UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

ABSTRACTS

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AIR FORCE RESEARCH LABORATORY

ABSTRACTS

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University of Illinois at Urbana-Champaign

Harley T. Johnson, Conference Chair
Iwona Jasiuk, Technical Chair

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Contents

Foreword

The University of Illinois, the Conference Organizing Committee and Symposia Organizers, and SES Officers and Board of Directors welcome you to the 45th annual technical meeting of the Society of Engineering Science (SES 2008).

SES conferences are forums for bringing together diverse, interdisciplinary groups of researchers from all engineering and science disciplines, as well as mathematics, to discuss advances in highly focused symposia. This year's conference features more than 30 symposia and over 500 presentations on research in a broad range of disciplines that includes solid and fluid mechanics, bioengineering and biological sciences, applied mathematics and computational science, dynamical systems, fluids and transport, imaging, multiscale and micro- and nano-mechanics of materials, and other engineering and science fields. To accommodate so many offerings, podium presentations will be held in 12 parallel sessions in 12 different rooms.

Attendees can also attend three Plenary Lectures from internationally known researchers (Professors R. James, S. Suresh, and P. Selvadurai) and one Special Keynote Lecture by Dr. Y. Rajapakse. A student paper competition with presentations by 16 finalists selected from more than 160 applicants will also be held on Monday morning. The winners will be announced at the conference banquet.

Three SES medalists will be recognized at the banquet: Richard James, recipient of the Prager Medal; Subra Suresh, recipient of the Eringen Medal; and Anthony Spencer, recipient posthumously of the Society of Engineering Science Medal. The new SES fellows will also be recognized at the banquet. Symposia in honor of R. James, S. Suresh, A. Spencer, and J. Goddard are also scheduled.

We wish you a great visit at the University of Illinois, and we hope that you will find this meeting interesting, intellectually stimulating, and personally enjoyable. Finally, we would like to thank the sponsors for their support and the symposia organizers and conference staff for all their time and effort in organizing this conference.

Harley Johnson (Conference Chair) and **Iwona Jasiuk** (Technical Program Chair)
Department of Mechanical Science and Engineering
College of Engineering
University of Illinois at Urbana-Champaign

Plenary Lecture Abstracts

Engineering Science and the Study of Human Diseases

Subra Suresh
School of Engineering
Massachusetts Institute of Technology

This lecture will provide an overview of recent advances and major opportunities in the application of engineering science to the study of human health and diseases. Scientific discoveries at the intersections of engineering, biology, genetics and medicine are examined with particular reference to experimental and computational studies of mechanobiology at the cell and molecular levels. Specific results will be discussed in the context of infectious diseases, hereditary blood disorders, and different types of human cancer. Potential applications for disease diagnostics, therapeutics and drug efficacy assays will also be examined.

Simulation of the Motion of Defects in Nanostructures

Richard D. James
University of Minnesota

The concept of Objective Structures gives a framework for looking at the structure of matter that encompasses both bulk structures like crystals and nanostructures like carbon nanotubes, buckyballs, and the parts of viruses. Mathematically, its usefulness derives from its intimate relation to the fundamental invariance of quantum mechanics. This invariance can be used to simplify both first principles calculations of energy and molecular dynamic calculations for these structures. We describe a method of doing exact molecular dynamics termed Objective Molecular Dynamics. It is well adapted to study the formation and motion of defects in nanostructures. We present some results on the study the failure of carbon nanotubes under conditions of constant strain rate and discuss failure mechanisms.

Joint work with Kaushik Dayal

The Spencer-Rivlin Function for Problems in Higher-Order Elasticity Theory

A.P.S. Selvadurai*
Department of Civil Engineering and Applied Mechanics
McGill University
patrick.selvadurai@mcgill.ca

The contributions of R.S. Rivlin, A.E. Green and A.J.M. Spencer to the development of non-linear continuum mechanics and in particular non-linear elasticity represent milestones in the history of the subject. Higher-order elasticity theories and second-order elasticity theory in particular, are procedures for obtaining approximate solutions to the non-linear equations governing the theory of finite elasticity. Although the theory of second-order elasticity was investigated by number of elasticians including Signorini, Stoppelli, Misiçu, Sheng and others, the work of Rivlin firmly placed the subject in the realm of engineering applications of the theory to rubber-like materials. The second-order theory in particular, provides suitable explanations for non-linear effects that can be observed in incompressible hyperelastic materials that are subjected to moderately large strains that are void of material instabilities. The formulation of problems in second-order elasticity theory can be approached in a variety of ways, including the extension of classical stress and displacement function techniques developed for formulating problems in linear elasticity. Four decades ago, Spencer proposed a method of solution of the second-order problem which reduced the governing equations for a displacement function, the *Spencer-Rivlin function*, and for the isotropic stress, to canonical equations. This lecture will focus on the application of the *Spencer-Rivlin function* for the solution of inclusion problems in torsion-less axial symmetry and to problems of torsion, where the second-order solution exhibits axial symmetry. Current availability of symbolic mathematical manipulation techniques provides the opportunity for extending the method of successive approximations to include terms beyond the second-order.

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* *William Scott Professor* and *James McGill Professor*

Abstracts for Sponsor Lectures

Composites Research for Marine Structures

Yapa Rajapakse
Program Manager, Solid Mechanics
Office of Naval Research

Naval structures operate in severe environments, in the presence of moisture, sea water, extreme temperatures, and hydrostatic pressure. They are subjected to wave slamming, and high sea states; they have to be designed to resist highly dynamic loading (due to air/underwater explosions, and hull slamming).

The Solid Mechanics Research Program of the Office of Naval Research (ONR) provides the scientific basis for the effective design of affordable and reliable Naval structures, and for the assessment of structural integrity. The current focus is on mechanics of marine composite materials and composite sandwich structures. The program deals with understanding and modeling the physical processes involved in the response of glass-fiber and carbon-fiber reinforced composite materials and composite sandwich structures to static, cyclic, and dynamic, multi-axial loading conditions, in severe environments (moisture, sea water, temperature extremes, and hydrostatic pressure). The establishment of these models, with predictive capabilities, requires multi-scale, multi-physics analysis. Avenues for enhancing the performance of marine composite structures through the introduction of nanoparticles (and nanotubes), and through the incorporation of novel design concepts, are also being explored. Research on multifunctional composites seeks to enhance performance through the incorporation of additional beneficial attributes, without compromising on the mechanical properties.

Recent achievements of the leading researchers in mechanics of composite materials and sandwich structures, supported by the ONR Solid Mechanics Program, will be summarized. Topics covered include: sea water effects on marine composites, long term durability, impact damage, fatigue and failure theories, strain rate effects, interfacial failure, interactions of multiple delaminations, failure and fatigue of foam core, fluid-structure interaction effects, damage detection, and concepts for the mitigation of damage.

Future directions of research include greater emphasis on the mechanics of shock/blast effects, implosions, and hull slamming. Other emerging areas of research include coupled phenomena (combined effects of sea water, temperature extremes, and dynamic loading).

Student Abstracts / Presentation Awards

Combined Experimental and Simulation Study of the Cure Kinetics of DCPD

Michael Aldridge[a], Chandrashekar Shankar[a], Lang Sui[a], John Kieffer[a], Mary Caruso[b], and Jeff Moore[b]

[a] University of Michigan, [b] University of Illinois at Urbana-Champaign

Dicyclopentadiene (DCPD) is used as a remediating agent in self-healing polymer matrix composites. Polymerization occurs via ring opening metathesis (ROMP) mediated by Ruthenium based Grubb's catalysts. In self-healing materials, DCPD is released from microcapsules embedded in the polymer when these are struck by propagating cracks. Once DCPD comes in contact with the catalyst, which is dissolved in the matrix, the healing reaction is initiated. The efficacy of DCPD in preventing continued crack growth under cyclic load depends on the rate with which mechanical resistance is re-established due to the polymerization of the DCPD that fills the crack[1,2]. Therefore, we investigated the cure kinetics of DCPD under various conditions using a combination of concurrent Brillouin and Raman light scattering and molecular dynamics (MD) simulations.

The two inelastic light scattering techniques allow us to monitor both the changes in visco-elastic properties and chemical signatures of DCPD in situ, while it is polymerizing. For both types of analysis the sample is irradiated by the same laser, and the inelastically scattered light is collected from the same sample volume. Thus the two analyses can be carried out simultaneously. Raman light scattering (RLS) is well established as a materials characterization tool that allows spectral features to be attributed to specific molecular geometries. Brillouin light scattering (BLS) probes the momentum of propagating acoustic phonons. As a result of photonphonon interactions, Brillouin peaks are Doppler shifted with respect to the frequency of the incident light. The magnitude of this shift is proportional to the velocity of sound in the scattering medium, and knowing the density of the material, one can easily extract its elastic storage modulus. The measurement also reveals a loss modulus, which can be derived from the line shape of the Brillouin peaks. Brillouin and Raman spectra are analyzed using instruments with different spectral resolution, a Fabry-Perot interferometer for the former and dispersive holographic gratings for the latter. The two measurements simultaneously provide information about chemical structure and the visco-elastic properties of the material. Because there never needs to be any mechanical contact with the sample, BLS and RLS provide a unique means of monitoring a reacting sample without disturbing the equilibrium of the reacting system.

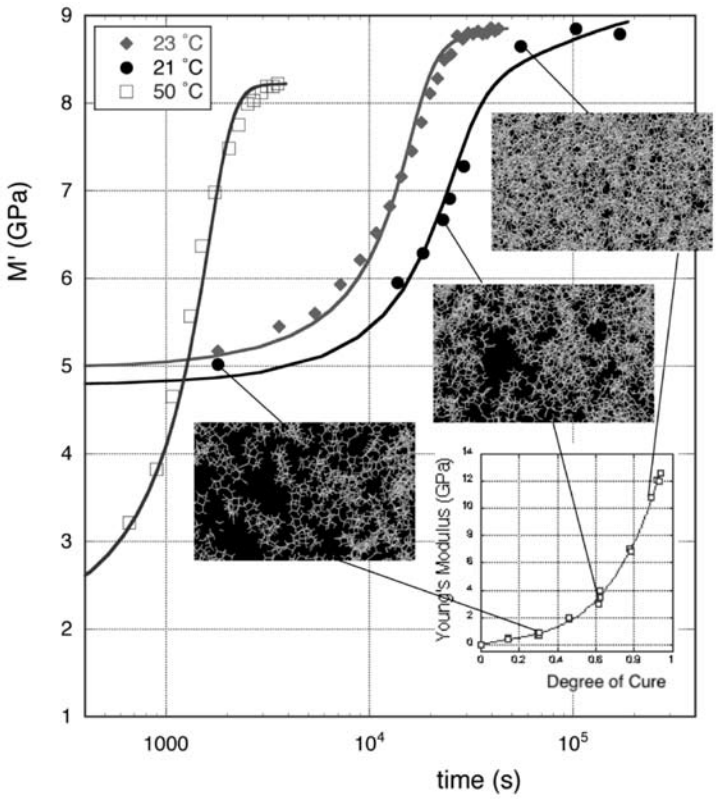

FIG. 1 • Elastic modulus as a function of time for different curing temperatures. Insets: Simulated DCPD structures and Young's modulus as a function of degree of cure.

To monitor the DCPD curing process, samples containing DCPD and Grubbs' 1st generation catalyst at various concentrations are prepared. The samples are then mounted into a miniature oven and placed into the optical path. Laser light of 532 nm wavelength is used for the measurements. The light scattered from the sample is directed towards the Fabry-Perot interferometer and

Raman spectrometer. By using the so-called platelet scattering geometry, in which the sample is contained between two parallel glass slides so that the plane of these slides evenly bisect the directions of incident and scattered radiation, it is not necessary to know the refractive index of the sample in order to determine the scattering wavevector. Thus, any changes in the refractive index that may result from the curing of DCPD does not affect our ability to determine mechanical properties of the polymer.

As the samples cure, Brillouin and Raman spectra are collected at regular intervals. The Raman data thus yield the temporal evolution of the chemical signatures of the sample. Likewise the Brillouin data provide the corresponding evolution of elastic moduli of the sample as it cures. Note that with BLS, moduli are determined at the nano-structural scale. The measurement is equivalent to performing oscillatory tensile tests on specimens 30 to 50 nm in length. Fig. 1 shows the elastic moduli so measured as a function of time for three different curing temperatures. Using these non-destructive techniques we directly probe the degree of cure in the bulk of the material

The complex mechanical modulus revealed by Brillouin scattering provides the most direct measure of the structural changes in the system. With increasing degree of cure, the elastic storage modulus transitions from that of a liquid to that of a solid, while the loss modulus exhibits a maximum during the phase when the storage modulus changes most rapidly. Thus, BLS yields a direct measure of the number of load bearing bonds in the structure per unit volume at the molecular level. However, to unequivocally relate this time dependent visco-elastic data to the cure kinetics of DCPD, we must establish the relationship between degree of cure and the elastic modulus of the resulting structure. To this end we carried out multi-scale molecular simulations. We generated DCPD networks using a combination of MD and a heuristic bond exchange protocol, recreating the ROMP process[3]. Mechanical properties of the simulated networks were evaluated at various stages during the polymerization, by subjecting them to uniaxial tension tests. By comparing the mechanical response of networks that result from realistic simulations of the ROMP process with that of structures created by random bond formation, we found that the modulus vs. degree of cure behavior indeed strongly depends on the reaction mechanism. The inset on the lower right of fig. 1 shows the dependence of the Young's modulus on the degree of cure obtained from simulation. Finally, we incorporated this simulation-derived modulus vs. degree of cure relationship into a numerical model of the cure kinetics to fit the modulus vs. time data. The model consists of coupled differential equations describing the reaction and heat release rates, respectively. This fitting procedure allows us to determine the overall reaction mechanism and corresponding rate coefficient. Best fits are shown as solid lines in fig. 1.

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Interfacial Self-Healing for Advanced Composites

B.J. Blaiszik[a], S.R. White[b,d], and N.R. Sottos[c,d]

[a] Department of Mechanical Science and Engineering—Theoretical and Applied Mechanics Program
[b] Department of Aerospace Engineering
[c] Department of Materials Science
[d] Beckman Institute for Advanced Science
University of Illinois at Urbana-Champaign

Fracture and fatigue damage in materials spans multiple length scales. In order to heal fiber reinforced composite microcracking damage, capsules and catalyst with smaller diameters were synthesized to allow self-healing materials to physically fit in the fiber interstitial spaces[1]. Since matrix microcracking and interfacial failure of reinforcing fibers are two of the key failure mechanisms in composite materials, healing this damage may allow for a substantial increase in expected material lifetime by preventing catastrophic growth of smaller flaws.

To investigate self-healing of an interface, a method was developed for sequestration of healing agent filled microcapsules and catalyst to the reinforcement-matrix interface. As shown in Fig. 1a, urea-formaldehyde (UF) capsules and nanocapsules containing a resin-solvent self-healing blend[2], or other monomeric healing agents[3] can be attached to the interface of standard glass fiber. Surface loadings above 15% have been achieved, which will allow sufficient healing agent release upon damage to initiate a self-healing response.

Microbond specimens, consisting of a single self-healing functionalized fiber embedded in a microdroplet of epoxy, are used to test the virgin and healed fiber-matrix interfacial properties[4,5]. By using the sample geometry shown in Fig. 1b, damage is initiated at the fiber-matrix interface, rupturing the attached capsules, and releasing the healing agent into the crack. A novel technique utilizing robotic controlled deposition of epoxy resin is used to prepare microbond specimens with controlled embedded lengths (L_e) ranging from 100 μm to 1 mm. The effect of self-healing material loading on the fiber-matrix interfacial fracture toughness, interfacial shear strength, and fiber-matrix load transfer is used to quantify the self-healing effect.

In order to test the self-healing microbond specimens, a custom-made single fiber testing frame is built and mounted under an optical microscope to provide simultaneous load-displacement and direct optical observation of the crack front propagation during debonding and subsequent healing events. A representative load-displacement curve obtained from the custom testing frame is shown in Fig 1c. In this work, we show promising self-healing results, control experiments,

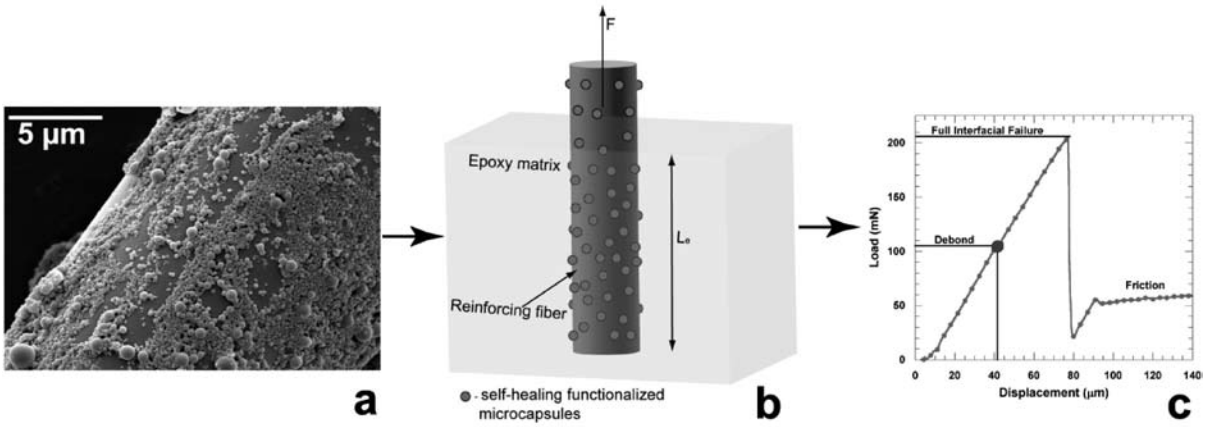

FIG. 1 • To test self-healing in a model composite, (a) microcapsules and nanocapsules are sequestered to the interface of standard E-glass fibers. (b) The functionalized fibers are then embedded in an epoxy matrix microdroplet, and (c) pulled out by a custom-built apparatus to determine interfacial toughness, interfacial shear strength, and load transfer between the fiber and matrix before and after healing.

and interfacial property data from microbond tests characterizing interfacial self-healing materials in a glass fiber-epoxy model composite system.

Achieving self-healing materials utilizing constituents smaller than 10 μm sequestered to the composite reinforcement interface will allow for a wide range of novel applications in advanced composites. With the additional self-healing functionality, these advanced composites will have the ability to overcome two of the earliest and most common failure mechanisms for reinforced composites, matrix microcracking and reinforcement fiber debonding. By healing at the microcracking and interfacial damage stage rather than allowing propagation of early flaws, the life span of reinforced composites could be extended.

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An Electrical Technique to Measure *In Situ* Contact Area Continuously during Instrumented Indentation and Its Application to Characterize Materials That Pile Up

Lei Fang[a], Christopher L. Muhlstein[b], Amber L. Romasco[b], James G. Collins[b], and Lawrence H. Friedman[a]

[a] Department of Engineering Science and Mechanics, Pennsylvania State University, University Park, PA, 16802
[b] Department of Materials Science and Engineering, Pennsylvania State University, University Park, PA, 16802

Instrumented indentation[1] using the Oliver-Pharr data analysis method[2] is a primary tool for mechanical characterization of materials. The resulting mechanical properties, such as hardness and the elastic modulus, are directly dependent on the *in-situ* projected contact area, A_c, between the indenter and sample; however, the Oliver-Pharr method lacks a direct measurement of A_c. This is a fundamental limitation that confounds instrumented indentation when characterizing dynamic properties of materials, thin films and materials that pile up around the indenter tip. An electrical technique was recently developed by the authors to continuously measure the *in-situ* contact area during instrumented indentation[3], and thus has the potential to overcome all the limitations in the Oliver-Pharr method when evaluating conductive samples. However, in [3] the technique was only applied to annealed Cu, a material to which Oliver-Pharr applies, and whether it can be extended to materials with Oliver-Pharr not applicable remains to be explored. Materials exhibiting pile-up, which have attracted much attention in the last two decades, represent such a case. The Oliver-Pharr method infers A_c based on an elastic contact model where sink-in always occurs, making it inapplicable for the case of pile-up. For materials that pile up, the Oliver-Pharr method was shown to underestimate the contact area, sometimes by as much as 60%[4], and overestimate hardness. Here, the electrical instrumented indentation technique is extended to characterize materials that pile up.

Work hardened Cu alloy 101 (oxygen-free, 99.99% pure) was indented to test the efficacy of the technique, because it was known to pile up and allowed direct comparison with annealed Cu. All samples were mechanically polished to 0.05 μm and cleaned with isopropyl prior to testing. An Instron microtester was modified to enable simultaneous electrical measurements during instrumented indentation. Details of the experimental apparatus were described in [3]. All indentation tests were conducted in a force-controlled mode; every test consisted of a linear loading up to the maximum force (P_{max}) over 100 s, a hold at Pmax for 20 s, and an unloading to zero force with the same rate as the loading. Ten indents were performed for each of five conditions with maximum forces ranging from 2 N to 6 N. Throughout each test, the electrical and mechanical contact responses between the indenter tip and sample were measured simultaneously. As a result, for each indentation test a force-displacement (P-h) curve and a series of current-voltage (I-V) curves were recorded synchronously.

As for annealed Cu, the measured *I-V* curves were found to be nonlinear for work hardened Cu (Figure 1a), making it impossible to apply the Holm's equation, which is essentially the only available analytic tool relating contact area to *I-V* curves. In 3, a new method was proposed to obtain *in-situ* contact area and hardness from the nonlinear I-V curves. Each *I-V* curve was characterized by the area under it, denoted by Γ, and Γ was subsequently correlated with A_c obtained from the Oliver-Pharr method at the start of unloading. Based on this correlation, the *in-situ* contact area and hardness were measured as a continuous function of applied force from the recorded contact *I-V* curves. This method was applicable to annealed Cu because the Ac-Γ relation can be calibrated using the contact area at the start of unloading via the Oliver-Pharr method. However, work hardened Cu exhibits pile-up, making the Oliver-Pharr method not applicable. To overcome this difficulty, an optical profilometer was used to image the residual indents, and an example image is shown in Figure 1a as an inset. The semi-ellipse method[5] was applied to determine the post-indent contact area, based on which the A_c-Γ relation was calibrated at the maximum forces for work hardened Cu. A_c was found to correlate well with Γ at the maximum forces, and the correlation was a power-law relation in the form of $A_c = A_0 \times \Gamma^n$ between 2 N and 6 N. This correlation function was also found to be comparable to the one for concurrently measured annealed Cu. With this calibrated correlation function, the insitu contact area and hardness were calculated from the contact *I-V* curves measured during loading. Hardness values from ten indents with the same maximum force were then averaged to obtain the average hardness for the four maximum forces (3 N to 6 N). The 2 N indents were omitted because the technique was only valid between 2 N and 6 N. As shown in Figure 1b, the average hardness values obtained from the electrical technique were almost constant during loading between 2 N and 6 N, and were 30 to 40 percent lower than the average Oliver-

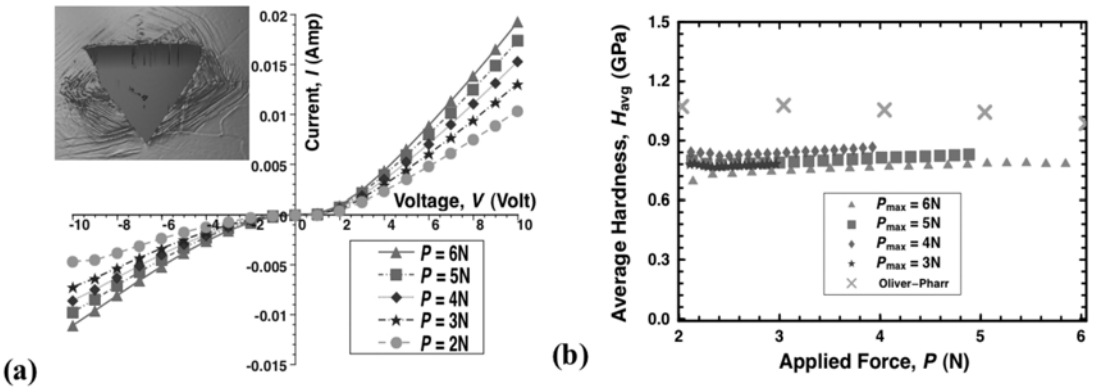

FIGURE 1 • Results from electrical instrumented indentation of work hardened Cu: (a) typical *I-V* curves and residual indent for an indent with P_{max}=6 N, and (b) average hardness *H* versus applied force *P*.

Pharr hardness. This was consistent with the finding that the contact area at the start of unloading from the Oliver-Pharr method was smaller than the optically measured post-indent contact area by as much as 35% due to pile-up.

In conclusion, this work demonstrated that the electrical instrumented indentation technique could be applied to characterize conductive materials exhibiting pileup, and extended the technique to materials to which the Oliver-Pharr method does not apply. Post-indent imaging was used along with electrical measurements to continuously access *in-situ* contact area and hardness while accounting for the pile-up effect. Furthermore, the fact that work hardened and annealed Cu have comparable A_c-Γ relation may not only allow us to use Oliver-Pharr for materials that pile-up, but also prove useful for other applications such as cyclic loading, indentation creep and indentation of thin films.

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A Stabilized Locking-Free, Two-Pass Finite Element Formulation of Contact

G. Haikal and K. Hjelmstad

University of Illinois at Urbana-Champaign

Introduction

The discrete node-to-surface gap function is typically used as a contact constraint to enforce the impenetrability condition between a "slave" node and a "master" surface. This type of formulation is usually sensitive to the choice of themaster/slave pairing and is generally not capable of representing a state of constant pressure, therefore failing thewell-known contact patch test[1,2]. When used as a two-pass method, the discrete node-to-surface gap function formulation has been shown to fail the Ladyzhenskaya-Babŭska-Brezzi (LBB) condition and therefore exhibits surface locking[1]. To address these issues, we propose a stabilization procedure in the formof a local enrichment of the contact surface that would eliminate the need for a master-slave definition while avoiding surface locking and insuring an accurate transfer of the pressure field across the contact interface.

Formulation

The aim of the proposed procedure is twofold: to transform the node-to-surface contact constraint to a node-to-node constraint withoutmodifying the existing mesh, and to ensure that the resulting formulation passes the contact patch test. To achieve the first objective, we adopt the following approach: If contact is detected between a point p and an element surface, a node can be inserted at the location of contact such that the gap function is reduced to a node-to-node constraint, as shown in Fig. 1a. Completeness of the finite element interpolation in the contact element can be preserved by updating the set of Lagrangian shape functions to account for the additional node. For example, the updated shape functions corresponding to the case illustrated in Fig. 1a are

$$N^5(\boldsymbol{\xi}^p) = \tfrac{1}{2}(\xi_1 + 1)\frac{(\xi_2 + 1)(\xi_2 - 1)}{(\xi_2^p + 1)(\xi_2^p - 1)} \qquad N^\alpha = N^\alpha_{Q_4} - N^\alpha_{Q_4}(\boldsymbol{\xi}^p)\, N^5 \tag{1}$$

for $\alpha = 1, \ldots, 4$,where $N^\alpha{}_{Q_4}$ are the shape functions of aQ4 element.This procedure can be repeated when multiple nodes contact a given element. The location of the additional node is determined by the process of contact resolution. As a result, the finite elementmesh of the contact element includes a node of moving reference. The added node has the effect of increasing the order of interpolation along the contact interface, thus providing the surface with an additional degree of freedom. This approach can therefore be safely implemented as a two-pass method, where the impenetrability constraints are enforced strongly at the contact locations using discrete Lagrange multipliers. The surface enrichment is local to the contact element, and the added degrees of freedom can be computed at the element level using a static condensation procedure.

For this formulation to pass the patch test, we implement stabilization approach, based on a Discontinuous Galerkin method, along the contact interface to account for the discontinuity in the displacement field and ensure the complete transfer of the contact pressure. The stabilization term is designed to take into account the continuity of displacement at the interface nodes, as enforced by the node-to-node contact constraints. The stabilized equations of motion take the form

$$\begin{aligned} &-\sum_e \int_{\Omega_e} \mathbf{S}\cdot\nabla\mathbf{w}^h d\Omega + \sum_e \int_{\Omega_e} \mathbf{b}\cdot\mathbf{w}^h d\Omega + \sum_e \int_{\hat{\Gamma}_{e_t}} \mathbf{t}_o\cdot\mathbf{w}^h\, d\Gamma + \sum_i \int_{\Gamma_i^+} \mathbf{Sn}^+\cdot\mathbf{w}^{h+}\, d\Gamma \\ &+\sum_i \int_{\Gamma_i^-} \mathbf{Sn}^-\cdot\mathbf{w}^{h-}\, d\Gamma - \sum_i \int_{\Gamma_i} [\mathbf{Sn}^+ + \mathbf{Sn}^-]\cdot\overline{\mathbf{w}}^h\, d\Gamma = 0 \qquad \forall\ \mathbf{w}\in\mathcal{V}^h \end{aligned} \tag{2}$$

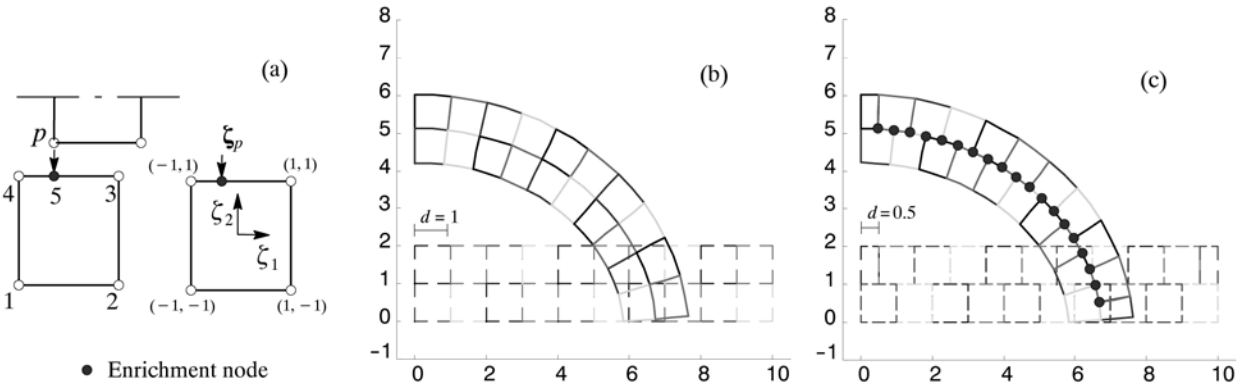

FIG. 1 • Double beam bending problem, (a) enrichment procedure (b) deformed configuration using conforming Q4 elements and (b) non-conforming (contact) enriched Q4 elements

where $\mathbf{Sn}^+$, $\mathbf{u}^+$ and $\mathbf{Sn}^-$, $\mathbf{u}^-$ are the traction and displacement vectors on each side of the contact interface interface and $\overline{\mathbf{w}}^h$ $(\mathbf{w}^{h+} + \mathbf{w}^{h-})2$ is the average of the variational displacement along the interface. This choice guarantees an unbiased method.

Results

The structure shown in Fig. 1 is composed of two 10 × 1 beams with material properties E = 1, ν = 0 [4]. The top and bottomsurface of the structure are initially subjected to a pressure of p = 0.1. Arotation α is then applied at the right end of the beams. The rotation angle is incremented quasi-statically from 0 to 90 degrees. Fig. 1b shows the the deformed configuration obtained using a conforming mesh with continuous nodes at the interface, in which case no contact events are involved. Fig. 1c shows the result obtained using a non-conformingmeshwhere the elements of the top beamare slightly shifted to the left and the nodes do notmatch at the interface. This configuration clearly involves multiple contact events and the applied pressure forces all contact constraints to be activated before rotation is applied. The deformed shape clearly matches that of the conforming mesh, and the interface pressure (not shown), before and after rotation, is also identical to the conforming case.

Conclusion

Surface locking is a phenomenon that hampers the two-pass node-to-surface contact formulation. To address this issue, we propose a stabilization procedure thatmakes use of a local enrichment of the contact surface. The stabilized formulation includes treating the contact interface using a special form of the DG method to guarantee an accurate transfer of the contact pressure field. The proposedmethod has the distinct advantage of treating the contact events as local phenomena that can be addressed at the element level. The result is a robust two-pass node-to-surface formulation that passes the patch test and strongly enforces the non-penetration constraint at contact locations without inducing surface locking[3].

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Effects of a Bio-inspired Interfacial Modification on the Properties of Polymer Matrix Nanocomposites

L. M. Hamming, P. Messersmith, and L. C. Brinson

Materials Science and Mechanical Engineering, Northwestern University

Marine mussels have the remarkable ability to attach to virtually any organic and inorganic substrate even in a tumultuous aquatic environment. The proteins responsible for their adhesion contain an unusual abundance of the amino acid L-3,4-dihydroxyphenyl-alanine (dopa)[1]. We have capitalized on dopa's role in adhesion by creating its synthetic analog for use in adhering polymer to metal-oxide surfaces[2]. After demonstrating that our adhesion method improved the interfacial shear stress between a metal wire and bulk polymer by 116%[3], we applied our method to polymer nanocomposites, a research area of growing interest to industries looking for a lightweight but strong alternative to metals.

One of the most important variables influencing a nanocomposite's properties is the quality of the interfacial interaction between the nanoparticles and the bulk polymer. Researchers have confirmed that there is a region near the surface of every nanoparticle in a nanocomposite system of altered molecular mechanics called an interphase zone[4, 5]. Polymer molecules near the surface of a nanoparticle will experience a reduction in their mobility if they are attracted to the nanoparticles or they will see an increase in mobility if they are repelled by the nanoparticles due to increased regions of free volume[6]. By modifying the surface of our nanoparticles with our synthetic version of dopa, we aimed to create a strong interphase region leading to improved mechanical and thermal properties of the composite. Since nanoparticles have extremely high surface area to volume ratios, only a few weight percent additions are potentially necessary to transform the macroscale properties with well dispersed nanoparticles that can lead to percolated interphase domains[4, 7].

The SEM images of fractured surfaces in Fig. 1 give a visual comparison of TiO_2 nanoparticles exhibiting a repulsive interaction with the surrounding polymer and TiO_2 nanoparticles modified with our biomimetic initiator exhibiting an attractive interaction with the surrounding polymer. To correlate the nanostructure observed in the SEM images to the overall mechanical and thermal properties of the composite, we employed differential scanning calorimetry (DSC), dynamic mechanical analysis (DMA), and ball-on-disc wear tests to measure several benchmark properties.

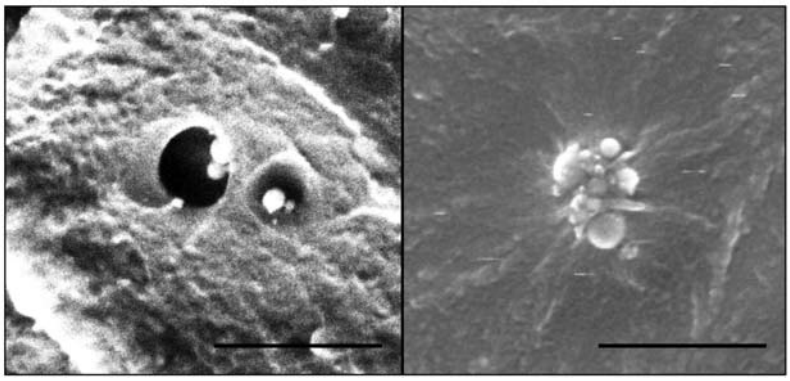

FIG. 1 • SEM images of (left) Unmodified TiO_2 nanoparticles exhibiting a repulsive interaction with the surrounding polymer and (right) TiO_2 nanoparticles modified with a dopainspired initiator exhibiting an attractive interaction with the surrounding polymer. Scale bar is 500 nm.

We determined the glass transition temperature, or the temperature at which the polymer molecules undergo relaxation from a glassy state to a rubbery state, of both our unmodified and modified composites using DSC and DMA. The attractive interaction between the nanoparticles and the surrounding polymer due to our interfacial modification likely leads to a reduction in local molecular mobility. Correspondingly, with only a 2wt% addition of modified nanoparticles, we measured an increase in Tg compared to neat PMMA from a mean of 116.4 °C to 119.2 °C. In contrast, the increased molecular mobility caused by a repulsive interaction between the unmodified nanoparticles and the surrounding polymer led to a depression of the Tg from a mean of 116.4 °C to 113.8 °C with only a 2wt% addition of unmodified nanoparticles. Student's T-tests indicate the probability of obtaining each of these results, assuming the null hypothesis, is less than 0.001.

We further examined the elastic modulus (E'), a measure of stiffness, and loss modulus (E"), a measure of energy dissipation, for our unmodified and modified samples using a temperature ramp test in DMA. We ran 14 tests and recorded the E' and E" values at a temperature in the glassy regime (30 °C) and at a temperature in the rubbery regime (140 °C). While there was no significant change in E" compared to neat PMMA for either the modified or unmodified composites, we did see a significant increase in E' in both the glassy and rubbery regimes for the modified samples and a decrease in E' for the unmodified samples compared to neat PMMA. The better interfacial adhesion of our modified composites allows for proper load transfer from the polymer to the stiffer nanoparticles and therefore manifests itself in improvements in bulk stiffness.

We have previously demonstrated through single molecule adhesion tests that the dopa to metal-oxide bond is strong and reversible even in the presence of water[8]. To determine whether our modified nanocomposites show superior hydrolytic stability, we are conducting long-term submersion tests. We have tested several samples that were soaked for 9 months at 37 °C. Interestingly, the glass transition temperature of our modified composites remained stable at the end of 9 months while all the unmodified composites failed to make it through the entire heating cycle. Additional data on water absorption for each type of composite over time is ongoing.

Our work highlights a biomimetic technique for increasing the reinforcement capability of nanoparticles in a polymer matrix. The superior performance of our biomimetic composites in terms of Tg, E', and hydrolytic stability is attributed to the unique adhesive properties of the amino acid dopa allowing for a robust interphase zone between nanoparticles and polymer. As medical implants as well as structural components are often subjected to aqueous environments, our technique opens up the possibility for increased lifetime and performance of these systems.

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Deformation in NiTiFe Shape Memory Alloys

R. M. Manjeri and R. Vaidyanathan*

Advanced Materials Processing and Analysis Centre (AMPAC), Department of Mechanical, Materials and Aerospace Engineering
*raj@mail.ucf.edu

The use of binary NiTi shape memory alloys in certain actuator applications is limited by specific requirements associated with hysteresis, fatigue and temperature of operation, among others. Addition of Fe to NiTi introduces an intermediate trigonal R-phase and lowers the monoclinic B19' martensitic transformation temperature. The presence of an intermediate Rphase further complicates an already convoluted array of deformation mechanisms in stresstemperature space. An understanding of the deformation characteristics of the R-phase is required to facilitate its use in low-temperature, low-hysteresis actuators, seals, switches, valves, etc. The deformation mechanisms in NiTi based alloys include inelastic modes such as detwinning (and/or martensite reorientation) and stress induced transformation, apart from conventional elastic and plastic deformations modes typically observed in metals. This study focuses on examining two competing

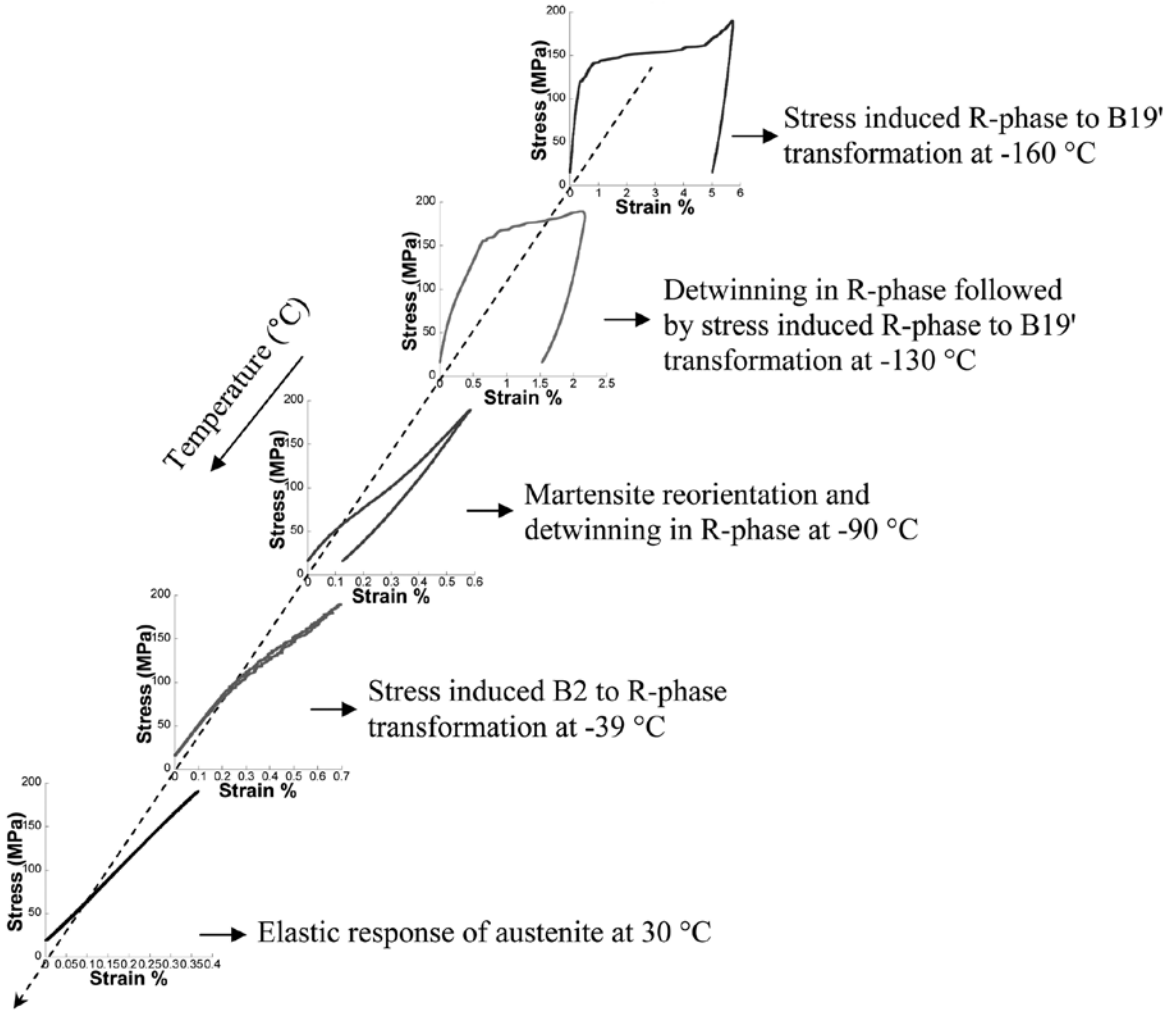

FIGURE 1 • Deformation mechanisms observed in a $Ni_{46.8}Ti_{50}Fe_{3.2}$ alloy at different temperatures. The results have implications for using the R-phase in low-temperature, low-hysteresis thermal switches on the moon and Mars. Financial support from NASA (NAG3-2751), NSF (CAREER DMR-0239512) and SRI is gratefully acknowledged.

mechanisms, i.e., detwinning and stress-induced transformation, that govern inelastic deformation in the R-phase in the temperature domain. Additionally, stress induced transformations in the parent austenite phase were investigated. Samples from a $Ni_{46.8}Ti_{50}Fe_{3.2}$ billet, fabricated by vacuum induction melting followed by vacuum arc melting, were cold worked by 30%, annealed at 600°C for 30 minutes and electrical discharge machined for subsequent testing. The resulting wires (rectangular cross section of approximately 130x125 microns and a gauge length of 20 mm) were electropolished and subjected to mechanical tests in a dynamic mechanical analyzer. Previous work that followed the aforementioned testing methodology has established that results from these wires are comparable to more conventional bulk specimens. The start and finish of the R-phase transformation from austenite and the corresponding reverse transformation to austenite from the R-phase, measured using a differential scanning calorimeter, were –36, –54, –49 and –33 (all ± 2°C), respectively. The temperature range in which the stress induced B2 to R-phase transformation occurs is very narrow, suggesting that the martensite desist temperature of the R-phase is very close to the austenite finish temperature. In the R-phase (below –54 °C), the sample underwent detwinning. However, when the sample was cooled to temperatures below –120 °C, detwinning was immediately followed by stress induced transformation to the B19' phase. The propensity of the R-phase to detwin decreased with decreasing temperature and at lower temperatures the R-phase underwent a direct stress induced transformation to the B19' phase. Figure 1 summarizes the phase dependent deformation mechanisms occurring in the NiTiFe system at different temperatures. The austenite phase, at room temperature, exhibits an elastic stress-strain response. A stress induced B2 to R-phase transformation is seen near the austenite finish temperature. Detwinning of the R-phase is observed at –90 °C (below R_f). At lower temperatures, detwinning was followed by stress induced transformation to the B19' phase. Finally, at even lower temperatures (–160 °C), the R-phase directly underwent a stress induced transformation to the B19' phase. It is important to note that the strain associated with the R-phase to B19' stress induced transformation (at –160 °C) is fully recoverable upon heating. The B2 to R-phase and the R-phase to B19' reversible stress induced phase transformations were analyzed within the framework of the Clausius-Clapeyron relation. The stress-temperature equivalence associated with the stress induced transformations under isothermal and isobaric conditions were in agreement, (6.6 MPa. K^{-1} for the B2 to R-phase and 1.8 MPa. K^{-1} for the R-phase to B19' transformation). Further, the stress-temperature equivalence of the B2 to R-phase stress induced transformation was larger than that of the R-phase to B19' transformation. Regions in stresstemperature space are identified based on detwinning in the R-phase followed by a stressinduced transformation to B19' martensite and a region where the onset of stress induced transformation occurs without any prior detwinning. By quantifying stresses and strains and identifying temperatures associated with various deformation mechanisms in NiTiFe alloys, this work has practical implications for using these NiTiFe alloys in applications that require lowtemperature, low-hysteresis actuators with superior fatigue behavior.

Bauschinger Effect in Unpassivated Freestanding Metal Thin Films

Jagannathan Rajagopalan, Jong H. Han, and Taher A. Saif

University of Illinois at Urbana-Champaign

Thin metal films, because of their unique dimensional and microstructural constraints, exhibit a substantially different mechanical response compared to their bulk, coarse-grained counterparts[1]. The yield stress of these films is, for example, often an order of magnitude larger than bulk metals, but their ductility is much lower[2]. Various theoretical models have been proposed to explain the strengthening effects associated with thickness and grain size of these films. Some of these models[3] and simulations[4] predict a distinct Bauschinger effect (BE) in passivated thin films with the stress-strain response deviating from elastic behavior during unloading, even when the films are still under tension.

Predictions of BE in passivated films have found support in various experimental studies[5,6] that have revealed early yielding in thin metal films on substrates during thermomechanical cycling. Early yielding in these passivated films has normally been attributed to the presence of stored dislocation energy, which assists reverse plastic deformation during unloading. Energy gets stored during the forward deformation because the dislocations are prevented from exiting the film by the passivation layer, resulting in dislocation pile ups or misfit dislocation segments being deposited at the film/passivation layer interface. In the absence of a passivation layer, dislocations are free to exit the film and hence it is accepted that unpassivated films should not show early yielding. Even recent experiments[7] that have provided direct evidence of BE in passivated thin metal films did not reveal any BE in similar unpassivated films. We show experimentally [BE paper] that unpassivated freestanding metal films, but with smaller thickness and grain sizes compared to films examined in the above studies, exhibit a distinct BE during unloading. These films, which were deformed under pure uniaxial tension, show large deviation from linear elastic behavior during unloading even at high values of overall tensile stress.

The stress-strain response of a 210 nm thick aluminum film with an average grain size of 170 nm is shown in Fig. 1a. The film had a large grain size distribution, with grains ranging from 60 nm to 400 nm. In cycle 1, the film was deformed to 0.67% strain and unloaded. During unloading, the initial slope was ~70 GPa, the bulk elastic modulus. But as the unloading progressed, there was a pronounced reduction in the stress-strain slope, leading to a plastic strain of just 0.14% upon complete unloading. On the other hand, if the film had traced an elastic unloading path the plastic strain would have been 0.42%. In other words, the early Bauschinger effect reduced the resultant plastic strain by 0.28%. During the second loading, the specimen exhibited slight residual hardening and showed even more pronounced Bauschinger effect during unloading. TEM observations of the film showed no noticeable change in the grain size after deformation. In

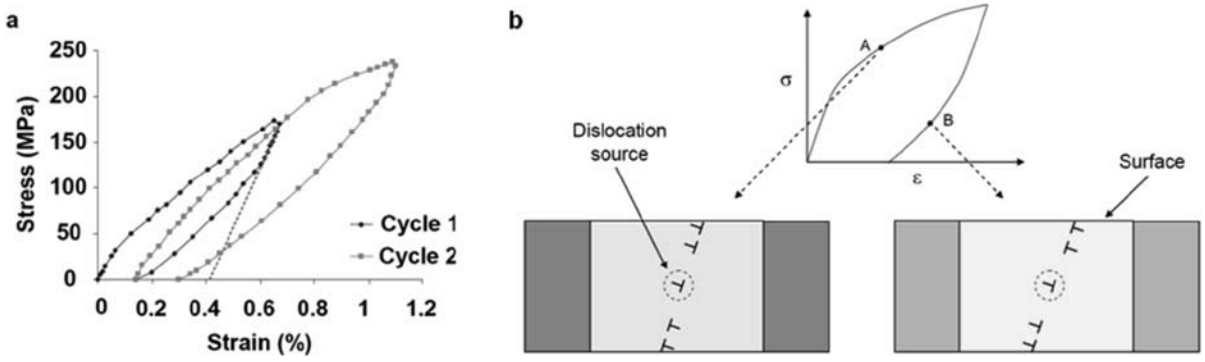

FIGURE 1 • a) Stress-strain response of a 210 nm thick aluminum film showing a distinct Bauschinger effect. b) A conceptual mechanism for BE in metal films with columnar grains. The figure shows the stresses in a large and two surrounding smaller grains. Grey and blue colors indicate tensile and compressive stress while darker shades represent higher magnitude. During loading (A), the large grain has lower stress as it deforms plastically. During unloading (B), the large grain undergoes reverse plastic deformation even though the overall stress is still tensile.

the experiments, both loading and unloading were done quasi-statically. The film was subjected to small increments/decrements in strain and the deformation was then halted for a period of one minute, after which the stress-strain data was recorded. The strain and stress resolutions were better than 0.005% and 5 MPa, respectively. Similar experiments[8] performed on two other aluminum films, with thickness of 360 nm (grain size 200 nm) and 400 nm (grain size 190 nm), respectively, and a gold film (thickness 240 nm, grain size 80 nm), confirmed the presence of BE in those films as well.

A conceptual mechanism that could lead to BE in unpassivated thin metal films is shown in Fig. 1b. The figure shows the stresses in a large and two surrounding smaller grains at two points, A and B, during loading and unloading, respectively. The large grain is representative of grains that are favorably oriented for plastic deformation while the smaller grains are symbolic of grains that undergo little plastic activity. During loading, the large grain starts deforming plastically at low stresses whereas the smaller grains accommodate the strain elastically. As the external load is increased, the stresses in the smaller grains keep increasing. However, the stress in the larger grain remains low (no hardening from dislocation entanglements) as the dislocations can escape to the surface. This leads to a highly inhomogeneous stress distribution in the film. Furthermore, once the larger grains start deforming plastically the stress-strain slope reduces markedly—the apparent strain hardening observed during loading is most likely the manifestation of such inhomogeneous (elastic and plastic) deformation. During the initial stages of unloading both the large and the smaller grains unload elastically. However, as the unloading progresses, the large grain goes into compression as it was under much smaller stress at the start of unloading. This compressive stress leads to reverse plastic deformation in the larger grain (the dislocations are of opposite sign now) and hence BE.

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Numerical Simulations of Wrinkling-Induced Delaminations in Multi-layered Thin-Film Systems

Kartik Srinivasan, Sanjay Goyal, Ganesh Subbarayan, and Thomas Siegmund

School of Mechanical Engineering, Purdue University

Film wrinkling is an instability occurring in thin-film systems comprising a compliant film/substrate capped by a stiffer film. During film wrinkling, patterns of periodic or labyrinth character emerge. Recent experimental studies[1, 2] provide evidence of a transition from film wrinkling at low compressive stresses, to the formation of folds at higher compressive stresses. During folding, a localization of the film deflection occurs. Such folding can be connected to the formation of delaminations at the film-substrate interface[1]. Numerical studies of wrinkling using 1-D beam models on non-linear foundations have shown that non-linearity in the foundation traction-separation response leads to localization effects[3, 4]. The first goal of the present work is to provide an understanding of the mechanics of such wrinkling-induced delaminations in the context of a more realistic plate theory. A secondary goal is to investigate the possibility of using folding experiments to obtain interfacial properties. This could potentially provide a convenient technique for the determination of interfacial properties in systems where stiff films are deposited on compliant substrates.

In the present approach, the stiff film is modeled using von Kármán plate theory. The combined effect of the interface and the underlying compliant film is modeled as a cohesive foundation which can possess a non-linear traction-separation relation. The non-linearity in the traction-separation relation of the foundation can be thought to be on account of damage or material separation at the interface. The governing equations are solved numerically using a spectral method. The spectral method used in the present work is an extension of the technique proposed by Huang et al.[5]. Extensions of this method are being described. We have developed an incremental solution procedure in the context of the spectral method such that irreversible interface relations can be considered. Also, we have allowed for the stiffness of the foundation to be dependent on the out-of-plane deflection and various forms of non-linearity in the foundation response (linear elastic, non-linear elastic, softening) have been implemented. The above extensions to the approach of Huang et al.[5] are essential in studying the transition from uniform wrinkles to delaminations.

The solution approach is now briefly described. An incremental form of the membrane strains[6] in von Kármán plate theory is used in the present work. Hooke's law relates the increments in membrane forces $\Delta N_{\alpha\beta}$ to the increments in membrane strains $\Delta\varepsilon_{\alpha\beta}$. On the interface between the stiff and the compliant film, let 3 T be the out-of-plane traction. Equilibrium requires that:

$$\Delta T_3 = -\frac{t^3\bar{E}}{12}\frac{\partial^4 \Delta w}{\partial x_\alpha \partial x_\alpha \partial x_\beta \partial x_\beta} + \frac{\partial}{\partial x_\beta}\left(\Delta N_{\alpha\beta}\frac{\partial w}{\partial x_\alpha} + N_{\alpha\beta}\frac{\partial \Delta w}{\partial x_\alpha} + \Delta N_{\alpha\beta}\frac{\partial \Delta w}{\partial x_\alpha}\right) \tag{1}$$

where w is the out-of-plane deflection (the wrinkling amplitude), $\bar{E}$ and t are the bi-axial modulus and thickness of the stiff film respectively. The increment in the out-of-plane traction ΔT_3 is related to the foundation stiffness $K(w)$ and the increment in out-of-plane deflection Δw by the relation:

$$\Delta T_3 = K\Delta w \tag{2}$$

Taking a Fourier Tranform of the above equations, a relation is obtained to update Δw:

$$F\left(\Delta w^{n+1}\right) = \frac{ik_\beta F\left(\Delta N^n_{\alpha\beta} w^n_{,\alpha} + N^n_{\alpha\beta}\Delta w^n_{,\alpha} + \Delta N^n_{\alpha\beta}\Delta w^n_{,\alpha}\right) - F\left(K^n \Delta w^n\right) + \zeta F\left(\Delta w^n\right)}{\left[K_1 + \left(t^3\bar{E}/12\right)k^4 + \zeta\right]} \tag{3}$$

where F denotes a Fourier Transform, Δw^n and Δw^{n+1} are the increments in the out-of-plane displacements at the n^{th} and $(n+1)^{th}$ iterations respectively, ζ is a numerical viscosity which is introduced solely for improving numerical convergence, k denotes a mode number and K_1 is the initial stiffness of the foundation.

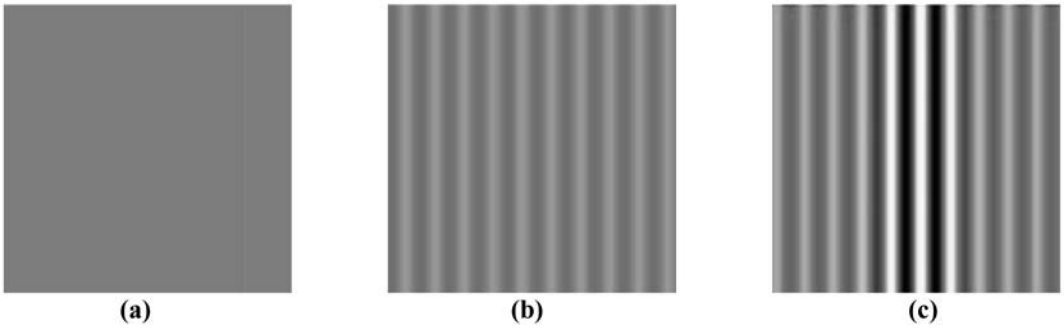

FIGURE 1 • Localization from uniform wrinkles to delamination-induced folding in uniaxial loading. Contours of the out-of-plane deflection. Unit cell has periodic boundary conditions. (a) Low applied strain-no wrinkling, (b) intermediate applied strain—wrinkling, (c) high applied strain—folding and localized delaminations.

Figure 1 shows contours of the out-of-plane deflection for a stiff film-compliant film system under uniaxial loading using the above solution procedure. Results shown in Fig. 1 are for a square unit cell with periodic boundary conditions. The foundation representing the compliant film is assumed to have a bi-linear softening traction-separation response. As the solution progresses, the foundation stiffness is updated by keeping track of the maximum out-of-plane deflection at each grid location. For low applied strains no wrinkling is observed, Fig. 1(a). As the applied strain magnitude is increased beyond a critical strain magnitude, the film wrinkles and the deformed shape is periodic, Fig. 1(b). As the applied strain magnitude is increased further, the uniform wrinkling mode transitions to localized fold formation enabled by the process of interface delamination, Fig. 1(c).

The critical strain for the transition from wrinkling to delamination-induced folding, as well as the width and height of the delaminations are related to the interfacial properties. Once relationships relating critical temperatures and fold geometry to interface properties are established, the findings of the present work can become particularly relevant to the microelectronic industry where stiff film-compliant film systems under compressive stresses occur widely during fabrication and processing.

Acknowledgement: Funding for this work was provided by SRC under grant number 1292.011.

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Simulation Model For Anisotropic Fibrous Materials

Anna Ask and Matti Ristinmaa

Lund University, Sweden

Introduction

Paper and paper-based materials such as cardboard are used in a variety of applications and accurate simulation models for these materials and structures are of major importance in computer based development and testing. Due to the manufacturing process, industrially made paper material typically has an orthotropic brous structure. Cardboard products such as packaging boxes are expected to deform plastically for instance when creased and folded. In this work a plasticity-based material model allowing for nite strains and suitable for materials with an anisotropic brous structure such as paper is developed. The general framework is based on separate mappings describing the deformations of the continuum and the substructure and a multiplicative split of these mappings into elastic and plastic parts.

Kinematic description

The anisotropic behavior of paper and paper materials is due to the brous substructure where the bers tend to align in certain preferred directions. These material directions are represented by vectors $v^{(\alpha)}$ and any planes of material symmetry can then be described by structural tensors $m^{(\alpha)} = v^{(\alpha)} \otimes v^{(\alpha)}$ [1]. These quantities are used to represent the substructure. It is assumed that the deformations of the continuum and of the substructure can be described separately[2]. For the continuum, the usual deformation gradient tensor F is used while a separate linear mapping is introduced for the director vectors

$$\boldsymbol{v}^{(\alpha)} = \boldsymbol{\Delta}^{(\alpha)} \boldsymbol{v}_0^{(\alpha)} \tag{1}$$

where zero subscript indicates the vector in the reference conguration. It should be noted that in general $\Delta^{(\alpha)} \neq F$ holds.

To allow for nite strains the formulation is based on a multiplicative split of the deformation gradient as well as the maps $\Delta^{(\alpha)}$ according to

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p \qquad \text{and} \qquad \boldsymbol{\Delta}^{(\alpha)} = \boldsymbol{\beta}^{(\alpha)} \boldsymbol{\alpha}^{(\alpha)} \tag{2}$$

into elastic (F^e, $\beta^{(\alpha)}$) and plastic (F^p, $\alpha^{(\alpha)}$) parts. It can be expected that the elastic parts of the deformation mappings are related in some sense; here this relation is chosen to be $\beta^{(\alpha)} = R^e$ where R^e is the orthogonal tensor obtained from polar decomposition of the elastic part of the deformation gradient, F^e.

Paper model

Due to the manufacturing process industrially made paper has two in-plane directions: one along and one across the direction of the bers and a third direction out of the paper plane. The elastic modulus as well as the yield strength are of an order two higher in the plane than out of it, with the strongest direction along the bers. The present model deals mainly with the in-plane properties and the out-of-plane behavior is assumed purely elastic. To describe the orthotropic material behavior the Helmholtz free energy function is taken as a quadratic form in the irreducible set of mixed invariants of the logarithmic strain and the structural tensors.

Associated plasticity is assumed for the continuum and a yield function proposed by Xia *et. al.*[3] is used. It is assumed that the yield surface is built up by yield planes related to loading in the material directions. The gradients n_ν to these yield planes are described by means of the direction vectors according to

$$\boldsymbol{n}_\nu = (n_{11})_\nu \cdot \boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(1)} + (n_{22})_\nu \cdot \boldsymbol{v}^{(2)} \otimes \boldsymbol{v}^{(2)} + (n_{12})_\nu \cdot (\boldsymbol{v}^{(1)} \otimes \boldsymbol{v}^{(2)} + \boldsymbol{v}^{(2)} \otimes \boldsymbol{v}^{(1)}) \tag{3}$$

where $(n_{ij})_\nu$ are constants to be calibrated. The gradients enter the yield function together with the Kirchho_ stress tensor so that

$$f(\boldsymbol{\tau}, \gamma, \boldsymbol{n}_\nu) = \sum_{\nu=1}^{6} \left(\chi_\nu \frac{\boldsymbol{\tau} : \mathbf{n}_\nu}{\tau_\nu(\gamma)} \right)^{2k} - 1$$

where the switching controller X_v activates or deactivates contributions depending on the direction of the loading and k is a regularization parameter. The hardening is described by $\tau_v(\gamma)$ where the internal variable γ is taken as the effective plastic strain.

Results

The material model is implemented into a nite element code using an explicit solver for the global equilibrium and an ode-solver for the local equations. It is then used to simulate the behavior of corrugated board, a commonly used packaging material consisting of wave-shaped layers of cardboard sandwiched between straight layers. The model is rst calibrated against uniaxial loading data; it is then tested against biaxial loading data and a good accuracy is obtained. To test the performance in simulating actual manufacturing steps, the model is used to simulate a creasing process in two and three dimensions with satisfactory results. The series in gure 1 shows a three dimensional simulation at three dierent stages.

FIGURE 1 • Simulation of the creasing process in three dimensions.

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Formation of Nanofibers by Capillary-Driven Thinning of Drying Viscoelastic Filaments

Jerome Crest, Jean-Christophe Nave, and Gareth McKinley

Massachusetts Institute of Technology

The fabrication of microscale and nanoscale polymer fibers has gained considerable interest because of its potential applications in nanoelectronics, nano-sensors, low-loss optical wave guides, filtration and biotechnologies[1]. Common fiber processes such as dry spinning or electrospinning don't allow precise, controlled placement of individual fibers on a substrate.

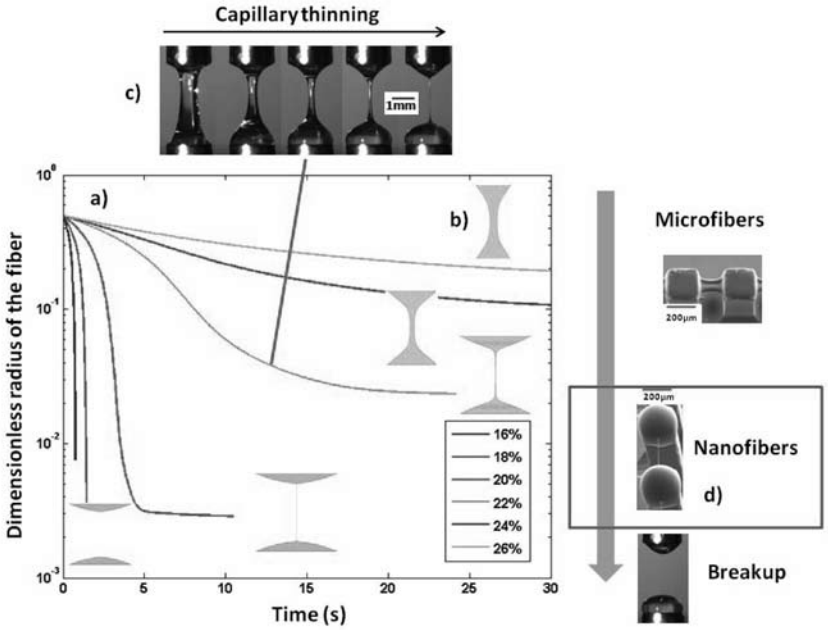

FIG. 1 • Numerical simulation of the CABER experiment for a drying filament at 23°C. Solutions of PMMA 996 000 g/mol in chlorobenzene with mass fraction ranging from 16% to 26% have been simulated and compared to experimental data. a) Dimensionless radius plotted as a function of time for different mass fractions of polymer; b) Profile of the fiber at equilibrium obtained by numerical simulation; c) Illustration of the CABER experiment at 22% mass fraction; d) SEM image of a nanofiber between two micropillars, from S. Pabba, University of Louisville.

Recent experiments have shown that it is possible to self-assemble very uniform polymeric nanofibers, illustrated on Fig. 1d, by exploiting elasto-capillary thinning of macroscopic liquid bridges[2]. We develop a model of this process that describes the simultaneous visco-elasto-capillary thinning and drying of cylindrical filaments of polymer solutions. The small size of the initial sample and the large viscous and elastic contributions to the total force ensure that gravitational body forces and inertia are negligible at all strains. The aspect ratio of the fiber being a small parameter, a slender body approximation is used.

The kinematics of the motion is therefore essentially one dimensional, and all variables can be averaged on a cross section and regarded as functions of the axial position and the time. The evolution in the kinematics, stress and composition of differential material elements are computed by numerical simulation on a fixed mesh using an explicit Eulerian scheme. The polymer rheology is described by a single mode Giesekus model with a concentrationdependent shift factor that accounts for compositional dependence of the zero shear rate viscosity and relaxation time of the fluid. To model evaporation of solvent, we suppose that internal diffusion is so rapid that there is no significant resistance to mass transfer within the liquid. All the resistance is external and arises from convection at the surface.

The test fluid used in this study is a high molecular weight poly(methyl methacrylate) (PMMA) dissolved in chlorobenzene, with mass fractions spanning both the semi-dilute entangled and concentrated regimes. The power law scaling of the rheological properties with concentration is determined experimentally with a shear rheometer. On Fig. 1, the computed dimensionless radius based on the characterization of the PMMA solutions is plotted as a function of time for different mass fractions. The simulations are compared to capillary breakup extensional rheometer (CABER) experiments,

illustrated on Fig. 1c, and semi-quantitative agreements have been found. For PMMA and chlorobenzene solutions, the entanglement network is evolving depending on the polymer concentration. At early times the solution has low viscosity and a minor elasticity due to low entanglement densities at high solvent concentrations. As the solvent evaporates, viscosity and elasticity increase, and at a critical concentration the mobility of the polymer chains dramatically decreases: a glass transition occurs, described by a Kelley-Bueche equation. Fig. 1a shows that the fiber diameter is a strong function of initial mass fraction of polymer, which can be explained by the evolving entanglement network. A rapid necking failure is observed at low initial concentrations. As the initial mass fraction increases, fibers of increasing diameters are obtained. Very large radius reductions—spanning three to four orders of magnitude—are attainable by careful control of the mass transfer rate, the extensibility of the dissolved polymer and the elastocapillary thinning dynamics. The simulations show that the nanofiber formation process can be conveniently parameterized by two dimensionless parameters which compare, respectively, the rate of capillary thinning, the rate of elastic stress relaxation and the rate of solvent evaporation[3].

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Matrix Mechanics and Cell Traction Regulate Integrin-Adhesion Ligand Bond Formation by Mesenchymal Stem Cells in 3D Micro-environments

Nathaniel D. Huebsch, Praveen Arany, Angelo Mao, José Rivera-Feliciano, and David J. Mooney

Harvard University School of Engineering and Applied Sciences

New materials used to fabricate scaffolds for tissue regeneration are designed around the idea that these scaffolds act not simply as passive delivery vehicles for cells but rather as synthetic analogs of the natural extracellular matrix (ECM), which plays a critical role in programming cell behaviors. A fundamental challenge for tissue engineers is to understand how the physicochemical structure of these materials influences the fate of cells they contact—and ultimately to leverage that understanding toward rational design. Studies relating cell fate to biomaterial composition often utilize hydrogel-forming polymers that interact specifically with cell receptors (e.g. integrins) through biomimmetic adhesion peptides. These studies have shown that adhesion ligand presentation (e.g. the density of peptides) strongly affects cell fate, (Kong 2006). Independent of adhesion ligand presentation, the mechanical properties (e.g. elastic modulus) of peptide-modified hydrogels has also been linked to a variety of cell behaviors, including lineage specification in mesenchymal stem cells (Engler 2006). However, the mechanisms linking ECM mechanics to cell fate are incompletely understood.

We hypothesized that one important means for cells to sense matrix stiffness is through mechanically-dependent changes in integrin-adhesion ligand bond formation, and further that sensing matrix stiffness would require active traction-force generation by cells. To test this hypothesis, we used synthetic ECM analogs comprised of alginate polymers covalently modified with the integrin-binding peptide sequence G4RGDASSKY-OH. Because of our ultimate goal of regenerating 3D tissues, many of the conventional tools available to study cell-matrix mechanics in 2D (e.g. atomic force microscopy) could not be applied to these studies. Instead, we used a set of novel biophysical and biochemical tools to assess bimolecular receptor-adhesion ligand interactions for cells encapsulated in 3D matrices.

Using a non-invasive FRET assay (Kong 2006, Huebsch 2007), we measured the relationship between matrix elastic modulus (E) and the number of bonds (N_b) formed between murine mesenchymal stem cells (mMSC) and RGD peptides presented by alginate. This revealed that N_b did indeed depend on both the density of available peptides and the elastic modulus (E) of the hydrogel (Figure 1a). Interestingly, the relationship between N_b and E was biphasic, in contrast to the monotonic relationship between cell adhesion and E typically observed in 2D studies, and likely represents a more physiologically relevant response of tissue cells to ECM compliance *in vivo*. Importantly, this biphasic relationship, and the peak in Nb at 20 kPa, was observed when E was varied over a wider range using a variety of different alginate polymers and crosslinking molecules (Figure 1b). A second FRET assay, which assessed nanoscale reorganization of RGD via cell traction forces, revealed that the matrices with the highest Nb were those in which ligand reorganization was most significant. Live-cell imaging of GFP-tagged α_5-integrins revealed that optimal cell-RGD bond formation was also coincident with localization of these receptors to the cell-matrix interface. Importantly, bond formation, along with intracellular integrin localization and matrix reorganization, was decoupled from matrix mechanics in the presence of drugs that inhibit cell traction forces (e.g. 1,3-butadiene monoxime, BDM).

To assess whether changes in N_b were mediated by multiple integrins, we developed a novel, ELISA-based method to measure integrin-subunit specific interactions with biotinylated RGD peptides. This revealed that both α5 and αV subunits acts as mechanosensitive RGD-receptors in 3D matrices, and provided the first experimental evidence that the RGD sequence alone is sufficient to bind α5-integrins in 3D matrices with the appropriate mechanical properties in cells capable of exerting traction on the matrix. Current efforts are aimed at linking observations on mechanical control of Nb to mMSC lineage specification in cells grown in 3D microenvironment. Preliminary gene transcription data (e.g. RT-PCR) suggest a shift towards osteogenesis, at the expense of adipogenesis, in mMSC within 20 kPa hydrogels that present RGD peptides to cells, whereas the same cells express adipogenic (fat) markers when hydrogel mechanics are not optimal to promote cell-RGD bond formation.

This work highlights a role for integrin-ligand bond formation in cellular mechanotransduction. Moreover, these results suggest that the biophysical manner in which adhesion ligands are presented to integrins may be equally important to the

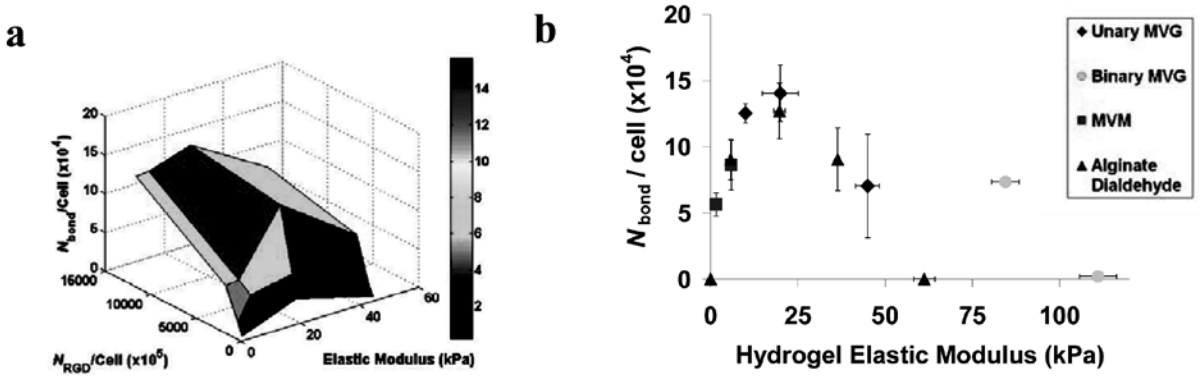

FIGURE 1 • Matrix Mechanics affect the Molecular Interface between Cells and Biomaterials. The number of bonds, N_b, measured with a FRET technique, between mMSC and RGD depends significantly on both the density of available RGD peptides, and the interaction between RGD density and matrix stiffness (E) (2-way ANOVA, $p < 0.01$). The biphasic relationship between N_b and E is maintained over a wide range of elastic modulus even when different alginate polymers and crosslinking molecules are used (b).

chemical structure of those ligands (in terms of their bimolecular interaction) providing insight into the widely observed differences in the biology of cells grown in standard tissue culture versus *in vivo*. This highlights a critical role for tissue engineering not only for therapeutic purposes, but also for engineering physiologically relevant micro-environments useful basic studies and drug screening. Perhaps the most important implication of these studies is a general design principal for engineering cell-programming biomaterials: cell-traction forces play an important role in the structure of biomaterials and can be harnessed in-situ to imbue simple template materials with complexity on both a molecular and functional level.

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A Simulation Model for Red Blood Cell Flow in Microcirculation

Amir H.G. Isfahani[a]*, Research Assistant; Hong Zhao[a], Postdoctoral Research Associate; Luke Olson[b], Assistant Professor; and Jonathan B. Freund[a,c], Associate Professor

[a] Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign
[b] Department of Computer Science, University of Illinois at Urbana-Champaign
[c] Department of Aerospace Engineering, University of Illinois at Urbana-Champaign
*ghalayan@uiuc.edu

Multi-cellular hydrodynamic interactions are important for much of the phenomenology of microcirculation where the flow length scales are comparable to cell dimensions. For example, leukocyte margination as a physiological response to inflammation[1], and detachment and metastasis of cancer cells appear to depend directly upon interactions with flowing red cells. We have developed a simulation model capable of representing large numbers of red cells interacting in the complex geometry confinement of capillaries. The cells are modeled as finite-deformation elastic shell membranes with strong resistance to surface dilatation and relatively small but finite resistance to bending.

The cell surfaces are discretized by marker points in a referential configuration. These points are interpolated by global spectral basis functions: Fourier modes in two dimensions and spherical harmonics in three, yielding optimal efficiency for a given accuracy. More importantly, this representation offers a rigorous treatment of de-aliasing without adding any

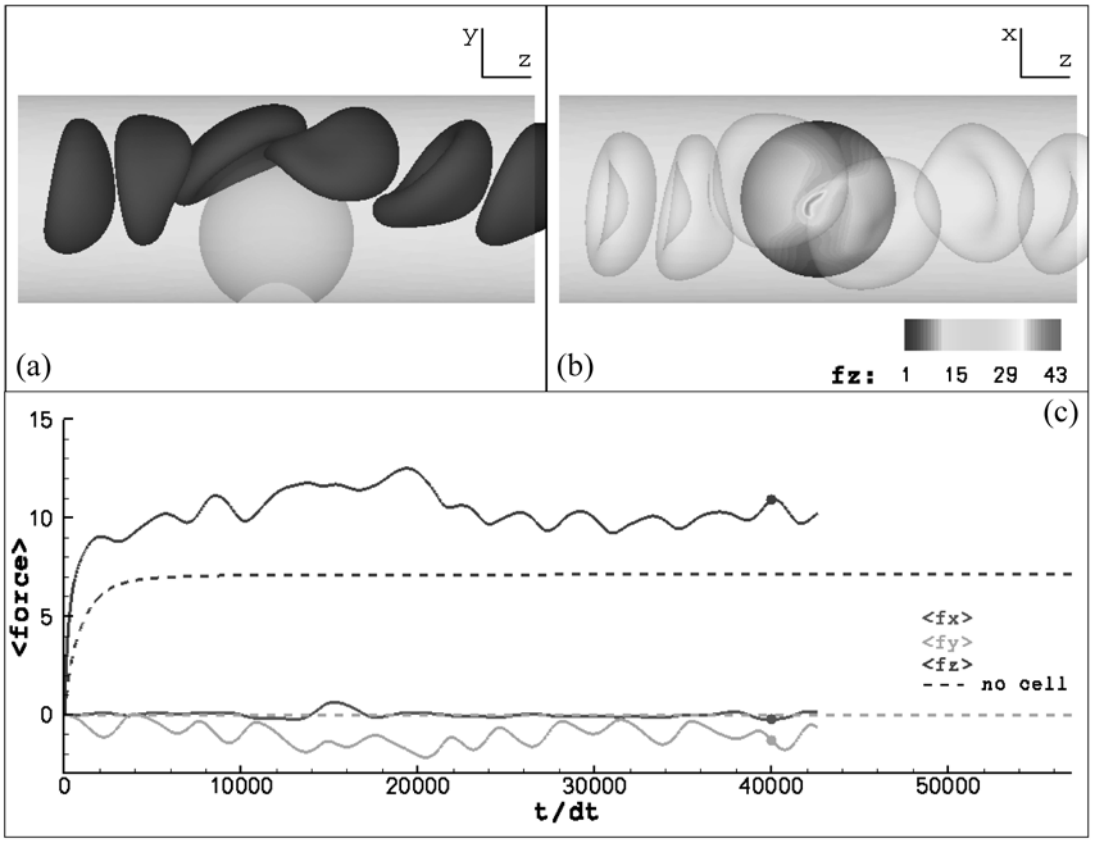

FIGURE 1 • (a) Visualization of the flow of red blood cells over a model cancer cell; (b) instantaneous local non-dimensional force on the surface of the wall-adhered cell; and (c) surface-averaged force history on the wall-adhered cells.

numerical dissipation. Aliasing which could lead to numerical instabilities arises due to geometric nonlinearities and would be compounded for more complex (nonlinear) constitutive models for the cells.

Stokes flow provides a realistic model for both the blood plasma and the red cell cytoplasm. To evaluate the boundary integral equation expressing the velocities on the boundary[2], Ewald[3] sum is a technique which does a remarkable job of splitting the very slowly convergent sum into two exponentially fast converging ones. To further enhance the performance of the algorithm, an O(NlogN) smooth particle-mesh Ewald method[4,5] is employed to decompose the periodic Green's functions of the Stokes operator into singular but integrable short-range and smooth long-range interactions. The length-scale parameter that defines the short-range interactions and the parameters associated with the discretization of each component do not yield independent errors, which makes the selection of these numerical parameters for efficient simulations a significant challenge. We have designed a process for selecting parameters like the number of points, Fourier modes, splitting factor, etc. to optimize computational efficiency for a desired accuracy.

Mismatched viscosity between the concentrated solution of hemoglobin inside red blood cells and the plasma on the outside gives rise to an implicit system, which is best solved iteratively. The impact of different physical configurations, such as the viscosity ratio between the fluids inside and out and the size of the system and hematocrit, as well as numerical enhancements, such as deflation of the system, on the performance and efficiency of several iterative strategies is outlined.

The vessel walls are modeled employing a penalty-like method, commonly used in finite element formulations, that enables simulation of complex geometries using free-space (in a sense) periodic Green's functions. This representation is then used to study the forces exerted on a cancer cell, modeled as a hump attached to the vessel wall (figure 1), in flow configurations which differ in hematocrit, hump radius, and vessel diameter. It is clear from figure 1(c) that the flow of red blood cells significantly affects the average forces that the model cancer cell experiences as compared to when the red cells are not present. These average forces have a direct impact in cell detachment mechanisms. On the other hand the local forces the cancer cell undergoes (as shown in figure 1(b)) could be much larger and potentially lead to mechanobiochemical stimuli within the cell that ultimately could translate to detachment. Understanding the detachment mechanisms could improve therapeutic methodologies to limit metastasis of cancer.

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Active Cooling of Polymer Structures Using Microvascular Networks

Brian D. Kozola[a], Vinay K. Natrajan[b], Kenneth T. Christensen[b], and Scott R. White[a]

[a] Department of Aerospace Engineering
[b] Department of Mechanical Science and Engineering
University of Illinois at Urbana-Champaign

Microvascular materials with interconnected three-dimensional networks offer an efficient method for active thermal control. The microscale of these networks offers advantages in convective cooling since the heat transfer coefficient scales inversely with channel diameter[1]. The effectiveness of active cooling using microvascular networks was examined in this study using thin fin polymer structures with embedded microvascular networks. The effects of channel diameter, single versus multiple layer networks, and varying flow rates from 0.5 to 10 ml/min were examined. In addition, the cooling fluid was also studied by using both water and also a MIL-PRF-87252 coolant based on a hydrocarbon oil.

The thin fin polymer specimens were created in bulk polymer material using direct-write assembly[2]. This process consists of writing the microvascular network with fugitive wax ink using robotic deposition. This wax structure is embedded in the bulk polymer matrix, and after the matrix is cured, the wax ink is removed using heat and vacuum. The final fin specimen dimensions were 19.5 mm high by 150 mm long by 3.5 mm thick, and four different microvascular networks were examined, each spanning 39.4 mm along the length of the specimen. First, control specimens were fabricated with no embedded microvascular network. A baseline specimen had 24 parallel channels of 200 μm diameter spaced 0.8 mm between channels. The third specimen had 12 parallel microchannels of 410 μm diameter spaced 1.6 mm between. Finally, an interconnected three layer network was created with three layers of 24 parallel, 200 μm channels with the middle layer perpendicular to the top and bottom layer.

The experimental setup consisted of mounting the fin to a heated copper plate with thermally conductive grease on the interface. The bottom of the specimen was heated to a constant 80° C while the top and sides of the fin were open to the environment at 23° C. The surface temperature was interrogated using a DeltaTherm 1560 infrared camera with a 256 by 320 pixel array of Indium Antimonide infrared detectors. After the heated equilibrium state was reached, the cooling fluid at 20° C was circulated at flow rates of 0.5, 1, 2.5, 5, and 10 ml/min using a syringe pump or diastolic pump depending on the volume of fluid necessary for the tests.

Two types of tests were performed on each specimen. First, the transient response from heated steady state to actively cooled steady state was examined by taking images at a rate of one frame per second. Then, the steady state cooled condition was examined averaging 20 seconds of data every five minutes for one hour. The results examined included horizontal averages over the height of the specimen and average field temperature of the entire surface over the network.

The control samples of solid polymer with no embedded microvascular network were compared to the thin fin analytical solution and a two-dimensional, steady state finite element model using ANSYS© software. The experimental results for the control samples correlated very well to the analytical and computational models with a maximum error of 2.2%. This verified the experimental procedure and validity of using the infrared camera in this study.

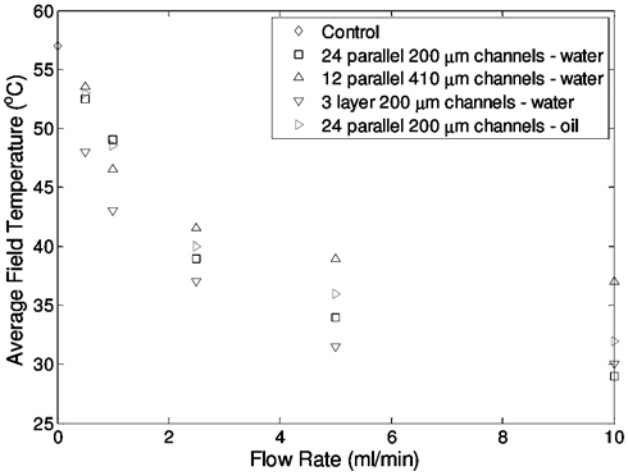

FIG. 1 • Average steady state field temperatures

The average temperature field results for all test cases are shown in Figure 1. For all test cases, higher flow rates produced faster cooling rates and lower steady state temperatures.

First, the effect of channel diameter was studied by comparing the results of the single layer 200 and 410 μm diameter channels networks. The experimental results verified that the smaller channel diameter yielded faster and more efficient cooling. The larger diameter channels took approximately 1.7 to 2.5 times longer to reach equilibrium and the field average of the steady state cooled specimen was 2 to 27% higher in temperature. The largest differences were seen in the higher flow rates.

The three layer specimens showed mixed results when compared to the single layer network with the same channel diameter. The transient response of the multiple-layer network was slower than the single layer network taking up to 25% longer to reach equilibrium at low flow rates. However, the multiple layer networks did show more efficient cooling, particularly at lower flow rates, with up to a 13% lower temperature when compared to the single layer network.

Water was the standard working fluid for these tests, but a military certified MIL-PRF-87252 cooling oil was also compared to results in the 24 parallel, 200 μm channel diameter specimen. The cooling trends were qualitatively similar between these two fluids, but water always exhibited a faster cooling response and also a lower steady state temperature at higher flow rates. However, at flow rates of 2.5 ml/min and lower, the military oil coolant is slower to cool but reaches a steady state temperature that is approximately equal to that of water. The military oil is better suited for real applications with a higher flash point and antioxidant additives properties.

Finally, the flow through the microvascular networks was examined using micro-PIV. Dilute quantities of 20 μm fluorescent particles were injected into the system and visually tracked to determine flow rates in all channels. At higher flow rates all channels are activated and have steady flow. However, flow rates below 2.5 ml/min exhibited a sharp decrease in cooling efficiency due to channel blockages preventing access to portions of the network. Incomplete network perfusion was accentuated in 3-D networks and with larger diameter channels.

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Intrinsic Indicators of Pathological States: Refractive Index Maps and Membrane Fluctuations in *P. falciparum* Infected Human Red Blood Cells

YongKeun Park[a], Monica Diez-Silva[c], Gabriel Popescu[b], George Lykotrafitis[c], Wonshik Choi[a], Michael S. Feld[a] and Subra Suresh[d]

[a]G. R. Harrison Spectroscopy Laboratory, MIT; [b]Department of Electrical and Computer Engineering, UIUC; [c]Department of Materials Science and Engineering, MIT; [d]School of Engineering, MIT

We present for the first time two intrinsic indicators that quantitatively and noninvasively elucidate the consequences on cell biomechanics of the malaria parasite *Plasmodium falciparum (P. falciparum):* three dimensional distributions of refractive index and the membrane fluctuations in *P. falciparum* infected red blood cells (*Pf*-RBCs). These properties can be used to systemically study the patho-physiology of human malaria disease. During the intra-erythrocytic development, *P. falciparum* causes structural, biochemical, and mechanical changes to host RBCs. Major structural changes include the growing of vacuole of parasites inside host RBCs, loss of cell volume, and the appearance of small, nano-scale protrusions on the membrane surface[1]. From the biochemical standpoint, a considerable amount of hemoglobin (Hb) is digested by parasites during development and converted into insoluble polymerized forms, known as hemozoin. Hemozoin appears as brown crystals in the vacuole of parasite in later maturation stages of *Pf*-RBCs. Two major mechanical modifications are loss of cell deformability and increased adherence of *Pf*-RBC membrane to vascular endothelium and other RBCs. These changes lead to sequestration in microvasculature in the later stages of parasite development, which is linked to vital organ dysfunction in severe malaria[2].

The refractive index maps of *Pf*-RBCs measured by tomographic phase microscopy[3] show the morphological alterations of host RBCs and the structures of vacuoles of parasites as well as growing of hemozoin. In addition, the refractive index is translated into quantitative information about Hb content of individual Pf-RBCs. During the intra-erythrocytic stages of *P. falciparum*, we show the decrease of both the total amount and the concentration of Hb in the cytoplasm of *Pf*-RBCs, as shown Figs. 1A-D. Thermally driven membrane fluctuations in *Pf*- RBCs are strongly correlated with the mechanical properties of cell, which is significantly modified by the specific proteins exported by *P. falciparum* during developmental stages. Fluctuations in *Pf*-RBCs membrane measured by diffraction phase microscopy[4], are used to characterize the membrane stiffness by determining the in-plane shear modulus. We show that membrane stiffness increases progressively with parasite development (Fig. 1E). In particular, the in-plane shear modulus at the schizont stage is up to an order of magnitude higher than that for healthy RBCs (Fig. 1F). These results indicate that parasite development stage directly correlates with the amplitude of membrane fluctuations. We also present experimental results of membrane fluctuations in *Pf*-RBCs over the full range of intra-erythrocyte stages at both normal body and febrile temperatures, representative of malaria fever episodes. Parasite interactions with host RBC strongly correlate with temperature-dependent and stage-specific alterations to membrane dynamics. We critically assess the hypothesis that after exposure to febrile temperature, *Pf*-RBCs at body temperature display deformability closer to those at febrile temperature.

In summary, we report the first experimental connections between these intrinsic indicators and pathological states. These intrinsic optical properties could provide insights into possible mechanistic pathways in the pathogenesis of malaria, as the parasite alters biomechanical properties of RBCs. Our systematic experiments cover all intra-erythrocytic stages of parasite development under normal body and febrile temperatures. These findings offer potential, and sufficiently general, new avenues for identifying, through cell membrane dynamics, pathological states that cause or accompany human diseases.

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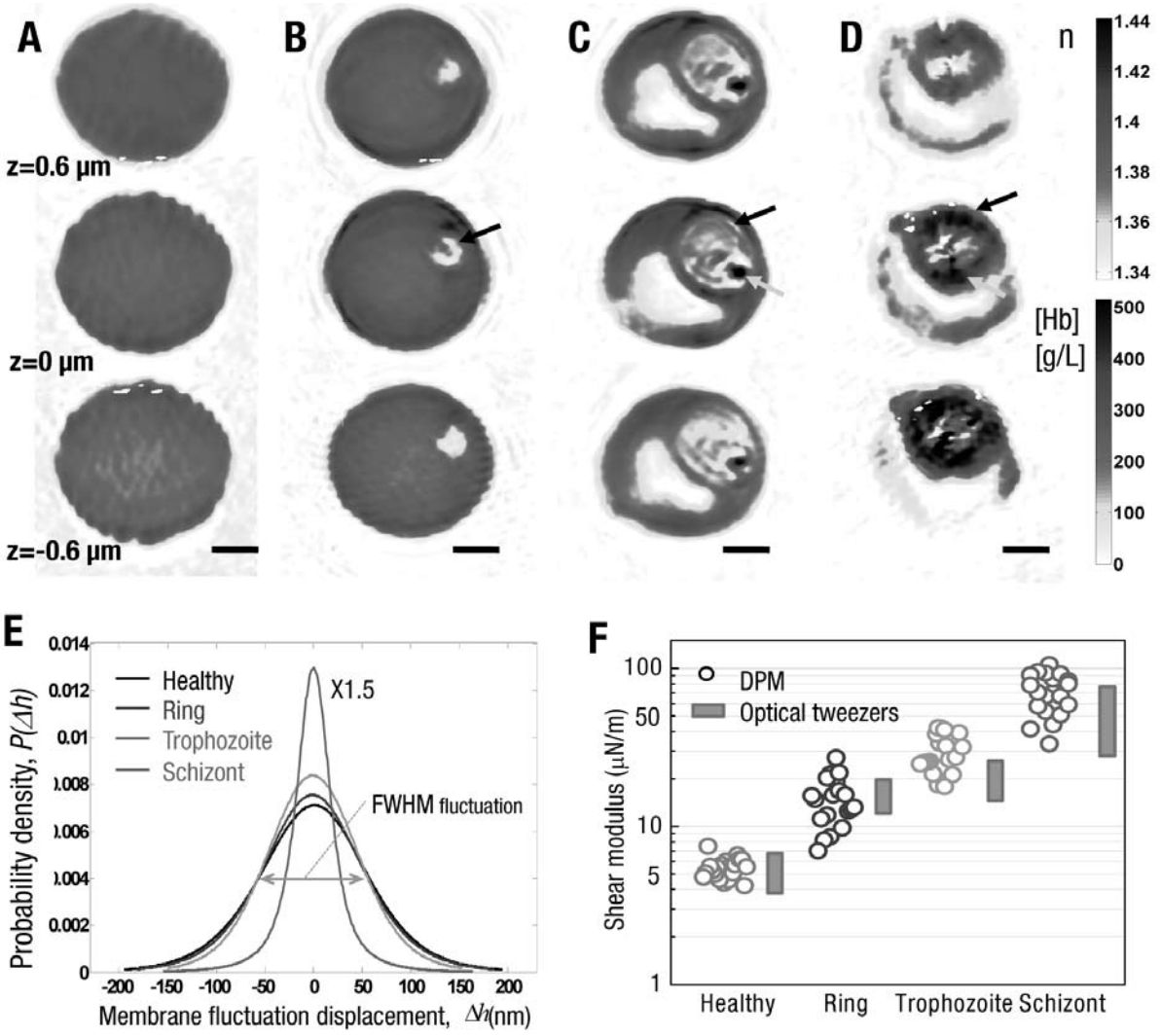

FIG. 1 • Three dimensional refractive index maps of *Pf*-RBCs during all intraerythtocytic stages reveal the structural modifications and the hemoglobin concentration of cytoplasm. (A-D). Membrane fluctuations and in-plane shear modulus at different intra-erythtocytic stages of *Pf*-RBCs. (E-F) (A) Healthy RBC. (B) Ring-. (C) Trophozoite-. (D) Schizontstage. Images in row show three different cross sections: 0.6 μm above (top), at the focused plane (middle), and 0.6 μm below the focused plane (bottom). Black arrows indicate the location of *P. falciparum*, and the gray arrows the location of hemozoin. Color-maps show the refractive indexes (top right) and Hb concentration. (E) Histograms of cell thickness fluctuation of *Pf*-RBCs. (Histogram of the schizont stage is scaled down by a factor of 1.5). (F) In-plane shear modulus of the RBC membrane versus developmental stage of *Pf*-RBCs. The in-plane shear modulus is calculated from the in-plane membrane displacement.. Also shown for comparison are the estimated from optical tweezers [2]. Scale bar 1.5 μm.

Towards Automated Breast Histopathology with Mid-IR Spectroscopic Imaging

Frances N. Pounder and Rohit Bhargava

Department of Bioengineering and Beckman Institute, University of Illinois at Urbana-Champaign

As breast cancer is treatable if diagnosed early, approximately 70% of women over forty have a mammogram every other year[1]. Upon observation of an abnormality, a biopsy is conducted to remove tissue for extensive pathology analysis. Pathology forms the gold standard in detection and grading of cancers. An estimated 1.6 million biopsies are conducted each year, and pathology evaluations cost around $240 per patient[2]. This expensive process is very timeconsuming: patients may wait over a week for a diagnosis[3], considerably heightening anxiety to clinically significant levels. As mammography is not a specific tumor detection technology, approximately 80% of these biopsies do not lead to a cancer diagnosis, leading to wasted effort and economic burden. Clearly the pathology evaluation process is sub-optimal, and automated techniques for analysis of breast tissue could improve the efficiency of cancer diagnosis.

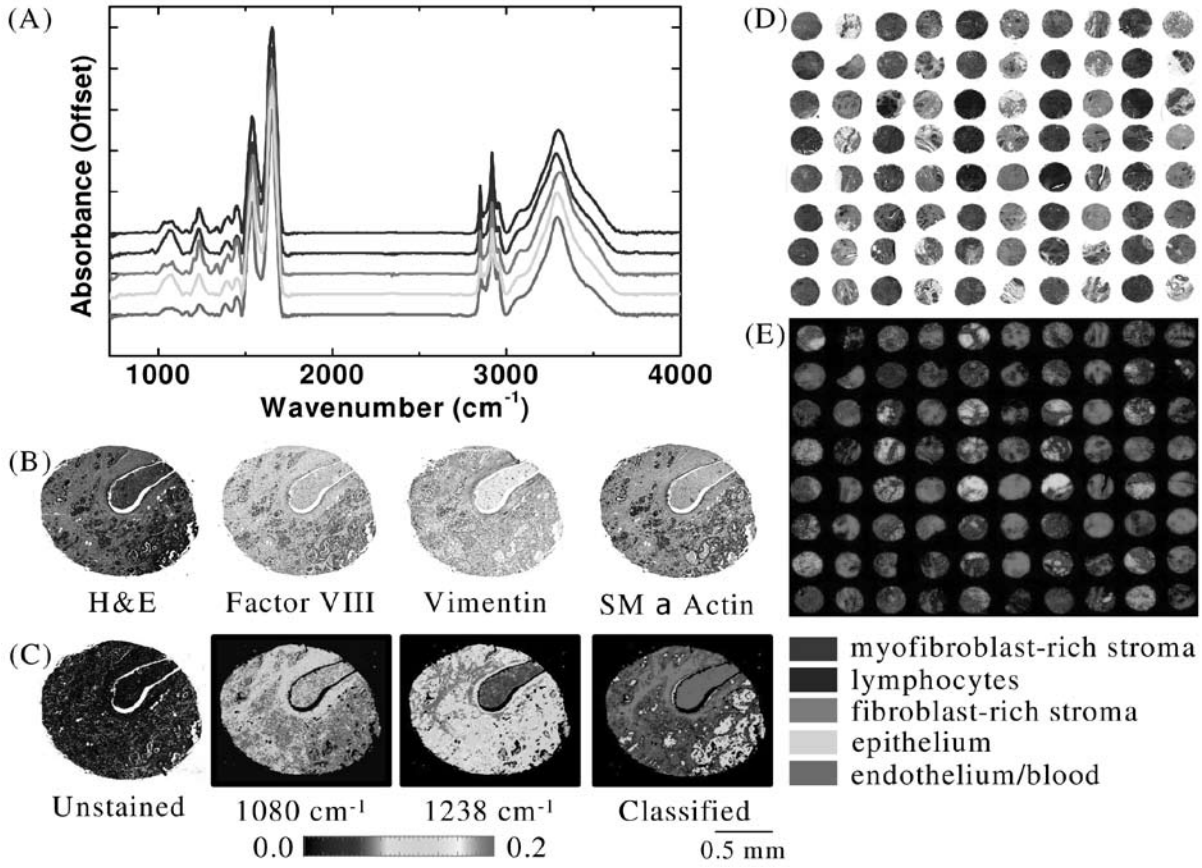

FIG. 1 • (A) Breast tissue IR spectra have distinct features. The distance between marks on the vertical axis is 0.1 a.u. (B) Pathology requires multiple stained tissue sections to characterize tissue. (C) Another approach involves collecting FT-IR images of a single unstained tissue section. Images at specific frequencies highlight different tissue features. FTIR images are classified to identify all tissues. (D-E) Staining and classification for 80 tissue sections demonstrate robust efficiency of the technology.

We hypothesize that Fourier transform infrared (FT-IR) molecular spectroscopy, extensively used in chemical analysis, may be applicable for breast pathology. IR spectra, shown in Fig. 1A, give a quantitative measure of tissue molecular composition. This can be numerically related to histopathology to identify tissue, including epithelium, fibroblast-rich stroma, myofibroblast-rich stroma, lymphocytes, and blood vessels. We use recent advances in instrumentation, combining FT-IR molecular spectroscopy with optical microscopy, to rapidly obtain spatial and spectral information with FT-IR imaging[4]. This technique produces tissue image datasets containing extensive morphological and biochemical information without the use of molecular probes or contrast agents[5]. In Fig. 1C, for example, two images of a single section of unstained breast tissue from a FT-IR dataset demonstrate visualization of different tissue components. The image at 1080 cm^{-1} highlights symmetric phosphate stretching vibrations associated with glycoproteins in secretory epithelium. The image at 1238 cm^{-1} highlights methylene wagging vibrations associated with glycine and proline side chains of collagen in stromal connective tissue.

FT-IR imaging datasets are then automatically classified by a supervised pattern recognition method to provide false-color images comparable to hematoxylin and eosin (H&E) and immunohistochemical (IHC) staining used for conventional diagnoses[6,7]. This computerized technique is robust and non-destructive, and is applied directly to fixed tissue sections employed in clinical practice today[8]. Current pathology evaluation requires a large panel of IHC stains to identify all types of tissue found in the breast and determine patient prognosis. As demonstrated in Fig. 1B and 1C, a single classified FT-IR image can provide similar information about breast tissue to that obtained from multiple IHC stained tissue sections employed to identify endothelium lining blood vessels with Factor VIII, fibroblasts with vimentin, and malignant myofibroblasts with smooth muscle actin (SM-Actin). In this false-color image an invasive epithelial tumor is visualized with adjacent lymphocytes, blood vessels, and myofibroblasts that accompany tumor growth. FT-IR imaging and automated classification could save time and money in pathology evaluation by streamlining the number of stained tissue sections required for each breast biopsy.

We employ tissue microarrays (TMAs), which offer a high-throughput approach to collect data and build a prediction algorithm from a large selection of cancer and normal tissue samples. The tissue section in Fig. 1B and 1C is a single 1.5mm core from a TMA with 80 tissue cores from 40 patients. H&E stained and classified images for the entire TMA in Fig. 1D and 1E demonstrate robust identification of breast tissue types. Automated tissue classification accuracy on this TMA is assessed by receiver operating characteristic (ROC) analysis and validation on additional TMAs and biopsy surgical resections. Results from three TMAs and several large fixed tissue sections demonstrate 99% accuracy for tissue histology classification. After identification of the type of breast tissue associated with each pixel of a FT-IR dataset, malignant TMA cores are identified with 98% accuracy by quantitative evaluation of epithelial content and structure. This high accuracy is unprecedented for an automated diagnostic tool; we are not aware of any other automated method that can provide human-competitive accuracy. This work demonstrates that FT-IR imaging and classification has the potential to provide preliminary diagnoses to streamline time-consuming pathology evaluations on millions of breast biopsy samples annually.

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Biorheology of Healthy and Diseased Human Red Blood Cells

David J. Quinn[a], Subra Suresh[a,b,c], Monica Diez[c], and Sophie Wong[c]

[a] Department of Mechanical Engineering (MIT), [b] Department of Materials Science and Engineering (MIT), [c] Department of Biological Engineering (MIT)

Hereditary hematological disorders and foreign organisms can introduce changes to the spectrin molecular network and membrane of human red blood cells (RBCs). These structural changes can lead to altered cell shape, deformability, cytoadherence and rheology, which may, in turn, promote the onset of vaso-occlusive events and crises that may ultimately cause pain, stroke, organ damage and possibly death. This work aims to experimentally investigate the connections among structure, mechanics, and disease states. Specifically, we examine quantitative experimental measurements of cell deformation and rheology by recourse to optical tweezers and in-vitro flow experiments in microfluidic channels. Previous work by our group and others[1, 2] has shown that the RBC membrane exhibits reduced deformability (i.e., increased stiffness) as a manifestation of diseases such as malaria, spherocytosis, elliptocytosis and sickle cell anemia. More recently, in the case of *P. falciparum* malaria, we have demonstrated that the plasmodial RESA (Ring-infected erythrocyte surface antigen) protein, may be largely responsible for the observed stiffening of RBCs during the earliest stages of the intraerythrocytic cycle of the parasite. Furthermore, it has been shown that the role of such proteins may be more pronounced at physiological temperatures of 37°C (normal body temperature) and 41°C (febrile). However, much of this previous work has modeled the RBC membrane as a purely elastic material and experiments are typically performed within the quasistatic deformation regime. Thus, the work presented here attempts to investigate this connection between disease, structure and function in a more physiologically relevant, dynamic context. This is done experimentally through two primary approaches: (1) in-vitro, microfluidic flow experiments and (2) dynamic/rheological characterization using advanced optical trapping techniques.

An in-vitro experiment has been designed to characterize the flow behavior of healthy and diseased cells with the aid of microfluidic channels designed to mimic individual capillaries in microcirculation. Healthy and diseased red blood cells are caused to flow under a constant pressure differential across a single microfluidic channel with characteristic widths and heights of 3-6μm. Using a high-speed camera system, flow velocities and traversal times as a function of pressure differential are characterized. Experiments are performed at room temperature, 37C and 41C. Current results, presented in Figure 1, indicate markedly impaired flow for infected cells versus uninfected cells in the Ring (0–24 hrs) stage of the parasitic cycle. This impaired flow behavior appears to be reduced in the absence of RESA and is more pronounced at physiologically relevant temperatures.

In order to more fully understand the source of these observed flow behaviors, advanced optical trapping techniques are used to measure fundamental RBC membrane properties. Several different types of experiments are performed to

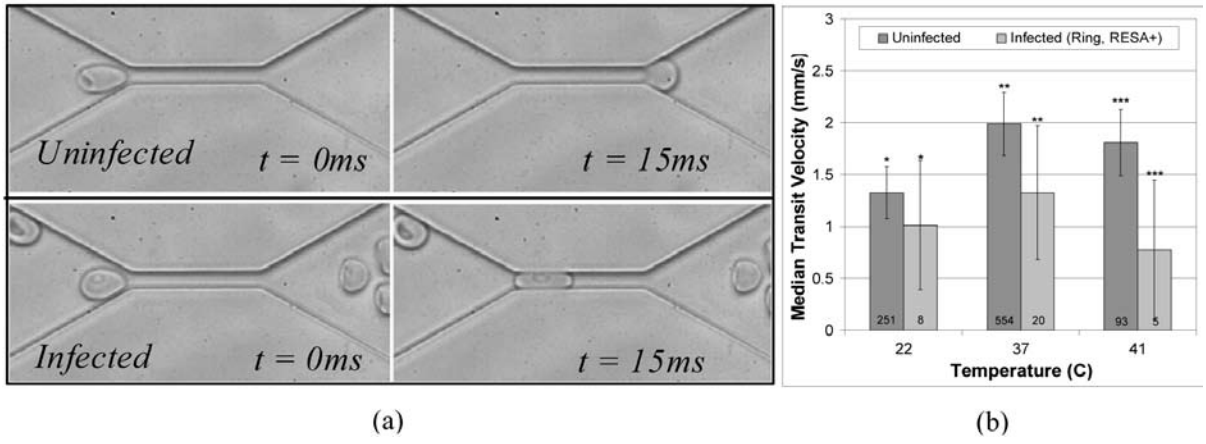

FIGURE 1 • (a) Uninfected and infected RBC flow across a 4μm wide x 3μm high x 30μm long channel (ΔP = 0.7kPa). (b) Median transit velocities across channel at room and physiological temperatures. (* p = 0.003,** p = 6.7x10-9,*** p = 5.8x10-4).

characterize the membrane, including uniaxial tension tests under variable stretching rates, stress relaxation experiments and active rheological characterization using a sinusoidal load application under frequencies ranging from 0-100Hz. The results from these experiments are compared to collaborative work using magnetic twisting cytometry (MTC) and passive rheology characterization using membrane fluctuation experiments as well as work presented in the literature[3-5]. Finally, if time allows, results from collaborative efforts to model the flow of RBCs in the microvasculature using dissipative particle dynamics (DPD) will be presented. These modeling efforts utilize the single-cell experimental results discussed above as primary inputs.

The combination of these results allow for the determination of the relative contributions of membrane elasticity, membrane viscosity, external viscosity and internal viscosity to the physiological flow behaviors of healthy and diseased red blood cells within the microvasculature. Furthermore, when considered in conjunction with the biochemical activity of parasitic proteins such as RESA, these and future results may provide additional insight into the molecular etiology and pathogenesis of malaria and other hematological disorders and diseases. Such insight may lead to new therapeutic approaches to treatment.

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Abstracts by Symposium

SYMPOSIUM
A

Advanced Mathematical Tools: A Frontier between Mathematics and Engineering

ORGANIZERS:

Jane Liu, *Tennessee Technological University*

Rafal Ablamowicz, *Tennessee Technological University*

Application of Brownian Motions in Modeling the Damage Density Evolution in Engineering Materials

Rezwanur Rahman
Aerospace Engineering and Mechanics, Graduate Student
University of Alabama

Anwarul Haque
Aerospace Engineering and Mechanics, Associate Professor
University of Alabama

Zhijian Wu
Mathematics, Professor
University of Alabama

This paper reveals a mathematical formulation for micro-damage damage density evolution in engineering materials (i.e. composite materials) under both mechanical and environmental degradation process. Evolution of micro-damages in materials (polymers, composites and metals) is quite random in nature [1]. A First Order Quasi-Linear Stochastic Partial Differential Equation (SPDE) was developed based on the concept of equilibrium in the damage phase space [2]. The significant phase variables are: damage location, crack length, moisture concentration, temperature, plasticization etc. These phase variables are dealt as deterministic terms in the SPDE. The net flux of damage density in the phase space comes out in terms of damage nucleation/annihilation rates. In this paper we defined the nucleation/annihilation rates as "Continuous Martingales (i.e. Standard Brownian motions). We incorporated this Brownian motion (at a certain probability state) in the governing SPDE. Eventually the generalized form of solution was shown. Finally, the Brownian motion was shown as "Continuous Random Walk model (limiting form)" and it was introduced in the generalized solution of the SPDE.

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Better Living through Simulation: Computer-Aided Tissue Scaffold Design

Ileana Carpen
Assistant Professor
Chemical Engineering, Tennessee Technological University

A tissue/organ donor may (upon demise) end up saving as many as 50 people, according to one government website [1]. Although the lives lost to lives saved ratio is heartening—the demise requirement is less so—and there are complicating medical and social factors. However, there are a number of avenues that are currently being explored with varying degrees of success: stem cell research, xenotransplantation (transplanting non-human organs into humans), and tissue engineering, all of which essentially avoid the ethical conundrum of donor death. Of these, tissue engineering (TE) is, as the name implies, best suited to an engineering approach: basic TE involves introducing the "appropriate" cells onto the "appropriate" scaffold material, and letting these cells grow and divide and (in theory) recreate the desired tissue. Current state-of-the-art TE is highly empirical, using a limited set of chemicals for scaffold design that have a previous record of being FDA-approved for use in humans, as well as the generic method of miming the natural scaffold found in actual tissue. A more rigorous process is proposed herein—using Brownian Dynamics simulations to optimize a soft, polymer-based scaffold for best initial cell dispersion. The scaffold considered is based on a dendrimer network—chosen because in practice, dendrimers are very well characterized and straightforwardly functionalized to produce desired interactions, and are also being considered for other biomedical uses (drug delivery/gene therapy). Cells are represented by interacting particles diffusing through the network. The effects of scaffold-cell interactions and scaffold structure are investigated in order to determine favorable scaffold designs. The method can be targeted to specific tissues and presents an opportunity for non-intuitive conceptual jumps in tissue engineering.

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Practical Finite Temperature Continuum Modeling with Applications to Film Evolution

Lawrence Friedman
Assistant Professor
Engineering Science and Mechanics, Penn State University

Continuum modeling is most often performed in a low-temperature approximation, meaning that thermal fluctuations are often neglected. Such models include phase-field model of crystal growth and other phenomena [1] or continuum models of strained crystal surfaces. [2] When modeling continua at the small scales, however, it may be desirable or necessary to augment existing models to include thermal fluctuations; for example, see Ref. [3]. In most instances, random fluctuations are neglected or random initial conditions are used as a surrogate for actual thermal fluctuations. Until recently, a general prescription for including thermal fluctuations has been lacking. However, in 2007, Lau and Lubensky [4] showed how to construct finite temperature models using stochastic differential equations with general white noise terms. Their proposed method uses Langevin or stochastic differential equations and guarantees that after a long time, an ensemble of systems approaches the Boltzmann distribution. Unfortunately, their approach works only for a finite number of degrees of freedom, not for continua.

Here it is demonstrated that applying Lau's method to continua is problematic and leads to bizarre divergences, but an alternative approach is feasible. Discretizations of nominally continuous low-temperature models can be constructed in the usual fashions such as the finite-difference method, the spectral (Fourier-Transform) method, or the finite element method. These discrete low temperature models can then be promoted to finite temperature models in a manner consistent with Ref. [4]. Practical implementations of all three mentioned discretization methods for thin film evolution are presented, and it is shown that the appropriate thermal equilibrium steady-state is achieved in each case. Finally, an alternative and mathematically simpler approach than Ref. [4] is presented.

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Temperature-Related Cauchy-Born Rule for Nanoscale Continuum Simulations

Maciej Rysz
Mechanical and Industrial Engineering, The University of Iowa

Shaoping Xiao
Mechanical and Industrial Engineering, The University of Iowa

A new homogenization technique, the temperature-related Cauchy-Born (TCB) rule, is proposed via considering free energy instead of the potential so that temperature effects at the nanoscale and on material stability can be investigated. In this paper, the TCB rule is verified via stress analyses of several crystalline solids. With the TCB rule, temperature effects on material stability are also analyzed. Furthermore, a new hierarchical multiscale method is developed through implementation of the TCB rule into meshfree particle methods to perform nanoscale continuum simulations. The problems of crack propagation in a nanoplate are studied, and the results compare well with the molecular dynamics outcomes. In addition, a thermo-mechanical coupling model through implementation of the thermal diffusion equation into nanoscale continuum approximation is developed. Therefore, temperature evolution will be investigated.

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Application of Algebraic Geometry to Vibration Control of Geometrically Nonlinear Hygrothermal-Elastic Composite Plates

Jane Liu
Associate Professor
Civil and Environmental Engineering, Tennessee Technological University

George Buchanan
Professor
Civil and Environmental Engineering, Tennessee Technological University

In recent years, with the increasing capability of symbolic computation, the advanced computational algebraic geometry has become a powerful mathematical tool and a feasible option for many scientific applications. One such advanced computational method—Groebner bases, has attracted more and more attention and gained a reasonable level of awareness in various scientific fields. However, this modern computational method has, until recently, had very little impact on engineering applications. With the increased use of advanced composite materials, nonlinear modeling and analysis become essential and unavoidable in the design of modern structures. However, nonlinear analysis always poses difficult research issues. All this has provided the motivation for this study.

The objective of this paper is to show a surprising application of Groebner bases to a vibration control problem of composite plates that has a complex, nonlinear, and highly coupled nature. The talk will focus on how the Groebner basis technique is employed to analytically solve nonlinear polynomial systems of equations, which usually are solved by numerical methods. This approach will allow us to find relationships, for the purpose of vibration control, among the hygrothermal coefficients, material properties, vibration amplitude, and natural frequencies, which are impossible to obtain by the numerical methods. The results obtained from the study show that the computational method of Groebner bases provides useful alternative and has a great potential in various engineering applications.

Solving Nonlinear Systems of Polynomial Equations

Troy Brachey
Mathematics, Tennessee Technological University

An overview of solving non-linear systems of equations using Groebner Basis techniques. Groebner bases provide an easy to use tool to find exact solutions for non linear systems of equations. The theory of Elimination and Extension is briefly discussed and a practical example shown in detail. This method can be applied to any non-linear system of equations found in many engineering problems.

Solving Systems of Polynomial Equations with Groebner Bases: Examples and Applications

Rafal Ablamowicz
Department of Mathematics,Tennessee Technological University

Jane Liu
Department of Civil and Environmental Engineering, Tennessee Technological University

Resultants have been used in engineering science to solve systems of polynomial equations in several variables. This method is applicable to systems of two equations although generalizations to larger systems have been considered. The method of Groebner bases is an efficient generalization of the method of resultants to any system of polynomial and rational equations. Unfortunately, the theory of Groebner bases including algorithms for their computation, which belongs to the area of computational algebraic geometry, is not usually taught in any engineering curriculum even at the graduate level. Thus, its power to exactly solve systems of polynomial equations remains only known to rather specialized fields of engineering science such as robotics. The aim of this talk is to present examples of finding exact solutions to problems appearing in a variety of applications, including Langrange multipliers, computational geometry, matrix algebra, robotics, etc., when using the Groebner basis method.

Using Maple Computer Algebra System in Teaching Mechanics Courses

Jane Liu
Department of Civil and Environmental Engineering, Tennessee Technological University

Rafal Ablamowicz
Department of Mathematics, Tennessee Technological University

Computer Algebra Systems like Maple or Mathematica impact traditional way of teaching science, mathematics, and engineering. Due to its symbolic manipulation capabilities, a variety of built-in packages, as well as its programming language, Maple provides a very powerful tool for teaching engineering courses. The first author has taught with Maple advanced mechanics of materials, theory of elasticity, plates and shells, the theory of finite element method, and composite materials.

Instead of using paper and pencil, derivation of formulas is greatly simplified and accelerated with Maple. Students still must understand the theory yet the actual computation they do in a Maple worksheet. For the instructor, Maple offers a reliable and fast tool to show many difficult derivations that otherwise would either not be attempted on a board or would take too much time in the classroom. In this approach, students play a much more active role as they are required to use Maple to derive formulas, write procedures and programs to solve various homework problems and special projects. Thus, they also learn an entirely new way of learning.

In this talk, several examples of Maple-based derivations of mechanics formulas in the theory of elasticity and laminate theory in composite materials will be demonstrated. Worksheets developed by the first author when teaching these courses are a foundation of special-purpose Maple packages that can be used by other instructors.

Analysis of Photo-Stimulated Luminescence Spectra Using Genetic Algorithms for Stress Measurements in Chromium-Doped Alumina

Seetha Raghavan
School of Aeronautics and Astronautics,
Purdue University

P.K. Imbrie
School of Aeronautics and Astronautics,
Purdue University

William A. Crossley
School of Aeronautics and Astronautics,
Purdue University

Spectral analysis methods to determine piezospectroscopic relationships in the emission spectrum of chromium-doped alumina have contributed significantly to the development of photo-stimulated luminescence spectroscopy (PSLS) as a stress measurement tool.

Besides the well-known R-lines, used widely today to establish stresses in the thermally grown oxide layer in thermal barrier coating systems, there has been growing interest in understanding stress effects on the weak bands of peaks accompanying these lines, also called the vibronic sidebands of the spectrum [1,2]. The behavior of the multiple peaks in these bands, characterized by their energies from the R-lines [3], have yet to be fully elucidated under uniaxial stress. The ability to deconvolute and monitor these peaks with stress, improves their potential to contribute to measurement of the complete stress state in chromium-doped alumina. Gradient-based algorithms have been used widely in the spectral analysis methods developed thus far. The use of genetic algorithms in the spectral analysis of R-lines and vibronic bands is a novel approach taken in this work. The overall spectral analysis procedure involved pre-processing, deconvolution and fitting of the spectra. This method was applied to spectra from our uniaxial compression tests on single crystal specimens and the resulting peakshifts obtained were validated with the existing data on piezospectroscopic coefficients of the R-lines [1,4]. The implementation of this method has led to significant new results in the quantification of peakshifts with uniaxial stress in the vibronic bands of the spectrum. The use of genetic algorithms was instrumental in the deconvolution and fitting of the numerous pseudo-Voigt peaks in these bands. Fitting statistics such as the fitness function and number of function evaluations were used to assess the effectiveness of the procedures used.

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Introducing the Implementation of Kruskal-Wallis Non-parametric One-Way ANOVA as a Statistical Tool in Image Analysis

Soumit Salman Rahman*
Microsoft Corporation, China
soumit.s.rahman@gmail.com

Joydip Saha
Department of Mechanical Engineering, Bangladesh University of Engineering and Technology

Image analysis has widespread use in different dimension of fields such as Remote Sensing, Surveillance Systems, Medical Diagnosis, Civil Infrastructure Inspection, Underwater Sensing etc. These different fields require the image analysis procedures provide different volumes and measures of output. An image analysis algorithms preformat the input data and extracts different kinds of information from them. But whatever the initial processing is, obtaining a result eventually comes down to a stage of comparison. We did some research on different comparison methods already in application. We found out that, this comparison methods depends almost entirely on the extracted data from the preformatted images. While going through different statistical methods, we came across one very strong yet simple tool named Kruskal-Wallis nonparametric one way ANOVA [1]. Unlike its analogous method of one way Analysis of Variance (ANOVA), Kruskal-Wallis tool does not assume the data sets to be a normal population. As a result this can be implemented as an ideal process for comparing a series of image sequence. In our experiment we considered the images to have three color layers (Red, Green and Blue) and analyzed them individually. With the outcomes derived from the experiment this paper presents a an approach that approximately states the locality of change in a scene, applying the Kruskal-Wallis nonparametric one way ANOVA as a tool for comparison.

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Computational Nonlinear Solid and Structural Mechanics

SYMPOSIUM
B

ORGANIZER:

Ilinca Stanciulescu, *Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign*

Multiscale Modeling of Indenter Penetration in Granular Media

Xuxin Tu
Postdoctoral Fellow, Civil Engineering
Northwestern University

Jose E. Andrade
Assistant Professor, Civil Engineering
Northwestern University

Indenter penetration in granular media is a generic problem of practical significance. At the field scale, this phenomenon corresponds to the bearing capacity issue for building foundations. At the nano-scale, a relevant application can be found when a nanometer indenter probes the fundamental structure of cement-based materials, to accurately characterize the nano-scale pore structure and to obtain critical elastic mechanical properties [1]. In this generic problem, microscopic interactions—including particle sliding and rolling, fabric rearrangement, force chain forming and breaking—play a crucial role for near-field material response, and thus greatly affect the mechanical response to the penetrating indenter. For high-resolution modeling, we use a micromechanically-based multiscale model [2] to simulate the near-field granular material. To make the problem tractable, we use a continuum model to simulate farfield material response. Coupling these two methods at different scales is based on a recent multiscale technique developed for granular materials [3, 4]. It is shown that such a multiscale approach provides a favorable framework for solving the generic indenter penetration problem.

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Toward Stable Treatment of Fluid/Solid Interaction in the Presence of Free Surfaces

Jessica Sanders
Department of Civil Engineering, Duke University

Tod Laursen
Department of Civil Engineering, Duke University

John Dolbow
Department of Civil Engineering, Duke University

Computational treatment of floating solids, in the presence of free surfaces and/or breaking waves poses several modeling challenges. Examples where these systems might be of interest could include off shore wave energy harvesting systems. Some such systems use buoys, while others ideas rely on flexible structures or joints where motion and elastic deformation is important to the optimization of energy capture. Many other systems exist in which interaction between free surfaces and deformable structures may be of interest, including some microfluidic systems. In this work, we take the first steps in developing a robust computational strategy for treating deformable bodies in a fluid environment with free surfaces, arbitrarily large fluid motion, and potentially finite deformation of the solid.

In the finite element community, fully coupled solid-fluid interaction is heavily researched and most commonly treated with ALE formulations, which tend to require special modifications or remeshing when motion is large. An immersed finite element method coupling an Eulerian finite element fluid grid with a Lagrangian finite element solid grid is also sometimes used [1]. The most sophisticated free surface solvers for computational fluids, however, exist in the finite difference communities [2] [3]. It is the purpose of this work to suggest a coupling between the capabilities of the finite difference solutions involving level set free surface descriptions and the finite element capabilities of large solid deformation.

The work is based on a finite difference and level set description of a free surface between two immiscible fluids (for example water and air) for incompressible flow by Sussman et. al. [2]. The addition of a deformable solid with a Lagrangian finite element mesh is investigated. Previous results by the authors suggest techniques for the stable enforcement of boundary conditions on the solid mesh by Nitsches method. Concepts and preliminary results will be presented.

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Finite Element Analysis of Inelastic Laminated Plates Using a Global-Local Formulation with Delamination

Hashem Mourad
Technical Staff Member
Theoretical Division–T3, Los Alamos National Laboratory

Todd Williams
Technical Staff Member
Theoretical Division–T3, Los Alamos National Laboratory

Francis Addessio
Technical Staff Member
Theoretical Division–T3, Los Alamos National Laboratory

The current work is part of an ongoing effort to develop analytical and computational tools which can be used to study the response and damage distribution within laminated composite plates subjected to complex/severe static and/or dynamic loads.

The proposed finite-element formulation [1] is based on the global-local laminated plate theory of Williams [2], which is founded on a generalized superposition of displacement fields associated with different length scales: (i) a global field, which varies continuously over the thickness of the entire laminate, and (ii) a local field whose definition varies from layer to layer. This layer-wise definition of the local field allows discontinuities between layers (due to delamination) to be incorporated in a straightforward manner, and affords much improved accuracy, but incurs a higher computational cost. However, the presence of a global field makes it possible to use the full global-local representation only in critical regions of the model, where high resolution is required (e.g. in the immediate vicinity of the collision site, in the case of a large structure impacted by a small high-speed projectile). A more economical global-only representation can be used to model the remainder of the structure, thereby maximizing overall computational efficiency.

Several numerical examples are presented to illustrate the advantages of the proposed approach, and to examine the performance characteristics of the proposed plate element.

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Application of the Generalized Finite Element Method with Global-Local Enrichment Functions to Local Plastic Analysis

Carlos Armando Duarte
Assistant Professor
Civil and Environmental Engineering,
University of Illinois

Dae-Jin Kim
Graduate Research Assistant
Civil and Environmental Engineering,
University of Illinois

Sergio Persival Proenca
Professor
Structural Engineering, University of São Paulo

The main feature of partition of unity methods such as hp-cloud, generalized and extended finite element methods is their ability of utilizing a priori knowledge about the solution of a problem in the form of enrichment functions. Linear combination of partition of unity shape functions can reproduce exactly the enrichment functions and thus their approximation properties are preserved. This class of shape functions enables, for example, the approximation of solutions in the neighborhood of cracks [3], inclusions, voids [4], etc. using finite element meshes that do not fit them. However, analytical derivation of enrichment functions with good approximation properties is mostly limited to two-dimensional linear problems. In this paper, we use the so-called generalized finite element method (GFEM) with global-local enrichment functions [2] to generate proper enrichment functions for problems with localized nonlinearities. This procedure involves the solution of boundary value problems around regions exhibiting nonlinear behavior and the enrichment of the global solution space with local solutions through the partition of unity framework used in the GFEM. This approach was originally proposed to efficiently handle crack propagation simulation [1], but it also has the potential to solve nonlinear problems accurately with a reduced computational cost compared with the conventional finite element method. Several nonlinear problems of the J2-based plasticity theory with linear isotropic hardening are solved using the proposed procedure to demonstrate its robustness, accuracy and computational efficiency.

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Some Ideas on Time Integration for the Simulation of the Dynamic Response of Soft Materials

Adrian Lew
Department of Mechanical Engineering, Stanford University

In this talk I will discuss some recent ideas on computational solid dynamics. I will first describe the main ideas behind variational time integrators for solid dynamics, and introduce one such integrator that enables each element of the mesh to advance with its own time step, and its associated scalable parallel extension. I will discuss some of its nice conservation and stability properties, and show recent results on an explicit contact algorithm that takes advantage of the algorithms asynchronous nature to both provide substantial computational savings and retain outstanding energy conservation properties through the collision. Additionally, I will introduce a novel shock-capturing technique. The performance of all these ideas are showcased in the simulation of the penetration of a soft gelatin by a projectile.

A Stabilized Locking-Free, Two-Pass Finite Element Formulation of Contact

Ghadir Haikal
Civil and Environmental Engineering, University of Illinois

Keith Hjelmstad
Professor
Civil and Environmental Engineering, University of Illinois

The discrete node-to-surface gap function is typically used as a contact constraint to enforce the impenetrability condition between a "slave" node and a "master" surface. This type of formulation is usually sensitive to the choice of the master/slave pairing and is generally not capable of representing a state of constant pressure, therefore failing the well-known contact patch test [1][2]. When used as a two-pass method, the discrete node-to-surface gap function formulation has been shown to fail the Ladyzhenskaya-Babuska-Brezzi (LBB) condition and therefore exhibits surface locking [1].

To address these issues, we propose a stabilization procedure in the form of a local enrichment of the contact surface that would eliminate the need for a master—slave definition while still satisfying the LBB condition. The enrichment is local to the contact element, and the additional unknowns can be condensed out at the element level. The impenetrability constraints are enforced strongly at the contact locations using discrete Lagrange multipliers. The stabilized formulation guarantees an accurate transfer of the pressure field across the contact interface. The result is a robust two-pass node-to-surface formulation that passes the patch test and strongly enforces the non-penetration constraint at contact locations without inducing surface locking [3].

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Large-Scale Parallel Multibody Dynamics with Frictional Contact on the GPU

Dan Negrut
Department of Mechanical Engineering, University of Wisconsin, Madison

Toby Heyn
Research Assistant
Department of Mechanical Engineering, University of Wisconsin, Madison

Alessandro Tasora
Department of Mechanical Engineering, University of Parma

Mihai Anitescu
Mathematics and Computer Science Division, Argonne National Laboratory

In the context of simulating the frictional contact dynamics of large systems of rigid bodies, this paper reviews a novel method for solving large cone complementarity problems by means of a fixed-point iteration algorithm. The method is an extension of the Gauss-Seidel and Gauss-Jacobi method with overrelaxation for symmetric convex linear complementarity problems. Convergent under fairly standard assumptions, the method is implemented in a parallel framework using a Single Instruction Multiple Data (SIMD) computation paradigm promoted by the Compute Unified Device Architecture (CUDA) library for GPU programming. The computational capability implemented will be demonstrated to support the simulation of problems with more than one million bodies in contact. This renders simulation as a viable tool in investigating the dynamics of complex systems such as ground vehicles running on sand, powder composites, and granular material flow.

Generalized Finite Element Method for Modeling Nearly Incompressible Bimaterial Hyperelastic Solids

Philippe Geubelle
Professor
Department of Aerospace Engineering, University of Illinois

Karthik Srinivasan
Graduate Research Assistant
Department of Aerospace Engineering, University of Illinois

Karel Matous
Principal Research Scientist
Computational Science and Engineering, University of Illinois

An extension of the generalized finite element method to the class of mixed finite element methods is presented to tackle heterogeneous systems with nearlyincompressible nonlinear hyperelastic material behavior. In particular, heterogeneous systems with large modulus mismatch across the material interface undergoing large strains are investigated using two formulations, one based on a continuous deformation map, the other on a discontinuous one. A bimaterial patch test is formulated to assess the ability of the two formulations to reproduce constant stress fields, while a mesh convergence study is used to examine the consistency of the formulations. Finally, compression of a model heterogeneous propellant pack is simulated to demonstrate the robustness of the discontinous deformation map formulation.

Mathematical Properties of Space Discretization that Guarantee Directional Isotropy: Examples in Crack Propagation and Random Microstructures

Katerina D. Papoulia
Department of Civil Engineering, University of Waterloo

Our focus is on mathematical properties of geometries that preserve directional isotropy, i.e., have no preferred directions. Typical finite element meshes specifically lack this property, e.g., a crack constrained to propagate along element edges is obviously restricted to a few preferred directions no matter how fine the mesh is. We present finite element meshes based on so-called pinwheel and quaquaversal tilings of the plane and 3D-space, respectively. These meshes possess the "isoperimetric property" that for any curve C in the computational domain, there is an approximation to C using mesh-cell edges that tends to C including a correct representation of the length of C, as the grid size tends to zero. We suggest that the isoperimetric property is a necessary condition for any possible spatial convergence of cracks constrained to propagate along mesh-cell edges in the general case that the crack path is not known in advance. Conversely we are able to establish that if a two-dimensional isoperimetric mesh is used, the discrete interface first activated in the finite element model will converge, as the mesh size tends to zero, to the theoretical initial crack. Convergence takes place in three senses: position of the interface, time of initiation, and orientation of the interface.

These meshes also possess the property that, in the limit as the mesh is refined, the orientations of the mesh-cell edges are uniform in the sense that for any open subset of the upper hemisphere, the probability that an edge's orientation will lie in that subset is proportional to the area of the subset. In fact, something even stronger is true: if one selects any interior point x of the domain and any interior ball B centered at x, then the orientations of the mesh edges that lie inside B are also uniform in the limit of refinement. We examine composites with randomly distributed short fibers and explore the possibility of fibers selected as randomly chosen edges of the matrix discretization. Our numerical experiments suggest that this results in isotropically distributed fibers, which amounts to much smaller models than the traditional approach of meshing around randomly positioned fibers.

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Vibration Suppression in a Traversing Mass-Cantilever Beam System

Birbal Singh*
Department of Mechanical Engineering, Lakehead University
Birbal.Singh@Lakeheadu.ca

Sultan Siddiqui
Department of Mechanical Engineering, Lakehead University

Yue Huang
Graduate Student
Department of Mechanical Engineering, Lakehead University

This paper is focused on the modeling and vibration suppression of a continuously distributed system interacting with a traversing spring-mass subsystem. The system has many applications such has design of bridges, robots traversing on space trusses, vibration suppression in stacker cranes carrying moving loads in large warehouses, and vibration suppression in space trusses. The equations of motion are derived using Hamilton's principle. To solve the resulting nonlinear partial differential equations, Galerkin method is used to discretize in the space and time domains to reduce them to nonlinear ordinary differential equations.

Vibration suppression strategy used in this study is based on enhancing the coupling in the system. The coupling in the system can be made stronger by establishing internal resonance. When internal resonance exists in the system, energy imparted initially to one of the modes involved in the internal resonance will be continuously exchanged among all the modes involved in that internal resonance. When all the modes in the system are strongly coupled, damping applied in one direction can directly suppress vibrations in that direction and indirectly suppress vibrations in the remaining directions. Internal resonance occurs if a commensurable or nearly commensurable relationship exists between the linear natural frequencies of the system. The novel feature of the vibration suppression technique presented in this paper is establishing internal resonance between the beam and the traversing spring-mass subsystem as a prerequisite condition before suppressing vibrations within a simple PD controller. In order to establish internal resonance, parametric analysis is carried out to identify regions where the natural frequencies are commensurable or nearly commensurable. Then, using a proportional gain controller, internal resonance is achieved. Having built up internal resonance and thus enhanced the coupling, damping is introduced in the traversing spring-mass subsystem via a derivative controller, resulting in rapid vibration suppression.

The vibration suppression technique developed is demonstrated using numerical simulation with the adaptive stepsize Runge-Kutta method and spectral analysis is carried out. Spectral analysis involves finding the response frequencies in the system using discrete Fourier transform. This approach gives the averaged behavior of the frequencies over the length of the time series for which the discrete Fourier transform was performed. However, the motion of the traversing spring-mass subsystem results in the change in the response frequencies with time. To investigate this effect, time-frequency analysis is carried out. Time-frequency analysis captures the changes in the frequency content of a signal with time.

It is found that after establishing IR states and applying two controllers in direction v and direction w, vibrations can be successfully and rapidly suppressed. The numerical simulation results from different solvers, models, and IR states indicate that there are minor differences between the Runge-Kutta method and AAF for the dimensional model. As for the non-dimensional model, Runge-Kutta method diverged due to numerical instability when the time range is increased, whereas AAF remains very stable. In addition to good numerical stability, the AAF method employs the actual DAE system and hence yields more accurate results. Further, the AAF algorithm produces evenly spaced data with desired accuracy.

A Generalized Finite Element Method for Steady-State and Transient Heat Transfer Problems Exhibiting Sharp Thermal Gradients

Patrick O'Hara
Research Assistant
Civil and Environmental Engineering, University of Illinois

Armando Duarte
Assistant Professor
Civil and Environmental Engineering, University of Illinois

Thomas Eason*
Air Vehicles Directorate, Air Force Research Laboratory
Thomas.Eason@wpafb.af.mil

Heat transfer problems exhibiting sharp thermal gradients are analyzed using the classical and generalized finite element methods. Convergence studies show that low order (linear and quadratic) elements require strongly refined meshes for acceptable accuracy.

A generalized FEM with global-local enrichments is proposed for the class of problems investigated. In this procedure, a global solution space defined on a coarse mesh is enriched through the partition of unity framework of the generalized FEM with solutions of local boundary value problems.

The two-way information transfer provided by the proposed generalized FEM is appealing to several classes of problems, especially those involving multiple spatial scales. The proposed methodology brings the benefits of generalized FEM to problems where limited or no information about the solution is known a-priori. The proposed GFEM may also be attractive for time dependent problems, which require high spatial resolution. Initial investigation shows that much larger time steps may be used in the proposed GFEM than in the FEM. The target application involves response prediction at elevated temperatures. As such, temperature-dependent materials as well as nonlinear solution strategies will need to be considered.

Discrete Method for Solid Mechanics

Jia Lu
Associate Professor
Mechanical and Industrial Engineering, The University of Iowa

Jian Qian
Graduate Research Assistant
Mechanical and Industrial Engineering, The University of Iowa

We present a new method for solving 2dn order boundary value problems such as elasticity. An underlining motivation was provide a solver that can be seamlessly connected to point cloud solid models which become increasingly popular in biomechanical applications. In this method, the domain is partitioned into node-based cells. On each cell, a linearly exact discrete gradient operator is defined. This gradient operator is subsequently employed in a weak form to yield a nodal-integration-like Galerkin formulation. The method works for both point clouds and domains originally discretized by polygon elements; a unified approach is devised to construct the gradient operators for both cases. The method has several advantages. First, the gradient operator is defined directly on discrete nodal values without introducing continuous approximation of the unknown variable. Thus, the method bypasses the often tedious computation of meshfree shape functions or polygon element shape functions. Second, the discrete gradient has the Kronecker-delta properties and can be directly interfaced to lower order finite elements. Thirdly, the method passes the linear displacement patch test by construction. The method over performs the lower order triangular or quadrilateral elements, and substantially alleviates numerical locking in the thin-element and incompressibility limits. Application of the method in middle- to large size biomechanical problems will also be presented.

Keywords: discrete method, meshless method, image-based analysis

A New Type of Theory for the Development of Multiscale Plate Theories

Todd Williams*
Technical Staff Member
Theoretical Division, T-3, Los Alamos National Laboratory
oakhill@lanl.gov

The theoretical development for a new type of general framework for nonlinear, multiscale plate theories is presented. The multiscale nature of the theoretical framework is due to the use of a superposition of both general global and local displacement effects. The forms and the orders of both the global and local displacement fields are arbitrary. Using this global-local displacement field the governing equations of the theory are obtained by satisfying the governing equations of nonlinear continuum mechanics referenced to the initial configuration. In particular, the equations of motion and the lateral surface boundary conditions are derived by using the method of moments over the different scales and an orthogonality constraint. The theory satisfies the interfacical constraints (displacement (dis)continuity and traction continuity) and the top/bottom surface boundary conditions in the strong sense. Delamination effects are incorporated into the theory through the use of cohesive zone models (CZM). The theory is sufficiently general that any type of CZM can be used to model delamination initiation and growth at the different interfaces. Furthermore, the theory is developed in a sufficiently general fashion that any type of constitutive theory for inelastic material behavior can be used. As a result of the formulation the global and local effects are fully coupled.

It is shown that the theory is capable of providing accurate predictions for all of the fields in perfectly bonded and delaminated plates even for relatively low orders of displacement approximations. In particular, the theory is shown to provide accurate predictions for the transverse stresses (in most cases less than a few percent) directly from the constitutive relations that are continuous across the interfaces.

Fatigue Crack Propagation Threshold and Paris Curve Determination Using Cohesive Element-Based Methodology

Spandan Maiti
Mechanical Engineering– Engineering Mechanics, Michigan Technological University

Aniket D. Utkur
Mechanical Engineering– Engineering Mechanics, Michigan Technological University

Bob Farahmand
Boeing

Designs that tolerate cyclically applied loading and avoid fatigue failure during their lifetime have been the quest of designers/researchers for a long time. With the variety of materials used in different structures, it will be very convenient to have a reliable analytical or computational scheme in place of expensive and tedious experimental methods for the estimation of fatigue and fracture allowables to be used in life estimation of structural parts. However, sub-critical nature of the fatigue crack growth makes it harder to apply classical fracture mechanics theory for the prediction of this form of failure.

Maiti and Geubelle [1] presented an irreversible cohesive model based method for the estimation of fatigue crack propagation in polymers in Paris region. Present study is an extension of that technique for the prediction of threshold of fatigue crack propagation in metallic materials employing a cohesive-volumetric finite element scheme. The computational method presented here is based on the energetics of the crack propagation. The fracture energy for crack extension GIC is estimated from the constitutive law of the material employing an extended Griffith theory [2, 3]. Further, this energy is partitioned into two parts in a cohesive modeling framework: Threshold energy Gth for fatigue crack initiation, and the energy required for the fatigue crack propagation after initiation. Gth is intrinsically tied with a cohesive law parameter Sinit, as will be presented. An in-depth parametric study of the effect of various materials, loading environment, and model parameters on the fatigue crack propagation in the threshold region will be discussed. The application of this technique will permit the virtual generation of fatigue crack growth curves, and will eliminate costly and time consuming experiments.

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Engineering Science across Disciplinary Boundaries: A Symposium in Honor of Eringen Medalist Subra Suresh

SYMPOSIUM C

ORGANIZERS:

K. Jimmy Hsia, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Zdenek P. Bazant, *Department of Civil and Environmental Engineering, Northwestern University*

Interfacial Plasticity Governs Strain Rate Sensitivity and Ductility in Nanostructured Metals

Ting Zhu
Woodruff School of Mechanical Engineering, Georgia Institute of Technology

Ju Li, Amit Samanta, Hyoung Gyu Kim
Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia

Subra Suresh
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Nano-twinned copper exhibits an unusual combination of ultrahigh strength and high ductility, along with increased strain-rate sensitivity. We develop a mechanistic framework for predicting the rate sensitivity and elucidating the origin of ductility in terms of the interactions of dislocations with interfaces. Using atomistic reaction pathway calculations, we show that slip transfer reactions mediated by twin boundary are the rate-controlling mechanisms of plastic flow. We attribute the relatively high ductility of nanotwinned copper to the hardening of twin boundaries as they gradually lose coherency during plastic deformation. These findings provide insights into the possible means of optimizing strength and ductility through interfacial engineering.

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Strength of Quasi-brittle Ceramics: Impossibility of Finite Weibull Threshold and Statistical Justification in Nano-mechanics

Zdenek P. Bazant
W.P. Murphy Professor and McCormick Institute Professor
Department of Civil Engineering, Northwestern University

Jia-Lian Le
Graduate Research Assistant
Department of CEE, Northwestern University

Sze-Dai Pang
Department of Civil Engineering, National University of Singapore

The experimentally observed deviations of the strength histograms of coarse-grained ceramics from the two-parameter Weibull distribution have recently led to a wide-spread adoption of the three-parameter Weibull distribution, which has a finite threshold. However, the misfit of the experimental histogram and of size effect curves is remedied only partly. It is shown that all the known experimental data can be fitted very well by a recently proposed theory [1,2], which was derived from Maxwell-Boltzmann type statistics and the stress-dependence of the activation energy barrier for the free energy potential of an atomic system of a rupturing nano-scale connection. According to that theory, the cumulative strength distribution of a small representative volume element (RVE) of a quasibrittle material must be a Gaussian (normal) distribution, onto which a power-law tail (or Weibull tail), reaching to the failure probability of about 0.0001 to 0.01, must be grafted from on the left. For an increasing structure size, the strength distribution must be deduced from a finite, rather than infinite, weakest-link model. This model indicates that, with an increasing structure size, the Weibull distribution expands from the left tail and its grafting point grows into the Gaussian core until, for a structure consisting of >10,000 equivalent RVEs, the entire distribution becomes perfectly Weibullian. It is demonstrated that the proposed model fits the observed strength histograms and size effect plots for quasibrittle industrial and dental ceramics as well as other quasibrittle materials. In closing, extensions to structure lifetime and applications to fiber and particulate composites are outlined.

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Experiments and Simulations in Twinning

Huseyin Sehitoglu
Department of Mechanical Science and Engineering, University of Illinois

This presentation will start with summarizing Subra Suresh's early accomplishments in fatigue. I will summarize his superb contributions to experimental studies of environment effects in fatigue, and roughness induced crack closure. I will then focus on our experimental work in fcc steels, the role of slip and twinning, and strengthening of steels with addition of nitrogen. New techniques of local deformation measurements using digital image correlation will be described to shed light into twin strains. Then, the presentation will focus on the use of atomistic simulations to establish the equilibrium spacing of partial dislocations and its variation with nitrogen content. We show that the separation distance of the partials correspond with the maximum strengthening observed near 1% N content. There has been significant work on twinning in the past but a theoretical framework to establish the nucleation stress is still missing. For the first time, we derive a twin nucleation stress without a-priori constants. The twin stress is established as a function of the generalized fault energy curve (γ-curve) along <112> direction. Our results show that the twin nucleation stress and critical aspect ratio of the twin nucleus depend strongly on the unstable stacking fault energy γus, unstable twin stacking fault energy γut and the stable twin stacking fault energy γtsf. The resulting relationship is very simple and shows the limitations of the twin stress theories that rely on the intrinsic stacking fault energy alone. A natural consequence of this model is that the predicted values of twinning stress for fcc metals are in excellent agreement with the experimental values reported in literature. Finally, we will discuss our recent work on the role of grain misorientations on grain boundary energies and its ramifications in mechanical response of metals and crystal plasticity modeling.

Virtual Melting as a Mechanism of Crystal-Amorphous and Crystal-Crystal Phase Transformations and Plastic Relaxation

Valery Levitas
Schaefer 2050 Challenge Professor
Departments of Mechanical Engineering, Aerospace Engineering, and Material Science and Engineering,
Iowa State University

A new mechanism of temperature- and pressure-induced crystal-amorphous and crystal-crystal phase transformations, as well as plastic relaxation via virtual melting was justified thermodynamically and kinetically [1-3]. Virtual melting occurs 100-1000K below the thermodynamic melting temperature and is operative when the classical mechanisms of plastic relaxation (due to dislocations and twinning) are suppressed. The energy of the internal elastic stresses, induced by large change in volume (transformation strain) for crystal-crystal phase transformation, increases the driving force for melting and reduces the melting temperature; under certain conditions, a barrierless melt nucleation occurs. Melting releases the internal stresses and the unstable melt solidifies into the stable crystalline (above the glass transition temperature) or amorphous (below the glass transition temperature) phase. A short-lived unstable melt (transitional state) is called the virtual melt. Virtual melting removes athermal interface friction, reduces kinetic barrier, increases atomic mobility and stabilizes subcritical crystalline nucleus or transforms supercritical crystalline nucleus to an amorphous nucleus. Two types of applications are considered. The first one is related to beta-delta transformation in energetic crystal HMX. In this case, virtual melting occurs at 120K below the melting temperature and is indirectly confirmed by sixteen nontrivial experimental phenomena. Kinetic equation for beta-delta phase transformation is currently used as a part of mechanochemical model for HMX decomposition with a rigid cylinder [4]. The second application is devoted to pressure-induced crystal-crystal phase transformation and amorphization in materials with a specific pressure-temperature phase diagrams. We combine virtual melting, stress analysis and non-equilibrium phase transformation diagrams to develop new scenarios of crystal-amorphous and crystal-crystal phase transformations. Results are applied for a new interpretation of melting, crystal-amorphous and crystal-crystal phase transformation mechanisms in ice Ih. Virtual melting is expected to be a main mechanism of amorphization in geological materials (e.g. quartz, coesite, and jadeite), in brittle semiconductors (e.g. Ge and Si), in materials leading to superhard phases (e.g. BN and graphite), as well as polymet. Recent calorimetric experiments (S. L. Randzio and A. Kutner, J. Phys. Chem. B, 2008) confirm the virtual melting for amorphization in rosiglitazone maleate (avandia), an important pharmaceutical substance used as an insulin enhancer.

In addition to the above examples, some indications were found about the existence of the virtual amorphization, and that virtual melting and/or virtual amorphization may serve as mechanisms of various structural changes. It includes: plastic flow under high-strain-rate and shock loading of HMX crystal, metals [5], and metallic nanowires; fracturing (crack propagation and void nucleation); nanofriction; sublimation; and grain growth and sliding.

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Protein Mechanics: A New Frontier in Biomechanics

Gang Bao
Professor
Department of Biomedical Engineering, Georgia Institute of Technology and Emory University

Proteins play essential roles in all aspects of cellular processes, such as biosynthesis, division, growth, motility, metabolism, signaling, and transmission of genetic information. Proteins, however, could deform under mechanical forces, thus altering their biological functions. Here we present protein deformation as a possible molecular basis for mechanosensing and mechnotransduction, elucidate the important features of protein mechanics including protein deformation mode and dynamics, illustrate how protein deformation could alter biological function, and describe the important roles of protein deformation in force-sensing, force transducing and mechanochemical coupling in cells. The experimental and modeling challenges in protein mechanics are discussed.

How Protein Materials Balance Strength, Robustness, and Adaptability

Sinan Keten
Massachusetts Institute of Technology

Markus J. Buehler
Esther and Harold E. Edgerton Assistant Professor
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Proteins constitute critical building blocks of life, forming biological materials such as hair, bone, skin, spider silk or cells, which play an important role in providing key mechanical functions in biological systems. The fundamental deformation and fracture mechanisms of biological protein materials remain largely unknown, partly due to a lack of understanding of how individual protein building blocks respond to mechanical load and how they participate in the function of the overall biological system. However, such understanding is vital to advance models of diseases, the understanding of biological processes such as mechanotransduction, or the development of biomimetic materials. Recent theoretical and computational progress provides us with the first insight into such mechanisms and clarifies for the first time how biology works at the ultimate, molecular scale, and how this relates with macroscopic phenomena such as cell mechanics or tissue behavior, across multiple hierarchical scales. Here we review how molecular dynamics (MD) simulations implemented on ultra-large computing facilities, combined with statistical theories, is used to develop predictive models of the deformation and fracture behavior of protein materials. This approach explicitly considers the hierarchical architecture of proteins, including the details of their chemical bonding, capable of accurately predicting their unfolding behavior and thereby providing a rigorous structure-property relationship. We exemplify the approach in the analysis of the deformation mechanisms of beta-sheets and alpha-helices, two prominent protein motifs that form the basis of many protein materials, including spider silk and intermediate filaments. Spider silk is a protein material that can reach the strength of steel cables, despite the predominant weak hydrogen bonding. Intermediate filaments are an important class of structural proteins responsible for the mechanical integrity of eukaryotic cells, which, if flawed, can cause serious diseases such as the rapid aging disease progeria or muscle dystrophy. For both examples, our studies elucidate intriguing material concepts that enable to balance strength, energy dissipation and robustness by selecting nanopatterned, hierarchical features. We present an analysis that reveals that the utilization of such hierarchical features in protein materials is vital to synthesize materials that combine seemingly incompatible material properties such as strength and robustness, self-adaptation and adaptability, by overcoming the physical limitations of conventional material designs. We discuss the general implications of our work for the science of multi-scale interactions and how this knowledge can be utilized to develop de novo biomimetic materials based on a bottom-up design.

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Quantitative Characterization of 3D Deformations of Cell Interactions with Soft Biomaterials

Guruswami Ravichandran
California Institute of Technology

Christian Franck
California Institute of Technology

Stacey A. Maskarinec
California Institute of Technology

David A. Tirrell
California Institute of Technology

The interactions between biochemical processes and mechanical signaling during cell migration and spreading play an important role in various cellular processes of biological systems. Recent studies have shown significant differences in cell behavior and morphologies of cells in 2-dimensional environments when compared to cells in 3-dimensions. Hence, 3-dimensional measurement techniques are needed to investigate cellular behavior under or close to in vivo conditions. This study developed a 3-dimensional full-field measurement technique for measuring large deformations in soft materials. The technique utilizes a digital volume correlation (DVC) algorithm to track motions of fluorescent particles in subvolumes using laser scanning confocal microscopy. The developed method is validated by comparing experimentally measured non-uniform deformation fields near hard and soft spherical inclusions under far-field uniaxial compression with the corresponding analytical solution. The technique is employed to map the full 3-D displacement fields during the migration of fibroblast cells on polyacrylamide gels. These results provide new insights into the dynamic mechanotransduction of migrating cells and the role of the mechanical properties of the substrate. Preliminary cell-matrix interaction results for migrating cells on artificial extracellular matrix proteins are presented. The results show that the proposed technique is well-suited for investigating the mechanics of cell-matrix interactions as well as for obtaining local constitutive and rheological properties of soft biomaterials in 3-dimensions.

The Stiffness of a Biomembrane Force Probe Vesicle

L.B. Freund*
Division of Engineering, Brown University
freund@brown.edu

The biomembrane force probe is an experimental apparatus that has been developed to measure the response of a single molecular bond to applied force [1]. A key element in the probe is a small vesicle that is held and manipulated by means of a pipette tip. The interest in this element is due to the fact that it is positioned in series with the bond being interrogated. As a result, the interpretation of data hinges on a knowledge of the mechanical properties, principally the load versus deflection behavior, of the vesicle. Under the assumptions that the vesicle has fixed membrane surface area and fixed internal volume, its load-deflection behavior is considered here. Because the deformation of the vesicle itself is severely constrained, energy storage in the vesicle is precluded and the compliance of the configuration derives from the air column in the pipette. The analysis is exact but the final result does not appear in closed form; consequently, it must be evaluated by numerical means. For a given geometry, the initial stiffness is found to scale with the pipette pressure and pipette channel radius [2].

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Beyond Bells Model: How Matrix Stiffness Can Alter Ligand-Receptor Kinetics

Krystyn Van Vliet
Professor
Materials Science and Engineering, MIT

Emily B. Walton
Materials Science and Engineering, MIT

Ranjani Krishnan
Biological Engineering, MIT

Sunyoung Lee
Materials Science and Engineering, MIT

It is well established by Bells model that in the forced unbinding of molecular pairs such as extracellular matrix ligands and cell surface receptors, the rupture force of the complex depends on the rate of loading. Here, we show experiments and simulations on individual complexes that demonstrate an additional factor in far from equilibrium unbinding of such complexes: the stiffness of the macrolmolecules to which the ligand and the receptor are tethered. We explain this increase in apparent rupture force with increasing tether stiffness in terms of the altered energy landscape of the complex, and discuss implications in terms of cell-matrix interactions including adhesion, migration, and cell response to matrix-presented growth factors.

Mechanical Insights into the Pathophysiology of Malaria

Chwee Teck Lim*
Division of Bioengineering and Department of Mechanical Engineering, National University of Singapore
ctlim@nus.edu.sg

Ang Li
Division of Bioengineering, National University of Singapore

Dr. Gabriel Yew Hoe Lee
Singapore-MIT Alliance

Dr. Kevin Shyong Wei Tan
Department of Microbiology, National University of Singapore

Plasmodium falciparum is the most deadly species of human malaria parasites. When the parasite invades and matures within a red blood cell, the parasite induced proteins are secreted and embedded in the host cell membrane. This gives rise to a phenomenon known as cytoadherence where infected red blood cells are found to adhere to endothelial cells that line the blood vessel walls [1-5]. Often, this phenomenon can cause severe consequences such as blood clogging. Here, we seek to quantify the molecular interactions between the endothelial receptor proteins TSP and CD36 and the adherent parasite exported proteins on the surface of the malaria-infected red blood cells using single molecular force microscopy. Functionalization of AFM tips with target proteins allows us to covalently attach the receptors of interest to the AFM tips under well controlled conditions. After obtaining force curves on the living malaria red blood cells with functionalized tips under different loading rates and temperatures, we perform a statistical analysis to find the most probable single bond forces and then curve fit our experimental data to obtain the energy landscape of the single molecular bond pairs. This study can better help us understand the molecular interactions involved in malaria pathophysiology arising from cytoadherence.

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Electronic Structure Calculations Using Hartree-Fock-Based Finite Element Method

K. Jimmy Hsia
Department of Mechanical Science and Engineering, University of Illinois

Rouholla Alizadegan
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

Electronic structure calculations are in general very computationally intensive, sometimes requiring substantial super-computer time just to compute the electronic structure of a single atom. Among all quantum mechanical methods, the quantum chemistry Hartree-Fock (HF) ab-initio electronic-structure method is the most mature one, capable of predicting the chemical and physical properties of a wide range of atoms, molecules, and compounds. Here we explore the use of the finite-element method (FEM) to the HF ab initio electronic-structure calculations in three dimensions. Roothaans extension of the HF method to the calculation of the molecular orbitals (MOs) is discussed and compared to this basis-free implementation. The method is shown to be efficient and robust for the selected test atoms and molecules. It has the potential to be used for large scale simulations of complex systems, particularly for coupled electro-mechanical phenomena.

Probing Cell Mechanics with Light

Gabriel Popescu
Assistant Professor
Electrical and Computer Engineering, University of Illinois

Huafeng Ding
Postdoctoral Associate
Electrical and Computer Engineering, University of Illinois

Ru Wang
Research Assistant
Mechanical Science & Engineering, University of Illinois

Zhuo Wang
Research Assistant
Electrical and Computer Engineering, University of Illinois

Light scattering is widely used in physics, biology, and medicine, as a complementary approach to microscopy, which has the benefit of providing information intrinsically averaged over the measurement volume. However, it is often the case that the spatial resolution achieved is insufficient in applications such as microrheology. "Particle tracking" microrheology alleviates this problem by measuring the particle displacements in the imaging (rather than scattering) plane. The drawback in this case is that relatively large particles are needed such that they can be tracked individually, which also limits the throughput required for significant statistical average.

We introduce a novel experimental approach, referred to as Fourier transform light scattering (FTLS), which combines optical microscopy and light scattering for studying cell structure and dynamics. The static scattering measurements from microspheres agree very well with predictions by Mie theory and the dynamic light scattering results from particles undergoing Brownian motion match the predictions by the Stokes-Einstein equation.

We employed FTLS to determine experimentally the scattering properties of red blood cells (RBCs), for the first time to our knowledge. FTLS provides an effective modality for studying live cell mechanics by measuring both intrinsic scattering from cell structures and scattering from probe particles. FTLS is used for studying dynamics over very large time intervals. Thus, at short times, the measurement is limited by the acquisition time of the CCD, and at long times by the total number of frames that the camera can transfer to the computer. We demonstrate this by measuring high-throughput red blood cell membrane rheology, on a time scale from milliseconds to minutes.

Formation of Creases on the Surfaces of Elastomers and Gels

Zhigang Suo
Professor
School of Engineering and Applied Sciences, Harvard University

Wei Hong
Professor
School of Engineering and Applied Sciences, Harvard University

Xuanhe Zhao
Professor
School of Engineering and Applied Sciences, Harvard University

When a block of an elastomer is bent, the compressed inner surface may form a crease. Similar creases appear when a gel swells. This paper determines the critical condition for creasing by comparing the elastic energy in a creased body and that in a smooth body. The model is developed for elastomers under general loading conditions and for swelling gels. The theoretical critical conditions are compared with experimental observations.

A Meso-structurally Based Continuum Model for the Dynamic Response of Woven Fabrics

Simona Socrate
Mechanical Engineering, Massachusetts Institute of Technology

Ethan M. Parsons
Mechanical Engineering, Massachusetts Institute of Technology

Woven fabrics are used in many applications, including soft body armor and fabric-reinforced composites. Modeling fabrics is challenging due to the need to capture the fabric response at different scales—both the macroscopic scale of the fabric and the "mesoscale" of the yarns that compose the weave. In earlier work [1] we proposed a modeling technique that captures relevant fabric behaviors at these two scales in a single modeling step. The technique relies on the selection of suitable unit cell geometry to represent the weave structure, and of physically motivated constitutive relations that describe the response of the unit cell to deformation. The macroscopic deformation gradient is then related to the configuration of the unit cell, either by using energy minimization techniques or by tracking internal degrees of freedom to satisfy local equilibrium. The mesostructural level forces and the corresponding macroscopic continuum stresses are then calculated. In the original model proposed in [1] the kinematical description of the fabric was simplified by introducing a constraint preventing transverse yarn slip of the crossing yarns, so that cross-over point could be considered material points of the continuum. This model was extended by introducing an innovative approach for capturing yarn slip in a continuum framework. The motion of the weave cross-over points, rather than the motion of the yarns, is directly tracked, and the motion of the yarns relative to the cross-over points is described by velocity fields. The most significant advantage of this approach is that it is easily integrated with the original formulation. When slip occurs, the unloaded configuration of the weave evolves with deformation according to a non-local theory. Driven by gradients in yarn tension, the transverse slip velocity is calculated via an experimentally determined constitutive relation. Gradients in the slip velocity result in an evolution of the amount of yarn associated with a given cross-over point, affecting the material response at that point. The role of transverse yarn slip in woven fabrics is analogous to the role of plasticity in the deformation of metals. By providing an additional mechanism of deformation, it increases the compliance of the material, and decreases stress concentrations, delaying failure. The model has been implemented in an explicit finite element code. Here we demonstrate the capabilities of the proposed modeling framework by comparing experiments and simulations of ballistic tests performed on single-ply Kevlar S706.

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Molecular Engineering of Cellular Environments: Cell Adhesion to Nano-digital Surfaces

Joachim P. Spatz
Department of New Materials and Biosystems, Max-Planck-Institute for Metals Research, Stuttgart & University of Heidelberg

Engineering of cellular environments has become a valuable tool for guiding cellular activity such as differentiation, spreading, motility, proliferation or apoptosis which altogether regulates tissue development in a complex manner. The adhesion of cells to its environment is involved in nearly every cellular decision in vivo and in vitro.

Our approach to engineer cellular environments is based on self-organizing spatial positioning of single signaling molecules attached to inorganic or polymeric supports, which offers the highest spatial resolution with respect to the position of single signaling molecules. This approach allows tuning cellular material with respect to its most relevant properties, i.e., viscoelasticity, peptide composition, nanotopography and spatial nanopatterning of signaling molecule. Such materials are defined as "nano-digital materials" since they enable the counting of individual signaling molecules, separated by a biologically inert background. Within these materials, the regulation of cellular responses is based on a biologically inert background which does not trigger any cell activation, which is then patterned with specific signaling molecules such as peptide ligands in well defined nanoscopic geometries. This approach is very powerful, since it enables the testing of cellular responses to individual, specific signaling molecules and their spatial ordering. Detailed consideration is also given to the fact that protein clusters such as those found at focal adhesion sites represent, to a large extent, hierarchically-organized cooperativity among various proteins. Moreover, "nano-digital supports" are capable of involvement in such dynamic cellular processes as protein ordering at the cell's periphery which in turn leads to programming cell responses.

Rate-Dependent Mechanics of Polymeric Nanofibers

Mohammad Naraghi
Graduate Student
Aerospace Engineering, University of Illinois

Ioannis Chasiotis
Assistant Professor
Aerospace Engineering, University of Illinois

Polymeric nanofibers, fabricated by electrospinning, are versatile building blocks for hierarchically structured materials, such as nanocomposites, high strength fabrics, high density filters, and scaffolds for tissue engineering. The mechanical behavior of nanoscale polymeric fibers in response to quasi-static and intermediate loading rates is unexplored. A novel experimental method that utilizes a MEMS-based mechanical property-testing platform was conceived to investigate the effect of strain rate during cold drawing of single electrospun polyacrylonitrile (PAN) nanofibers with 200-500 nm diameters and tens of microns in length. The mechanical strength of the PAN nanofibers at their glassy state was as high as 200 MPa while their ductility was larger than 200%. The fiber ductility was found to vary consistently with macroscale expectations, increasing with reducing strain rate. Curiously, the fiber strength did not vary monotonically with the drawing rate. At slow drawing rates ($<10^{-4}$ s^{-1}), the fiber strength increased dramatically compared to faster strain rates ($<10^{-2}$ s^{-1}), establishing a minimum at about 10^{-3} s^{-1}. This seemingly conflicting behavior was the result of two different mechanisms of deformation. At slow stain rates, the fibers underwent homogeneous deformation and strain localizations were suppressed by material relaxations. This behavior permitted large fiber deformations and molecular chain alignment, and therefore large fiber strengths. At faster strain rates ($>10^{-3}$ s^{-1}), the formation of (non-propagating) periodic surface instabilities along the nanofibers allowed for large fiber stretch ratios, while maintaining the high fiber strength.

Scale-Dependent Contact Strength of Gold Nano-asperities

Shuman Xia
Research Associate
Division of Engineering, Brown University

Kyung-Suk Kim
Professor
Division of Engineering, Brown University

Compression tests of single crystal gold pyramids with {114} facets on (001) surface plane [1] have shown a wide spectrum of contact strength from a few hundred MPa to 3 GPa, depending on the contact edge length ranging from 600 nm to 100 nm. Based on molecular dynamics simulations [2], it is believed that the size-dependent strength of asperities can reach even higher values (3–10 GPa), when the contact size goes below 100 nm. Both the experiments and MD simulations have shown that the contact strength has a power-law dependence on the contact edge length, with the scaling exponent of –0.75 for the experiments and -0.32 for the MD simulations. A theoretical study on the contact strength of these nano-asperities is performed based on a dislocation nucleation model [3]. Heterogeneous surface dislocation nucleation due to a wedge stress singularity is analyzed as the incipient plastic deformation mechanism for asperity contact size smaller than about one hundred nanometers. The dislocation nucleation is assumed to obey the Rice-Thomson criterion. The driving forces on dislocations are calculated with the 2-D and 3-D conservation M-integrals. Both the quasi-analytic asymptotic analysis and full numerical simulation are performed based on anisotropic elasticity and dislocation mechanics. The contact strength is found to be scaled with the contact size with a scaling exponent of –0.497 for the contact edge length range between 10nm and 100nm. The validity of the model is supported by the comparison with the MD and experimental results.

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Plastic Strain Recovery in Freestanding Nanocrystalline Metal Films

Jagannathan Rajagopalan
Graduate Student
Mechanical Science and Engineering, University of Illinois

Jong H. Han
Mechanical Science and Engineering, University of Illinois

Taher A. Saif
Professor
Mechanical Science and Engineering, University of Illinois

In nanocrystalline metals, the paucity of intragranular dislocation sources leads to unconventional deformation mechanisms. However, plastic deformation, irrespective of the size scale or the underlying deformation mechanism, is expected to be permanent. We present results from uniaxial tensile experiments and post deformation annealing experiments on freestanding nanocrystalline aluminum and gold films which show that a large fraction (50-100 %) of plastic strain in these films is recoverable after unloading [1]. This strain recovery is time dependent and is expedited at higher temperatures. The aluminum and gold films, both 200 nm thick, had average grain sizes of 65 nm and 50 nm respectively and were deformed using a MEMS based micro testing stage. The strain recovery appears to be driven by residual internal stresses since the films are macroscopically stress-free during strain recovery. The deformation behavior of these films during loading is analyzed in the context of strain recovery [2] and a mechanism for plastic strain recovery is put forth.

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Constrained Deformation in Thin Metal Films: A Modeling Perspective with Case Studies

Yu-Lin Shen
Professor
Department of Mechanical Engineering, University of New Mexico

Mechanical behavior of materials at small length scales has received significant attention in recent years, due mainly to the development of devices and components having micro- and nano-scale feature sizes. For thin films bonded to a substrate and/or other dissimilar layers, deformation is heavily influenced by the physical confinement imposed on the films [1-3]. This presentation is devoted to the analysis of constrained plastic deformation in thin metal films. We apply continuum-based numerical modeling to establish a baseline mechanistic understanding. In particular, several modeling scenarios with different geometric and loading configurations will be addressed. These include: tensile loading of the film/substrate system, bending deformation of microbeams, and nanoindentation behavior of multilayered composites. Special emphasis is on the evolution of local deformation pattern and overall mechanical response, and their implications in the experimental practice. Certain unique features discovered from the modeling analysis will be highlighted.

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Mechanical and Interface Properties of Single Carbon Nanofibers for Polymer Nanocomposites

Tanil Ozkan
Research Assistant
Mechanical Engineering, University of Illinois

Qi Chen
Research Assistant
University of Illinois

Ioannis Chasiotis
Assistant Professor
University of Illinois

Carbon-based nanostructures are effective means to improve the mechanical, thermal, and electrical transport properties in advanced and conventional carbon fiber composites. Three grades of pyrolytically stripped and heat treated Pyrograf-III carbon nanofibers, with average diameter of 150 nm, were tested for their tensile strength and interface adhesion properties by a novel MEMS-based mechanical testing platform. The applied force was measured by a surface micromachined device with an accuracy of 50 nm. The nominal tensile strengths of the pyrolytically stripped nanofibers and the heat-treated nanofibers followed Weibull distributions varying between 2-5 GPa. The true material strengths excluding the hollow fiber cores were twice the nominal strengths tending towards that of single crystal graphite. These are the first properties measurements of these fibers which, to date, were assumed to have the strength of carbon fibers in laminate composites. SEM images of matching ruptured surfaces pointed to failure geometry that agrees with the "dixie cup" structure of Pyrograf III. Furthermore, the nanofiber fracture surface had all the elements of brittle fracture with an additional slip of the angled graphene layers comprising the nanofibers. These strength data established a reference for fiber pull-out tests from an epoxy matrix. Recent individual carbon nanofiber pull-out measurements from an epoxy, cured at room temperature, gave values larger than 30 MPa for the average interfacial shear strength. The pull-out experiments showed a non-linear dependence of the pull-out force with respect to the embedded fiber length and an even stronger effect of matrix curing time on the nanofiber pull-out force.

Length Scales in Deformation and Fracture of Amorphous Alloys

Upadrasta Ramamurty
Professor
Materials Engineering, Indian Institute of Science

Plastic deformation and fracture in crystalline metals are associated with a hierarchy of structural features that can be categorized into different length scales on the basis of the extent of their operation. Connections between these, i.e. how processes at one length scales affects the next higher level one, etc. is well understood—qualitatively, if not quantitatively. In the context of amorphous alloys, while the consensus is emerging on the length scale of various operating mechanisms, the connections between various length scales, is yet to be agreed upon. For example, how the unitary processes of deformation, shear transformation zones, combine to form shear bands -the raison d être for inhomogeneous plasticity in metallic glasses at relatively low temperatures and high stresses—is not clear. At the meso/macro-scopic level, what controls the minimum spacing between shear bands or the sizes of plastic zones at the crack-tips is also an important question that is yet to be sorted out. These are the key issues not only from the scientific stand-point of view, but also from the technological perspective. For example, an excellent correlation was reported for the toughness and plastic zone in amorphous alloys, thus, if one knows ways and means of enhancing the plastic zone size ahead of a crack-tip, it will be possible to design very tough metallic glasses. In this presentation, I shall first review the length scales of various operating micromechanisms in metallic glasses. Then, I will present results of our recent efforts—experiments as well simulations—for understanding the connections between them. Finally, I shall enumerate questions that remain outstanding within the context of fracture of metallic glasses.

Improving Both Strength and Ductility of Nanostructured Materials with Nanoscale Twins

Ming Dao
Research Scientist
Department of Materials Science & Engineering, MIT

A review of the systematic experiments on the effects of nano-scale twins in ultrafine crystalline copper demonstrated that increasing the nano-scale twin density, while keeping the grain size fixed, results in significant increases in strength and strain-rate sensitivity. It is also found that the activation volume associated with this deformation process significantly decreases with increasing twin volume fraction. These results point to the trend that refining structural dimensions through the introduction of nano-scale twins has the same effect on strength and hardness as grain refinement. On the other hand, nano-scale twins were found to significantly improve ductility with decreasing twin spacing.

A comprehensive computational analysis of the deformation of ultrafine crystalline pure Cu with nanoscale growth twins is presented. This physically motivated model accounts for high plastic anisotropy by treating the twin boundary as an internal interface and allowing special slip geometry arrangements that involve soft and hard modes of deformation. This model correctly predicts the experimentally observed trends of the effects of twin density on flow strength, rate sensitivity of plastic flow and ductility, in addition to matching many of the quantitative details of plastic deformation reasonably well. The analysis also offers some useful understanding of why the nanotwinned Cu with high strength does not lead to diminished ductility with structural refinement involving twins, whereas nanostructured Cu normally causes the ductility to be compromised at the expense of strength upon grain refinement.

An Atomistic-Continuum Field Theory, Its Relation with Microcontinuum Theories, and Its Applications in Multiscale Simulation

Youping Chen
Department of Mechanical and Aerospace Engineering, University of Florida

Liming Xiong
Graduate student
Department of Mechanical and Aerospace Engineering, University of Florida

Classic continuum mechanics views a crystalline material as a homogeneous and continuous medium, in which the basic structural unit of the crystal is taken without structure and is idealized as point mass. Micromorphic theory views a material as a continuous collection of deformable point particles; each particle has finite size and additional 9 internal degrees of freedom describing the stretches and rotations of the particle. This paper presents a multiscale field theory that views a crystalline material as a continuous collection of lattice points, while embedded within each point is a group of discrete atoms. The atomistic formulation of the field theory is briefly introduced. Its relation with the well-known Micromorphic theory is derived. The applicability of the classical continuum theory, Micromorphic theory and the generalized continuum field theory is discussed. Numerical examples, including constitutive response and critical pheneomena like dislocation nucleation and motion, crack iniation and propagation, will be presented.

Interfacial Gradient Plasticity Governs Scale-Dependent Yield Strength and Strain Hardening Rates at Decreasing Microstructural Length Scales

Rashid K. Abu Al-Rub
Department of Civil Engineering, Texas A&M University

The emerging areas of micro- and nano-technologies exhibit important strength differences that result from continuous modification of the material microstructural characteristics with changing size, with smaller being stronger. There are many experimental observations which indicate that, under certain specific conditions, the size of micro/nano-systems significantly affect their strength such that a length scale is required for predicting such size effects when using the classical theories of continuum mechanics. For example, experimental works have shown increase in strength by decreasing: (a) the particle size in nano-composites; (b) the diameter of nano-wires in torsion and uniaxial compression; (c) the thickness of thin films in micro-bending and uniaxial tension; (d) the grain size of nano-crystalline materials; (e) void size in nano-porous media; (f) the indentation depth in micro/nano indentation tests, etc.

The effect of the material microstructural interfaces increases as the surface-to-volume ratio increases. It is shown in this work that interfacial effects have a profound impact on the scale-dependent yield strength and strain hardening of micro/nano-systems even under uniform stressing. This is achieved by developing a higher-order gradient-dependent plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces. Those nonstandard boundary conditions relate a microtraction stress to the interfacial energy at the interface. In addition to the nonlocal yield condition for the material's bulk, a microscopic yield condition for the interface is presented, which determines the stress at which the interface begins to deform plastically and harden. Hence, two material length scales are incorporated: one for the bulk and the other for the interface. Different expressions for the interfacial energy are investigated. The effect of the interfacial yield strength and interfacial hardening are studied by analytically solving a one dimensional Hall-Petch-type size effect problem. It is found that when assuming compliant interfaces the interface properties control both the material's global yield strength and rates of strain hardening such that the interfacial strength controls the global yield strength whereas the interfacial hardening controls both the global yield strength and strain hardening rates. On the other hand, when assuming a stiff interface, the bulk length scale controls both the global yield strength and strain hardening rates. Moreover, it is found that in order to correctly predict the increase in the yield strength with decreasing size, the interfacial length scale should scale the magnitude of both the interfacial yield strength and interfacial hardening.

Effects of Transformation Strain and Elastic Contrast on Directed Assembly of Nanostructures

Yucun Lou
PhD student
Department of Mechanical Engineering and Applied Science, University of Pennsylvannia

John Bassani
Department of Mechanical Engineering and Applied Science, University of Pennsylvannia

Microstructure evolution in a multi-phase solid is influenced by the temporal and spatial-varying elastic energy arising both from intrinsic transformation strain as well as externally-imposed stress field. The latter can be potentially utilized on forming highly ordered nano-structures. In this paper, we investigate the effects of elastic energies on aggregation in alloy films guided by patterned indentation, including a systematically variation of transformation strain, contrast in the elastic bulk moduli between the phases, and the magnitude of external traction. These effects are interpreted qualitatively by coupling the ideas of Eshelby and Mura on self and interaction energies with the thermodynamics and kinetics of aggregation.

Prager Medal Symposium in Honor of Richard James: Using Mechanics to Discover New Materials

ORGANIZERS:

Kaushik Bhattacharya, *Division of Engineering and Applied Science, California Institute of Technology*

Kaushik Dayal, *Carnegie Mellon University*

Antonio DeSimone, *SISSA*

SYMPOSIUM **D**

New Perspectives on Texture Evolution

David Kinderlehrer
Professor
Mathematical Sciences, Carnegie Mellon University

Shlomo Taasan
Professor
Mathematical Sciences, Carnegie Mellon University

Nearly all technologically useful materials are polycrystalline, consisting of small crystallites, called grains, separated by interfaces, the grain boundaries. The energetics and arrangement of this network, its texture, are important factors in material behavior, and constitute the basic problem of microstructure. Experimentally, the inverse relationships between grain boundary populations and energy have been observed for many years. We introduce the grain boundary character distribution (GBCD), a new statistic, and offer compelling evidence for its strong dependence on grain boundary energy. In addition we demonstrate that there are natural laws for texture and the GBCD using large network simulations. This is joint work with the MIMP group at Carnegie Mellon University.

Equilibrium Configurations of Epitaxially Strained Crystalline Films: Existence and Regularity Results

Irene Fonseca
Department of Mathematical Sciences, Carnegie Mellon University

Strained epitaxial films grown on a relatively thick substrate are considered in the context of plane linear elasticity. The total free energy of the system is assumed to be the sum of the energy of the free surface of the film and the strain energy. Due to the lattice mismatch between film and substrate, flat configurations are in general energetically unfavorable and a corrugated or islanded morphology is the preferred growth mode of the strained film. New regularity results for volume constrained local minimizers of the total free energy are established, leading to a rigorous proof of the zero contact-angle condition between islands and wetting layers.

On the Symmetry of Energy Minimizing Deformations in Nonlinear Elasticity: Compressible Materials

Scott J. Spector
Professor of Mathematics
Department of Mathematics, Southern Illinois University

Jeyabal Sivaloganathan
Reader in Mathematics
Department of Mathematical Sciences, University of Bath

Consider a homogeneous, isotropic, hyperelastic body that occupies a three-dimensional, thick spherical shell, S, in its reference state and is subject to radially symmetric displacement boundary conditions on its inner and outer boundaries. It is shown [1,2] that, to each deformation of the shell, there corresponds a radial deformation that has less elastic energy than the given deformation, whenever the stored-energy function is polyconvex and grows sufficiently rapidly at infinity.

The key ingredient is a new radial-symmetrization procedure that is appropriate for problems where the symmetrized mapping must be one-to-one in order to prevent interpenetration of matter. The radial symmetrization of an orientation preserving diffeomorphism, u:S—>S*, between shells S and S* is the radial deformation

v(x)=(R(r)/r)x, where r=|x|,

that maps each sphere Sr of radius r>0, centered at the origin into another such sphere that encloses the same volume as u(Sr). Since the volumes enclosed by the surfaces u(Sr) and v(Sr) are equal, the classical isoperimetric inequality then implies that the surface area of u(Sr) is bigger than the surface area of v(Sr). The equality of the enclosed volumes together with this reduction in surface area is then shown to give rise to a reduction in total energy for many of the constitutive relations used in nonlinear elasticity.

These results are also extended to classes of Sobolev deformations and applied to prove that the radially symmetric solutions to these boundary-value problems are global energy minimizers in the class of (possibly non-symmetric) deformations of a three-dimensional thick spherical shell.

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Shape Control of Polymeric Sheets Using SMA Wires

Dr. Raffaella Rizzoni
Department of Engineering, University of Ferrara

Mattia Merlin
Department of Engineering, University of Ferrara

We investigate, both from an experimental and a theoretical point of view, the behavior of SMA composites fabricated by bonding thin pre-deformed SMA wires to a polymeric matrix. The motivation of this study is primarily the design of a structure changing shape to change operating characteristics. Some relevant material properties are experimentally determined. A large number of tests are carried out on Ti-50.5at.%Ni wires, in order to describe the stress-temperature and the strain-temperature relations. In particular, the transformation temperature ranges of the wires are obtained via differential scanning calorimetry (DSC) tests and the latent heats on heating and cooling are calculated. The elastic moduli of the martensite and austenite phases are

determined by tensile tests at low and high temperatures. Constant stress tests and constrained recovery tests are also performed, in order to determine the relation between stress and the transformation temperatures, and the maximum recovery stress, respectively. The mechanical properties of the polymeric matrix are also studied. To simulate the behavior of the composite, a simple model is presented, which assumes classical plate theory for the composite. The behavior of the SMA wires is described by the theory for heterogeneous thin wires developed in [2], which, using ideas of the constrained theory of martensite [1], is specialized to phase transforming materials with high elastic moduli [3]. Simulations of the composite change of shape for different arrangements of the SMA wires are given. Experimental results on an epoxy resin composite plate with SMA embedded wires are also presented, showing that an appreciable bending can be obtained during wires activation.

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Solutions to the Periodic Eshelby Inclusion Problem in Two Dimensions

Liping Liu
Postdoc
California Institute of Technology

We consider the classic Eshelby inclusion problem on a finite unit cell with periodic boundary conditions. We give solutions in terms of Cauchy-type integrals to this problem in two dimensions for general shapes of inclusion and nonuniform but divergence-free eigenstress. This representation formula is reminiscent of the familiar Greens representation formula. More, it is shown that a Vigdergauz structure does not have the Eshelby uniformity property for non-dilatational uniform eigenstress unless it degenerates to a simple laminate.

Modeling the Forced Separation of a Molecular Bond

L.B. Freund*
Division of Engineering, Brown University
freund@brown.edu

Interest in this topic derives from the observed behavior of the non-covalent molecular bonds that account for adhesion of eukaryotic animal cells to extracellular matrix [1]. For purposes of modeling, bonding is understood to be the confinement of the configuration of the the system within an energy well, which arises as a principal feature of an overall energy landscape [2]. One consequence of application of a force on the bond is to distort this landscape over time. The system functions in a thermal environment, and the depth of the bond well is assumed throughout to be significantly greater than the thermal energy unit kT. The bond state is characterized by a probability distribution over the energy landscape and, as the landscape distorts, its evolution is governed by a partial differential equation. The system is analyzed in order to extract information on the most probable time for bond separation, the maximum force that can be sustained by the bond, and the sensitivity of bond separation behavior to loading rate, for example. The goal of experiments in which molecular bonds are separated under force is to infer magnitudes bond characteristics. The purpose of this discussion is to consider the relationships between measured quantities and properties of the bond itself, as modulated by an intervening loading apparatus [3].

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A Path-Integral Formulation of DNA Looping Probabilities

Ludovica Cotta-Ramusino
IMA, University of Minnesota

John H. Maddocks
Professor
Ecole Polytechnique Fédérale de Lausanne

DNA looping is a biologically important phenomenon in which the probability of loop formation depends on the sequence of the fragment in question. I will show how such looping probabilities can be modelled using a semi-classical path integral formalism to evaluate approximations to the stationary probability density function for the location and orientation of one end of a continuum elastic rod, or polymer. The expression obtained involves the energy of a solution to the associated Euler-Lagrange equations arising from elasticity plus a fluctuation correction in terms of a volume of a basis of solutions to the associated Jacobi equations.

Modeling the Mechanics of Viral Capsids

William S. Klug
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

Melissa M. Gibbons
Graduate Student
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

Lin Ma
Graduate Student
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

As revealed by techniques of structural biology, the protein shells of viruses (capsids) are some of natures most beautiful and robust examples of highly symmetric multiscale self-assembled structures. The ability of viral capsids to respond structurally and mechanically to physical and chemical stimuli also gives them tremendous potential as components for the design of synthetic materials with adaptive properties, as has been demonstrated recently by the creation of virus-based nanowires. A series of recent indentation experiments using atomic force microscopy (AFM) has shown that capsids also possess impressive mechanical properties of strength and elasticity. In this talk I will present some theory and numerical modeling of viral capsids based on continuum mechanics and Ginzburg-Landau theory of phase transitions, and I will discuss what weve learned about the elastic response and mechanical failure of viral capsids, and coupling of global capsid mechanical response to local protein conformational change. Overall the talk will highlight our ongoing efforts to push the limits of usefulness of continuum theory via coupled continuum-atomistic multiscale modeling of capsids and other large protein assemblies.

A Model for T4 Tail Sheaths

Isaac Chenchiah
Lecturer
Department of Mathematics, University of Bristol

Valeriy Slastikov
Lecturer
Department of Mathematics, University of Bristol

Building on the insights of Falk and James [1] we present a model for bacteriophage T4 tail sheaths. The model predicts helical configurations, phase transitions and non-uniform states—these are analysed and compared with experiments.

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Effective Relations for Inhomogeneous Elastodynamics and Electrodynamics

John Willis*
Professor
University of Cambridge, Centre for Mathematical Sciences
J.R.Willis@damtp.cam.ac.uk

The theory underlying effective constitutive relations for inhomogeneous elastodynamics is largely complete, even though there may remain practical difficulties in implementation. In contrast, there appears still to be some resort to ad hoc prescription in the case of inhomogeneous electrodynamics, even in the "homogenization limit". The purpose of this talk will be to follow, as faithfully as possible, a route recently developed and explored for elastodynamics [1,2], in the context of electrodynamics, to establish correspondences and differences and perhaps improve thereby appreciation of the structure of electrodynamic effective relations.

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Minimization Variational Principles for Acoustics, Elastodynamics, and Electromagnetism in Lossy Inhomogeneous Bodies at Fixed Frequency

Graeme Milton
Professor
Mathematics, University of Utah

Pierre Seppecher
Professor
Institut de Mathématiques de Toulon, Université de Toulon et du Var

Guy Bouchitte
Professor
Institut de Mathématiques de Toulon, Université de Toulon et du Var

The classical energy minimization principles of Dirichlet and Thompson are extended as minimization principles to acoustics, elastodynamics and electromagnetism in lossy inhomogeneous bodies at fixed frequency. This is done by building upon ideas of Cherkaev and Gibiansky, who derived minimization variational principles for quasistatics. In the absence of body forces the primary elastodynamic minimization variational principles have a minimum which is the time-averaged elastic energy dissipated to heat in the body. The variational principles provide constraints on the boundary values of the fields when the moduli are known. Conversely, when the boundary values of the fields have been measured, then they provide information about the values of the moduli within the body. This should have application to tomography. We also derive saddle point variational principles which correspond to variational principles of Gurtin, Willis, and Borcea.

Minimum Principles for the Trajectories of Systems Governed by Rate Problems

Michael Ortiz
Department of Aeronautics and Mechanical Engineering, California Institute of Technology

The evolution of many physical systems is the result of a balance between dissipative and energetic forces. This balance results in evolutionary equations that govern the time-dependence of the state of the system. The classical treatment of these equations tends to break down when applied to strongly nonlinear systems that develop evolving microstructures. In these cases, the energy of the system lacks lower-semicontinuity and equilibrium solutions that minimize the energy do not exist in general. In particular, time-incremental formulations suffer from a restart problem, i.e., the incremental problem becomes ill-defined when a microstructure has been previously established in the system and the initial conditions for the future evolution of the system are only defined in the sense of Young measures. However, it is possible characterize entire trajectories of the system as minimizers of certain energy dissipation functionals, thus entirely circumventing the restart problem of the classical rate and time-incremental problems. Because of the minimizing property of the trajectories of the system, tools of the calculus of variations such as the direct method for establishing existence, relaxation and optimal scaling can be applied. Selected examples illustrate how those tools shed light into microstructural evolution and on the effective kinetics governing the macroscopic evolution of the system.

Nanomechanics of Carbon Nanotubes

Traian Dumitrica
Professor
Department of Mechanical Engineering, University of Minnesota

Advances in condensed matter physics and theoretical chemistry have made possible a comprehensive modeling of materials. We can adapt and apply these theoretical methods to study the amazing properties of nanostructures. I will discuss two examples where such theories helped the understanding of the mechanical response of carbon nanotubes (generally viewed as a paradigm for nanoscale materials).

In materials modeling the most common way to implement molecular dynamics is via translational periodic boundary conditions. This is not the natural choice when modeling carbon nanotubes. Using the helical and rotational symmetries of the nanoscale graphitic tubules, molecular dynamics and structural relaxation can be done in a simplified way, on a modest number of atoms. This new method [1], termed objective molecular dynamics [2, 3], is compatible with quantum mechanics under the Born-Oppenheimer approximation. The utility of objective molecular dynamics will be presented in the context of studying the carbon nanotubes under bending and twist.

Combining a probabilistic approach of the rate theory with detailed quantum mechanical computations of failure nucleation and transition-state barriers, allows for a comprehensive analysis of the underlying atomic mechanisms and evaluation of the yield strain for arbitrary nanotubes under realistic conditions [4]. The numerical results are captured in a concise set of equations for the breaking strain, and reveal a competition between two alternative routes of brittle bond breaking and plastic relaxation. The employed probabilistic approach ultimately allows for the creation of a "strength map", which plots the likelihood that a nanotube will break—and how its likely to break.

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Phonon Analysis of Carbon Nanotubes with Arbitary Chirality by the Objective Structures Framework

Kaushik Dayal
Department of Civil and Environmental Engineering, Carnegie Mellon University

Ryan S. Elliott
Department of Aerospace Engineering and Mechanics, University of Minnesota

Normal modes of vibrations of collections of atoms, called phonons, provide important information about thermodynamic properties of materials. Further, they can be exploited to predict equilibrium crystal structures as a function of temperature and other environmental variables using bifurcation techniques [1,2]. However, computing the normal mode spectrum is extremely expensive, except in the special case of periodic crystals where Fourier techniques simplify the calculation. Recently, R. D. James observed a close analogy between crystals and certain complex atomic structures as well as biological structures [1]. Structures that satisfy this analogy are termed "Objective Structures". They include carbon nanotubes of all chiralities, buckyballs, as well as many biological virus components. This analogy brings in the idea of "Objective Boundary Conditions". The Objective Boundary Conditions allow for the same efficiencies that have made crystalline structures accessible to efficient calculation with periodic boundary conditions (ex. [4]), by allowing treatment of a single unit cell representative of the entire structure. Here, we develop the Objective analog of the Fourier transform to analyze phonon modes in carbon nanotubes. It allows us to treat carbon nanotubes with great efficiency by providing a basis that decouples the modes. Further, previous calculations of phonon spectra apply conventional periodic boundary conditions along the length of the nanotube. Hence chiral nanotubes require very large fundamental domains and the associated large computational cost. The use of the Objective Structures framework allows us to consider very small fundamental domains, regardless of chirality, with minimal computational effort. Further, our efforts are a step toward implementing a framework [1,2] to understand the equilibrium structures of carbon nanotubes under applied loads.

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Mathematical Foundations and Algorithms for the Quasicontinuum Method

Mitchell Luskin
Professor
School of Math, University of Minnesota

Marcel Arndt
School of Math, University of Minnesota

Matthew Dobson
School of Math, University of Minnesota

We will give an overview of the current state of numerical analysis and algorithms for the quasicontinuum method. We will present results for atomistic-to-continuum coupling error, rates of convergence for iterative solution methods, a posteriori error estimation, and adaptive algorithms for atomistic-continuum modeling and continuuum coarsening.

Thermoplastic Elastomers: Multiscale Modeling and Microstructure Evolution

Pedro Ponte Castañeda
Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

O. Lopez-Pamies
Department of Mechanical Engineering, S.U.N.Y.

Dr. V. Racherla
Laboratoire de Mécanique des Solides, École Polytechnique

Thermoplastic elastomers (TPEs) are block copolymers made up of "hard" (glassy) and "soft" (rubbery) domains that self-organize on a length scale of a few tens of nanometers. Under typical processing conditions, TPEs also develop a "granular" structure at the micron level, which is similar to that of metal polycrystals. Therefore, TPEs can be described as materials with (continuum) heterogeneities at two different length scales. In this talk, we will develop constitutive models for TPEs with lamellar morphology, where the grains are made up of the same, perfect, lamellar structure (single crystal) with randomly varying lamination directions (crystal orientations). In particular, based on experimental evidence, we consider two types of such materials: "oriented" and "unoriented" samples. The oriented TPEs are highly ordered, near-single-crystal systems with slightly varying grain orientations, while the unoriented samples are initially isotropic due to an initially random distribution of orientations in the sample. For oriented TPEs, it is found that under certain loading conditions; namely, under those with sufficiently large compressive deformations applied in the direction of the layers within the individual grains?the overall behavior of the material becomes macroscopically unstable (i.e., it loses strong ellipticity). The unoriented samples are also susceptible to loss of strong ellipticity, especially for large contrast in mechanical properties of the hard and soft domains. Finally, these instabilities will be related to the evolution of the underlying microstructure, which can be tracked experimentally (via small X-ray scattering measurements) in these systems.

High Pressure Mechanochemistry: Multiscale Theory, Experiment, and Search for New Materials

Valery Levitas
Schaefer 2050 Challenge Professor
Departments of Mechanical Engineering, Aerospace Engineering, and Material Science and Engineering,
Iowa State University

Yanzhang Ma
Department of Mechanical Engineering, Texas Tech University

High pressure mechanochemistry studies the effect of large plastic shear on high pressure phase transformations and chemical reactions. We developed rotational diamond anvil cell (RDAC) technique to study in situ strain-induced phase transformations in various material systems [1], including BN, Si, SiC and iron. Synchrotron X-ray diffraction and Raman spectroscopy is used. A three-scale continuum thermodynamic theory and closed form solutions are developed to describe observed mechanochemical phenomena [2,3]. Finite element simulations are performed as well [4]. At the nanoscale, a model for strain-induced nucleation at the tip of a dislocation pile-up is suggested and studied. At the microscale, a simple strain-controlled kinetic equation for the strain-induced phase transformations is thermodynamically derived. It depends (among other parameters) on the ratio of the yield strengths of phases. A macroscale model for plastic flow and strain-induced phase transformations in RDAC is developed and finite element solutions are found. These models explain why and how the superposition of plastic shear on high pressure leads to: a) a significant (by a factor of 3-10) reduction of the phase transformations pressure, b) reduction (up to zero) of pressure hysteresis, c) the appearance of new phases, especially strong phases, which were not obtained without shear, d) pressure growth during phase transformations (despite the volume decrease), and e) strain-controlled (rather than time-controlled) kinetics. Some methods of characterization and controlling the phase transformations are suggested and the unique potential of plastic straining to produce high-strength metastable phases is predicted. Some new phenomena are predicted theoretically and confirmed experimentally. Thus, phase transformations induced by rotational plastic instability was revealed and used to reduce pressure for irreversible phase transformations from hexagonal to superhard cubic BN from 55 GPa to 5.6 GPa [5]. Transformation-induced plasticity was revealed [1] which serves as a positive mechanochemical feedback for intensification of phase transformations.

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A Quasicontinuum for Multilattice Phase Transforming Materials

Ellad Tadmor
Professor
Aerospace Engineering and Mechanics, University of Minnesota

Ryan Elliott
Professor
Aerospace Engineering and Mechanics, University of Minnesota

Viacheslav Sorkin
Postdoctoral Research Fellow
Aerospace Engineering and Mechanics, University of Minnesota

The quasicontinuum (QC) method [1-2] is applied to materials possessing a multilattice crystal structure. Cauchy-Born (CB) kinematics, which accounts for the shifts of the crystal basis, is used in continuum regions to relate atomic motions to continuum deformation gradients. To avoid failures of the CB kinematics, QC is augmented with a phonon stability analysis that detects lattice period extensions and identifies the minimum required periodic cell size [3]. This augmented approach is referred to as "Cascading Cauchy-Born kinematics". Applications to one- and two-dimensional test problems that highlight the salient features will be presented. In particular, an effective interaction potential material model for a prototypical shape memory alloy is used to simulate a complete shape memory cycle. The results capture both temperature- and stress-induced martensitic transformations.

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About Stress-Induced Phase Transformations in Shape-Memory Polycrystals

Dr. Anja Schlömerkemper
Max-Planck-Institute for Mathematics in the Sciences

Kaushik Bhattacharya
Division of Engineering and Applied Science, California Institute of Technology

Above the phase transformation temperature, shape-memory alloys show a superelastic behavior upon an applied stress. This is due to a phase transformation induced by the applied stress. It is interesting to know the onset of stress-induced transformation from a general perspective as well as with respect to applications. Our aim is to determine and study this onset mathematically within the framework of energy minimization and homogenization theory [1].

We study a model case of scalar materials, give appropriate definitions of the transformation yield set in polycrystalline materials and show that the Sachs bound is a sharp bound on the yield set. That is, the Sachs bound turns out to characterize the onset of phase transformation in this case.

Furthermore we derive bounds on stress-strain curves of polycrystalline scalar shape-memory alloys; these bounds are based on an approach by Milton and Serkov [2], which was developed to bound currents in nonlinear conduction composites. To give specific examples, we consider four variant materials with special textures.

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Combinatorial Approach to Materials Discovery

Ichiro Takeuchi
Associate Professor
Materials Science and Engineering, University of Maryland

I will describe the applications of the combinatorial approach for rapidly optimizing and fine tuning physical properties of multifunctional materials. In particular, we have applied this technique to search for thermoelastic shape memory alloys with minimal hysteresis widths. Synchrotron microdiffraction was performed on ternary composition spreads of Ni-Ti-Cu in order to track the continuous change in lattice parameters across a large region of the phase diagram mapped on a single Si wafer. A clear relation between the transformation matrix (determined by the lattice parameters) and the thermal hysteresis of the shape memory alloys were observed across a large compositional region which verified the non-linear theory of martensite.

Breaching the Work Output Limitation of Ferromagnetic Shape Memory Alloys

Dr. Doron Shilo
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Yaniv Ganor
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Tom. W. Shield
Department of Aerospace Engineering and Mechanics, University of Minnesota

Richard D. James
Department of Aerospace Engineering and Mechanics, University of Minnesota

In recent years, a special class of active materials known as ferromagnetic shape-memory (FSM) alloys has received much attention due its large actuation strains and fast response. Despite of the large strains, the work output of FSM alloys are limited by their relatively low blocking stress of 2-6 MPa, above which magnetic field induced strain is not possible. This level of stress impedes the utilization of these alloys in practical applications where high work output by small components is required. To date, attempts to enhance the work output limitation are mainly focused on changing the concentrations of the off stoichiometric compounds of the FSM alloys, as they set the level of the magnetocrystalline anisotropy energy constant. In this paper we suggest that the work output limitation can be breached by reducing the size of the actuator, and present an indication of a possible fundamental relationship between size and work output capabilities.

Overall, the behavior of FSM alloys involves motion of twin boundaries and is significantly influenced by its microstructure. Based on a theoretical model, we have shown that down-scale specimens have finer twin boundary microstructure that consequently may increase the blocking stress. In light of this, a novel experimental method was realized to establish this conjecture and to provide comprehensive information on the behavior of micro-scale actuators. A series of tests demonstrated no actuation strain reduction up to extraordinary loads of 10MPa, which is we believe to be related to the size reduction of the FSM alloy in our experiments.

An Effective Interaction Potential Model of Stress- and Temperature-Induced Martensitic Transformations in Perfect Bi-atomic Crystals

Ryan Elliott
Department of Aerospace Engineering and Mechanics, University of Minnesota

Nick Triantafyllidis
Department of Aerospace Engineering, University of Michigan

John A. Shaw
Department of Aerospace Engineering, University of Michigan

Solid-to-solid martensitic phase transformations are technologically important phenomena that result in unique macroscopic material properties such as the shape memory effect, ferromagnetism, and ferroelectric behavior. In shape memory alloys, such as CuAlNi and NiTi, the martensitic transformation can result from a change in temperature or the application of stress. In fact, both temperature-induced and stress-induced transformations are essential for the existence of shape memory behavior.

An Effective Interaction Potential model for bi-atomic shape memory alloys, based on a set of temperature-dependent atomic pair-potentials, is presented. The equilibrium solutions of the governing nonlinear equations are found, as functions of temperature and applied stress, using symmetry arguments and Branch-Following and Bifurcation techniques. To check if a given equilibrium path is observable, its stability against perturbations of arbitrary (with respect to interatomic distance) wavelengths is investigated. This requires continuum-level energy calculations as well as a lattice-level phonon spectra analysis. Our work predicts the existence of a hysteretic two-step temperature-induced proper martensitic transformation from the high-temperature B2 cubic austenite phase, to an intermediate alpha-IrV orthorhombic phase, to a final B19 orthorhombic martensite phase. Stress-induced transformation to the alpha-IrV phase is predicted, at high temperatures, and characteristic properties such as tension-compression asymmetry are captured. Additionally, the transformation stress is found to increase with increasing temperature in agreement with experiment. The existence of both temperature- and stress-induced transformations indicates the possibility for shape memory behavior. Finally, the predicted transformation parameters show good correspondence with experimental values for the shape memory alloys CuAlNi and AuCd.

Nanoscale Piezoelectricity

Pradeep Sharma
Department of Mechanical Engineering, University of Houston

Crystalline piezoelectric dielectrics electrically polarize upon application of uniform mechanical strain. Inhomogeneous strain, however, locally breaks inversion symmetry and can potentially polarize even non-piezoelectric (centrosymmetric) dielectrics. Flexoelectricty—the coupling of strain gradient to polarization— is expected to show a strong size-dependency due to the scaling of stain gradients with structural feature size. In this study, using a combination of atomistic and theoretical approaches, we investigate the "effective" size-dependent piezoelectric and elastic behavior of inhomogeneously strained non-piezoelectric and piezoelectric nanostructures. We argue, through computational examples, the tantalizing possibility of creating "apparently piezoelectric" nano-composites without piezoelectric constituents. Further, to obtain analytical results and tease out the novel physical insights, we analyze a paradigmatic nanoscale cantilever beam. We find that in materials that are intrinsically piezoelectric, the flexoelectricity and piezoelectricity effects do not add linearly and exhibit a nonlinear interaction. The latter leads to a strong size-dependent enhancement of the apparent piezoelectric coefficient resulting in, for example, a "giant" 500% enhancement over bulk properties in $BaTiO_3$ for a beam thickness of 5 nm. Correspondingly, for non-piezoelectric materials also, the enhancement is non-trivial (e.g. 80 % for 5 nm size in paraelectric $BaTiO_3$ phase). Flexoelectricity also modifies the apparent elastic modulus of nanostructures, exhibiting an asymptotic scaling of $1/h^2$ where "h" is the characteristic feature size. Our major predictions are verified by quantum mechanically derived force-field based molecular dynamics for two phases (cubic and tetragonal) of $BaTiO_3$.

Stability of Shape Memory Alloy Honeycomb under Finite-Strain Isothermal Compression Cycles of Various Amplitudes

Nicolas Triantafyllidis
Professor
Aerospace Engineering Department, University of Michigan

Petros Michailidis
Aerospace Engineering Department, University of Michigan

John Shaw
Professor
Aerospace Engineering Department, University of Michigan

Metallic foams and honeycombs, with their light-weight, high specific stiffness, and well-developed energy absorption characteristics, are of obvious utility in engineering applications. However, these structures, often made of aluminum, suffer permanent deformation after crushing. Cellular structures made from shape-memory alloys (SMAs) are particularly intriguing for their potential to deliver shape memory and/or superelasticity in a light-weight material. Realization of open-celled Nitinol has recently become possible via a (newly discovered by Profs. D. Grummon at Michigan State Univ. and J. Shaw at Univ. of Michigan) transient-liquid reactive brazing system for creating robust metallurgical Nitinol-Nitinol bonds. With this technique, prototype sparse cellular honeycomb structures have been made and tested, showing up to 50% repeatedly recoverable strains.

Of particular interest here, in addition to modeling experiments on SMA's, is an in-depth investigation of the isothermal, hysteretic response of these honeycomb materials and the stability of their deformation patterns at finite strains. A detailed investigation of the influence of the material constitutive law on the macroscopic stress-strain behavior of these honeycombs is presented. It is found that instabilities—in the form of departure from the principal solution where all cells deform in the same pattern—appear with the increase of macroscopic strains as the cell-wall alloy transforms from austenite to martensite and then eventually disappear, upon further macroscopic straining, as all the cell-wall alloy is all in the martensitic phase. Upon unloading, where the cell-wall alloy material reverses this transformation, similar instabilities appear and disappear. The stability of honeycomb structure is addressed i) by using one-cell Bloch wave calculations for the infinite perfect case, ii) by using large perfect-geometry samples to account for specimen boundary conditions and finally iii) by using large imperfect-geometry samples to compare and contrast with experimental results.

Some Two-Phase Problems of Nonlinear Elasticity in the Presence of Small Interfacial Energy: A Global Bifurcation Approach

Tim Healey
Professor
Theoretical & Applied Mechanics, Cornell University

We consider several different physical problems, having a common mathematical structure: a non-convex energy in the lower-order terms plus a higher-order regularization (or singular perturbation), the latter characterized by a small parameter (or parameters). We study the equilibria of such systems, focusing on local minima of the total energy. We propose a novel approach based upon techniques of global bifurcation and a-priori bounds—with the reciprocal of the small parameter playing the role of a "large" continuation parameter. We indicate applications to shape-memory solids, thin flexible sheets and lipid bi-layer membranes.

Transmission Electron Microscopy Studies of Novel Ni-Ti-based Shape Memory Alloys

Dominique Schryvers*
Department of Physics, University of Antwerp
nick.schryvers@ua.ac.be

Rémi Delville
Department of Physics, University of Antwerp

The quest for new shape memory alloys better suited for particular applications usually follows a path where numerous extra constituents are added to the basic alloys in smaller or larger amounts. Though the choice of elements and ratios is normally based on their known effects in similar systems, this approach is essentially still trial-and-error based. Recently, a new approach has been suggested by R. James et al. in which a dedicated search for alloys with a low hysteresis was coupled with measurements of the austenite-martensite transformation matrix [1]. A low or zero hysteresis is expected when the middle eigenvalue lambda2 of this transformation matrix equals 1. At the same time, this condition implies a perfect fit at the habit plane so that no microtwinning in the martensite is necessary. Moreover, this condition also divides the remaining phase space into two parts, one with Type I and II twins (lambda2 > 1) and one with compound twins (lambda2 < 1). One such system is Ni-Ti-Pd in which Ni is replaced by Pd.

The present contribution focuses on transmission electron microscopy (TEM) work of Ni-Ti-Pd alloys with different compositions with lambda2 varying around 1. The TEM micrographs clearly confirm the existence of Type I and II twins at lambda2 > 1 with a decreasing twin density when approaching lambda2 = 1. In one sample, a twinless habit plane could be observed to grow during an in-situ cooling experiment. However, on some occasions also compound twins are observed in samples with lambda2 > 1.

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Mechanics of NiTi Fatigue for Vascular Stent Design

Brian Berg*
Senior Research Fellow
R&D Cardiovascular, Boston Scientific
Brian.Berg@bsci.com

Nitinol has become a frequently used medical implant material despite its notorious complexity, especially with respect to fatigue [1]. This intermetallic compound, NiTi, when designed & manufactured into a femoral arterial stent is able to spring out of a intra-vascular catheter, hold the diseased artery open, and undergo millions of cycles of large deformation due to walking, sitting-standing, et cetra without failure, usually. This talk will elucidate how mechanics is used to measure and model the use conditions in-vivo, and the fatigue life of a NiTi stent.

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A Macroscopic Constitutive Relation for Polycrystalline Shape-Memory Alloys

Kaushik Bhattacharya
Department of Mechanics and Materials Science, California Institute of Technology

Alex Kelly
California Institute of Technology

We present a constitutive model to describe the macroscopic behavior of shape-memory alloys. Though the model is phenomenological, it incorporates concepts that arise from the multi-scale experimental and theoretical studies of polycrystalline shape-memory alloys. In particular, it recognizes that the initiation and saturation of transformation are controlled by different mechanisms. We describe the model in detail, describe the mathematical setting and a numerical implementation. We use examples to demonstrate that the model is valid for a broad range of temperatures, for diverse loading pathways and for various textures. Finally, we use the model to propose some new experiments.

SES Medal Symposium in Memory of A. J. M. Spencer, FRS

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A.P.S. Selvadurai, *Department of Civil Engineering and Applied Mechanics, McGill University*

SYMPOSIUM
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Strain Gradient Plasticity Applied to Composites and Polycrystals

John Willis*
Professor
Centre for Mathematical Sciences, University of Cambridge
J.R.Willis@damtp.cam.ac.uk

Recent work of the presenter, in collaboration with N.A. Fleck, has formulated strain-gradient theory, employing a potential for the plastic strain-rate (or, more generally, rate of plastic distortion) and its gradient, together with a similar term which governs the jump conditions across interfaces. The theoretical structure is given concise expression in terms of variational principles. The theory admits both "energetic" and "dissipative" variables, work-conjugate to the plastic strain-rate and its gradient. The theory will be outlined and examples of its application to the homogenization of model composites and polycrystals will be presented, with emphasis placed on response to load reversal.

Effect of Surface Stress on Elastic Field of a Nanoscale Layer

Nimal Rajapakse*
Professor
Department of Mechanical Engineering, University of British Columbia
rajapakse@mech.ubc.ca

X.J. Zhao
Department of Mechanical Engineering, University of British Columbia

There is growing interest in studying the mechanics of nano-scale structures and devices. The surface-to-volume ratio of nano-scale elements is relatively high compared with that of macro-scale elements. The energy associated with atoms at a free surface is different from that of atoms in the bulk, and therefore the effect of surface free energy becomes important in the case of nano-scale elements [1]. Surface energy effects are generally ignored in traditional continuum mechanics, as the energy of the bulk material governs the response. Gurtin and Murdoch [2,3] developed a theoretical framework for the mechanics of a continuum that includes the effects of surface stress and interfacial energy. In this paper, the two-dimensional elastic field of a nano-scale elastic layer bonded to a rigid substrate is investigated using the modified continuum theory presented by Gurtin and Murdoch [2, 3]. Fourier integral transforms are used and the general solution for the elastic field is presented. Analytical solutions corresponding to selected surface loading are presented. The influence of the surface stress effect is discussed and a closed-form solution is obtained for the limiting case of a semi-infinite medium. Selected numerical results are presented to show the influence of surface tension, surface elastic properties and layer thickness on the elastic field. The general solution presented in this study also provides the basis for examining the classical indentation problems in the presence of surface stress.

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Adhesion of a Charged Particle to an Electronically Responsive Charged Substrate

Tian Tang*
Assistant Professor
Mechanical Engineering, University of Alberta
tian.tang@ualberta.ca

Oxana Malysheva
Research Assistant
Mechanical Engineering, University of Alberta

Peter Schiavone
Professor
Mechanical Engineering, University of Alberta

Adhesion of a charged particle to an electronically responsive substrate is important to many applications such as biosensors [1] and recently developed technique to separate carbon nanotubes using single-stranded DNA [2]. In this work, the equilibrium separation between a charged particle in an electrolyte solution and a substrate with an initially uniform surface charge density is obtained using the classical Derjaguin-Landau-Verwey-Overbeek (DLVO) theory [3]. The electrostatic free energy is obtained by coupling the electric response of the substrate with the electric potential obtained from the solution of the Debye-Huckel (DH) equation [4-5]. The van der Waals free energy is calculated by integrating the 6-12 Lennard-Jones (LJ) potential [3]. Metallic, dielectric and semiconducting substrates are considered in turn. Our results demonstrate a distinct response to the charged particle in each case. For example, in the case of a metallic substrate, the attached state (corresponding to equilibrium separation at short range) is always close to the van der Waals energy minimum. In addition, the application of a surface charge of opposite sign to that of the particle facilitates the transition from the detached state (corresponding to large separation at which the interaction between the particle and the substrate is negligible) to the attached state but scarcely changes the equilibrium separation. In the case of a dielectric substrate, the attached state is located at a distance of two orders of magnitude larger than that for a metallic substrate and this equilibrium separation reduces as the (opposing) surface charge increases.

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Boundary Integral Equations for Inhomogeneous Elastic Materials

David Clements
Mathematics, University of Adelaide

Boundary integral equations are obtained for the numerical solution of the partial differential equations governing deformations of inhomogeneous elastic materials. Some particular examples are considered to illustrate the application of the integral equations for the solution of crack and contact problems for inhomogeneous materials.

Dislocation-Based Metal Plasticity: Temperature and Rate Effects

Sia Nemat-Nasser
Professor
CEAM/Mechanical and Aerospace Engineering, University of California, San Diego

Excluding high-temperature creep, the plastic deformation of metals occurs by the motion of dislocations that produce slip on various slip planes in various slip directions. It is thus natural to seek to develop constitutive relations for metal plasticity, based on the concept of dislocations and their kinematics and kinetics. Such an approach has been successfully used by a number of investigators over the past several decades. More recently, however, the development of the recovery plate-impact tests by Clifton and his students at Brown University, and the recovery Hopkinson techniques by this writer and his coworkers at UCSD's CEAM, has provided important experimental tools to obtain reliable data on stress-strain response of variety of metals over broad ranges of strain rates and temperatures. A wealth of information thus has become available to guide and verify constitutive models that are proposed to describe metal plasticity. Using such data, I have been able to create a class of dislocation-based models which involve a few material constants, and seem to accurately characterize the response of a large number of metals over strain rates from 10^{-4} to 10^{5}/s strain rates, and from 77 to 1,300K temperatures. Some of the essential properties of these models are: They involve several length scales that are directly associated with the dislocations and their evolution, having clear physical bases which then allow their direct modeling without a need of arbitrary phenomenological quantities, such as plastic strain gradients and couple stresses.

• All constitutive parameters in these models can be estimated using a few simple experiments, rendering the models useful for immediate application to real materials.

• The effective plastic strain rate, gamma dot, is expressed in terms of the effective stress and other state variables that are routinely calculated in all large-scale numerical codes, thus allowing a direct implementation into such codes without any special numerical demands, e.g., a need for special algorithm to compute the strain gradients or other numerically troublesome quantities.

• They can be, and have been, successfully used in continuum as well as crystal plasticity.

• They have been extensively verified using an immense body of experimental data.

In this presentation, I will give a summary of these developments with specific illustrations.

Towards Scaling Laws in Random Polycrystals

Shivakumar Ranganathan
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

Martin Ostoja-Starzewski
Professor
Department of Mechanical Science and Engineering, University of Illinois

We demonstrate a methodology to set up unifying scaling laws in the response of a variety of random polycrystals. Within the framework of stochastic mechanics, we introduce the concept of a scaling function that governs the scaling behavior of both elastic and inelastic crystalline aggregates. It turns out that the scaling function depends on a mesoscale (scale of observation relative to grain size) and an appropriate universal measure quantifying the single crystal anisotropy; such a measure is introduced here. Based on the scaling function, we construct a material scaling diagram with whose help one can determine the size of RVE for a whole range of polycrystals made of various crystal classes (cubic, tetragonal, hexagonal,...). We demonstrate this approach on scaling of the fourth order elasticity tensor and the second order thermal conductivity tensor.

A Comparative Study of Damage Variables in Continuum Damage Mechanics

George Voyiadjis
Professor
Civil and Environmental Engineering, Louisiana State University

Peter I. Kattan
Civil and Environmental Engineering, Louisiana State University

In this work various definitions of the damage variables are examined and compared. In particular, special emphasis is given to a new damage variable that is defined in terms of the elastic stiffness of the material. Both the scalar and tensorial cases are investigated. The scalar definition of the new damage variable was used recently by many researchers. However, the generalization to tensors and general states of deformation and damage is new and appears here for the first time. In addition, transformation laws for various elastic constants are derived. Finally, the cases of plane stress, plane strain, and isotropic elasticity are examined in detail. In these cases it is shown that only two independent damage parameters are needed to describe the complete state of damage in the material.

In this work a physical basis is sought for the damage tensor that is used to link the damage state of the material with effective undamaged configuration. The authors and numerous other researchers have used different paths including fabric tensors (Voyiadjis and Kattan, 2006) to connect the two configurations. However, the approach presented here provides for a strong physical basis for this missing link.

Conditions on the Instantaneous Elasticity Tensor and Their Implications

Gearoid Mac Sithigh
Department of Mechanical and Aerospace Engineering, Missouri S & T

A hierarchy of convexity-type conditions are, in various contexts, imposed on the instantaneous elasticity tensor. These are, in order of increasing stringency, strong ellipticity, Agmons condition, Chens condition, and positivity. In this talk, I will explore the implications of these conditions and the ranges in which they hold for some simple families of deformations in an isotropic material.

The Double Shearing Model and Its Generalizations in the Mechanics of Granular Materials

David Harris*
School of Mathematics, University of Manchester
david.harris@manchester.ac.uk

The significance of the achievement in developing the double shearing model, Spencer [1], [2] thereby allowing the solution of quasi-static problems involving the flow of rate independent granular materials to be solved cannot be underestimated. In terms of theory, as a physically based flow rule, rooted firmly in the Coulomb yield criterion, it provides a mechanism with which to envisage the manner in which granular materials flow. In terms of mathematics, an equally significant achievement was the demonstration, in numerous papers, that the equations are a rich source of analytic solutions to boundary value problems.

A further achievement of the double shearing mode has been its ability to be developed and generalised further. It turns out that, Harris [3] and [4] that the double shearing model may be combined with the plastic potential model, the latter being used almost universally in geotechnical and civil engineering. This significantly widens the applicability of both models. The double shearing model was initially developed for rigid-perfectly plastic materials. In addition to a double shearing, the model also incorporates a double rotation, combining the rotation rate of the major principal stress axis and the vorticity. By replacing the stress rate by an intrinsic rotation term, Harris and Grekova [5], a new double shearing type model, embedded in a Cosserat continuum, enables net grain rotation effects to be incorporated.

In this talk we present here the generalisation to elasto-plastic work-hardening materials, incorporating intrinsic rotation. The model is formulated in several ways and various properties are developed. Some applications of the model are considered.

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Anisotropic Plastic Flow Rules with Microstructural Evolution

John L. Bassani*
Professor
Mechanical Engineering and Applied Mechanics, University of Pennsylvania
bassani@seas.upenn.edu

Haizhen Pan
Graduate Student
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

We consider a class of elastic-plastic materials that possess local orthotropic symmetry which is naturally represented in terms of second-order orientation tensors that can evolve with deformation. At finite strain, the standard multiplicative elastic-plastic decomposition is adopted, and the flow rule is defined in the intermediate configuration. The microstructural spin, i.e. the spin of the orthotropic axes, is defined to be the difference between the material and plastic spin. Spencer's (1971) theory of invariants coupled with representations for tensor-valued functions due to Wang and Smith (1969-1971) are utilized to develop phenomenological constitutive relations, including an equation for plastic spin. For yield functions that are quadratic in the components of stress, the classical normality flow rule leads to generators for the plastic part of the rate of deformation that only depend linearly on the stress tensor. In constructing a constitutive equation for plastic spin in the intermediate configuration, we assume similar dependencies on stress tensor in addition to nonlinear dependencies on the invariants of stress and orientation tensors. Comparisons with experimental data for textured polycrystals under uniaxial tension and simple shear loading are promising. Significant effects of microstructural evolution on limits to ductility are predicted.

On the Heat Flux Vector for Flowing Granular Materials

Mehrdad Massoudi*
U.S. Department of Energy, National Energy Technology Laboratory, Pittsburgh
Massoudi@netl.doe.gov

Heat transfer plays a major role in the processing of many particulate materials. The heat flux vector is commonly modeled by the Fourier's law of heat conduction and for complex materials such as non-linear fluids, porous media, or granular materials, the coefficient of thermal conductivity is generalized by assuming that it would depend on a host of material and kinematical parameters such as temperature, shear rate, porosity or concentration, etc. We will give a brief review of the basic equations of thermodynamics and heat transfer to indicate the importance of the modeling of the heat flux vector. We then propose and subsequently derive a properly frame-invariant constitutive relationship for the heat flux vector for a (single phase) flowing granular medium. Standard methods in continuum mechanics such as representation theorems and homogenization techniques are used. It is shown that the heat flux vector in addition to being proportional to the temperature gradient (the Fourier's law), could also depend on the gradient of density (or volume fraction), and Dij (the symmetric part of the velocity gradient) in an appropriate manner. The emphasis in this paper is on the idea that for complex non-linear materials it is the heat flux vector which should be studied; obtaining or proposing generalized form of the thermal conductivity is not always appropriate or sufficient.

Nonlinear Viscoelasticity, Strain Clocks, and Shear

Alan Wineman*
Professor
Mechanical Engineering, University of Michigan, Ann Arbor
lardan@umich.edu

Experimental evidence in the literature indicates that the stress relaxation response of viscoelastic materials is affected by deformation. Several constitutive equations have been proposed in which stress relaxation is accelerated by volume change. There is also experimental evidence that stress relaxation can be accelerated by shear. This phenomenon is introduced into the constitutive equation by replacing the physical time variable with a reduced time variable that depends on the deformation. There is little work that explores the implications of this phenomenon on mechanical response.

In the present work, a constitutive equation is constructed for nonlinear viscoelastic response that allows the study of the influence of both shear and dilatation on stress relaxation. The constitutive equation combines the Pipkin-Rogers single integral framework for nonlinear viscoelasticity, the Blatz-Ko model for compressible nonlinear elasticity and a time variable that can be accelerated by dilatation and/or shear. This constitutive equation incorporates the features discussed in the literature into a finite deformation framework.

This constitutive equation is used to study the response to the homogeneous deformation of shear superposed on triaxial extension. Several cases are considered: (i) simple shear under both shear and stress control, (ii) shear superposed on equal biaxial step elongation or contraction and (iii) shear in the absence of normal tractions. Results in this latter case illustrate time dependent dimensional changes that arise from the normal stress effect.

Nonlinear Anisotropic Magnetoelasticity

Ray Ogden
Professor
Mathematics, University of Glasgow

Roger Bustamante
Ingenieria Mecanica, Universidad de Chile

This talk concerns the theory underlying the mechanical behaviour of so-called magneto-active elastomers, which are regarded as smart materials. They are composed of a rubber-like matrix material containing a distribution of magneto-active particles. Due to the highly elastic behaviour of the rubber-like matrix the mechanical response of these materials is capable of significant change upon the application of external magnetic fields. In this talk we provide a theoretical basis for analyzing the nonlinear properties of a particular class of these materials, namely the class of transversely isotropic magneto-active elastomers. The particular characteristic of these materials is that during the curing process, when the magneto-active particles are added to the rubber-like material, an external field is applied, and as a result the particles are aligned in a preferred direction. Available experimental data suggest that the capacity of the material to deform in the presence of an external magnetic field is then enhanced significantly by comparison with the situation in which no external field is applied during curing, when the distribution of particles is essentially random. The general constitutive for such transversely isotropic magnetoelastic materials is developed following the theory of invariants of Spencer [1], and based on the formulation of magnetoelasticity due to Dorfmann and Ogden [2]. Application of the theory to a simple prototype problem is used to illustrate the effect of a magnetic field on the mechanical properties of a magneto-active material in the nonlinear regime.

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Fracture Initiation within the Atheromatous Plaque

Dr. Dimitrios Eftaxiopoulos
Applied Mathematical and Physical Sciences, National Technical University of Athens

Colin Atkinson
Department of Mathematics, Imperial College—South Kensington Campus

Atherosclerosis is a widespread disease of the arterial wall. During the process of it, plaque is accumulated within the arterial wall, as a result of the deposition of lipids that are transported by the circulating blood. Plaque, essentially develops as inflation and cellular transformation of the intima mainly and of the media secondarily. Intima and media are the inner and middle layers of the arterial wall respectively. In the early stages of its development, the plaque is relatively compliant, while later on it transforms to fibrous and calcified, becoming gradually stiffer. The presence of the plaque alters the stress field in the arterial wall, leading possibly to local stress concentrations, which eventually may cause fracture of the plaque. Fracture may emerge in the form of a radial crack, emanating from the innermost boundary of the arterial wall towards the media, or as a circumferential delamination between the infected intima and the healthy media.

In this work, a plane strain model of a curved strip of a diseased intima (plaque), loaded with uniform far field tensile stresses, is considered, as an approximation to the three dimensional case. This loading can be due to a deliberate intervention such as balloon angioplasty, or merely due to the blood pressure in the artery. The principle of local action enables us to work locally, at a point where a crack is imminent, but not present at the moment. At this location, which may be on the inner boundary of the plaque, we can replace the system of local orthogonal curvilinear coordinates, by a local system of Cartesian coordinates. Further, locally the curved strip of the plaque, looks like a half plane. The material property, namely the strain energy density function for the plaque and the uniform tensile stresses acting in the half plane, can be found in the literature.

An edge crack of small length, generating an extra field of small displacements, is introduced in the plaque, at this location. The theory of small deformations superimposed on large deformations, is implemented in this work, in order to study the energy release rate due to this starter fracture. The plaque is now considered under the linear, small displacement, anisotropic, elasticity theory, but with altered material properties, produced by small deformations on large. These properties depend on the preexisting stress field due to the large deformations. The problem of the small edge crack, rescaled locally, is then solved for the energy release rate or the stress intensity factor to be found.

Material Symmetry Characterization of Soft Tissue Deformation by Sets of Vectors

Stephen Cowin*
Professor
The New York Center For Biomedical Engineering, Mechanical and Biomedical Engineering Departments,
The City College of the City University of New York
scowin@earthlink.net

Many contemporary developments of constitutive relations for the large deformation behavior of soft tissues have employed sets of vectors to characterize the material symmetry rather than Noll's (1958) definition of material symmetry in terms of invariance of the constitutive relations under one of the specific crystallographic symmetry groups. The present work shows that this contemporary development of using sets of vectors to characterize material symmetry is fully equivalent to the group theoretic crystallographic viewpoint and provides a geometrically intuitive view of the elastic symmetries as a companion to the group theoretic crystallographic viewpoint. In this work it is shown that the different forms of the elasticity or compliance tensors that represent the different material symmetries in the generalized Hooke's law, at a point in the deformation process, may be obtained by assuming the strain energy depends on a set of structural unit vectors as well as the strain tensor or deformation gradients. The particular set of structural unit vectors is different for each of the eight linear elastic symmetries. This method permits the direct and evolving calculation of the changes in symmetry as a result of a deformation, a feature not contained in the traditional approach. The determination of the development-induced changes in the material symmetry employs results from the theory of an infinitesimal strain superposed on a finite strain in an elastic material.

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Homogenization-Based Estimates for Elastomers Reinforced with Short Fibers

Pedro Ponte Castaneda
Professor
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

O. Lopez-Pamies
Professor
Mechanical Engineering, S.U.N.Y. at Stony Book

In this talk we present the application of a recently developed "second-order" homogenization technique [1] to generate estimates for the effective behavior, microstructure evolution and loss of ellipticity in fiber-reinforced elastomers that are subjected to finite deformations. The main concept behind the method is the introduction of an optimally selected "linear comparison composite," which can then be used to convert standard linear homogenization estimates into new estimates for the nonlinear hyperelastic composite. Explicit results are provided for materials with isotropic and strongly elliptic constituents. The dependence of the macroscopic response on fiber concentration, shape and orientation is elucidated. It is found that the overall behavior may lose ellipticity at sufficiently large deformations, which corresponds to the possible development of shear band-type instabilities. The reasons for this result have been linked to the evolution of the microstructure, which, under appropriate loading conditions, can induce "geometric softening" leading to the overall loss of ellipticity.

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Small Longitudinal Oscillations of a Load on an Incompressible, Isotropic Limited Elastic Spring

Millard F. Beatty
Professor Emeritus
Engineering Mechanics, University of Nebraska, Lincoln

The small amplitude, free longitudinal vibrational motion of a load supported above by an incompressible, isotropic and homogeneous rubberlike spring is studied for a general class of materials having limited extensibility. First, a simple general frequency equation for small motions about a static equilibrium state is derived without specification of the constitutive nature of the spring. The normalized oscillational frequency of the small superimposed motion of the load is then determined for all materials in a broad class of limited elastic materials. This frequency depends on the limiting extensibility constant and the static stretch, but it is independent of any other physical properties of the spring. It is shown that, for the same static stretch, the normalized vibrational frequency of a load on a neo-Hookean support is a lower bound for its normalized vibrational frequency on any limited elastic spring in the general constitutive class. Specific equations for the Gent and Puso limited elastic models are derived, the frequency for the latter being smaller than that for the former under the same static conditions. The effects of their limited extensibility are described both analytically and graphically, and their connection with experiments on certain rubber materials and biological tissue is noted.

Boussinesq Indentation of an Isotropic Elastic Halfspace Reinforced by a Membrane with a Bilateral Inextensibility Constraint

A.P.S. Selvadurai*
William Scott Professor and James McGill Professor
Civil Engineering and Applied Mechanics, McGill University, Montreal
patrick.selvadurai@mcgill.ca

The class of problems that deal with the mathematical modelling elastic regions reinforced with arrays of closely spaced inextensible reinforcing elements can be traced back to a classical study presented by H.M. Westergaard in 1938. Other expositions of constrained media are also given by Wieghardt and Vlazov (see e.g. Selvadurai[1]). Modern continuum treatments of non-linear elastic media with inextensibility constraints were presented by Adkins, Rivlin and Pipkin and co-workers in connection with the study of rubber-like elastic materials reinforced with inextensible fibres. The treatise by Spencer [2] is a comprehensive study of the continuum theory of materials elastic reinforced with families of inextensible fibres. Further reviews of the topic are given by Spencer [3, 4]. This paper examines the linear elasticity problem related to the axisymmetric surface indentation of an isotropic elastic halfspace that contains an inextensible elastic membrane that is located at a finite depth. The problem can be regarded as a generalization of the classical Boussinesq indentation problem to include the inextensible elastic membrane inhomogeneity. When the inextensibility constraint for the membrane is bi-lateral, the resulting mixed boundary value problem can be reduced to the solution of a Fredholm integral equation of the second kind. Although an exact closed form analytical solution of the integral equation is not evident, it can be solved using a numerical technique. The numerical approach can be used to evaluate the axial stiffness of the indentor. It is shown that there is an optimum location of the inextensible membrane that leads to the greatest stiffness of the indentor and that this location is a function of Poison's ratio of the elastic medium. The limiting cases for the position of the inextensible membrane can, however, be obtained as exact solutions.

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Integral Transform-Based Solutions for Thermoelastic-Dynamic Problems in Functionally Graded Materials

Quentin Z.Q. Yue*
Department of Civil Engineering, The University of Hong Kong
yueqzq@hkucc.hku.hk

Functionally graded materials (FGM) are natural or man-made materials with their properties spatially variable to best accommodate the external loading such as force and heat. A majority of the common FGM are the solid materials that exhibit their mechanical properties continuously variable with depth from material surface. The prediction of the thermoleastic dynamic responses in the FGM is important in order to better design the materials and evaluate their integrity [1]. This paper presents a set of Fourier transform-based solution for thermoelastic dynamic problems in FGM. The FGM is assumed to occupy a three-dimensional space of either infinity extent or a semi-infinity extent or laterally infinity extent and finite thickness in depth. The basic partial differential equations governing the linear thermoelastic-dynamic response of FGM with body forces and heat source are examined with the classical two-dimensional Fourier transform and Laplace transform techniques. It is found that the basic partial differential equations can be re-written into two sets of ordinary differential equations with the depth independent variable z in the Fourier and Laplace transform domain. The ordinary differential equations can be solved analytically for some special cases of the non-homogeneity in the depth direction. By taking into account the boundary and initial value conditions, analytical solutions are derived for the displacements, stresses, strains and temperature in the Fourier and Laplace transform domain. Solutions for the field variables in physical domain can be obtained via the inversions of the analytical solutions in the transform domain [2-6]. It is expected that many new results can be computed using the proposed method for thermoelastic-dynamic problems in FGMs.

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Towards a New Generation of 2D Mathematical Models in the Mechanics of Thin-Walled Fiber-Reinforced Structural Components

Kostas P. Soldatos*
Theoretical Mechanics, University of Nottingham
kostas.soldatos@nottingham.ac.uk

Pioneering 1D and 2D mathematical models that describe the mechanical behaviour of elastic beams, plates and shells are associated with the names of the Bernoullis, Euler, Kirchhoff, Love and Timoshenko. From the early times of their existence until the beginning of the second half of the twentieth century, such models continued to appear under the adequate, for the times, assumption that the material of the thin-walled structure considered is homogeneous and isotropic. The appearance of highly anisotropic, fibre-reinforced materials and their extensive subsequent use and exploitation in the thin-walled structures industry necessitated the development of another generation of relevant 1D and 2D mathematical models, capable of taking those new, advanced material features into consideration. Initiation of that new generation of thin-walled structures mathematical models is attributed to Reissner and Stavsky [1] who, together with many others added afterwards a substantial number of relevant contributions (e.g. [2] for additional references).

Although development of that second generation of mathematical models for thin-walled structures still continues, it is based on the simplifying assumption that fibres have negligible thickness and they are perfectly flexible. This assumption is a valid approximation in many cases of interest, but is not invariably applicable. It is worth mentioning in this connection that micromechanics considerations reveal that there are cases in which fibres can resist bending to an extent necessitating the use of asymmetric theory of elasticity (stress tensor stops being symmetric). Resistance of fibres in bending gives therefore rise to asymmetric elasticity theory effects, consideration of which is expected to influence developments towards the generation of a new class of mathematical models, appropriate for the study of the mechanical behaviour of thin-walled structures and "smart" structural components.

In some detail, a relevant finite elasticity theory developed recently [3] produced, as a particular case, a version of asymmetric linear elasticity theory that takes into consideration the effects of fibres bending stiffness (resistance of fibres in bending). The latter, asymmetric theory of linear elasticity is currently available in a form appropriate to the material symmetries of transverse isotropy only. It can however serve as a means for incorporation of the aforementioned micromechanics effects into accurate 2D thin-walled structures modeling, in a manner similar to that followed already in developing conventional and advanced relevant models on the basis of the classical (symmetric) 3D theory of elasticity. The manner in which this aim may be pursued is outlined in another recent publication [4] but the present study is the first real attempt towards it. As such, it deals only with the simple geometrical configuration of a flat, plate-type structural component, the fibre-reinforced material of which contains however fibres that resist bending.

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Complex Variable Solutions for an Inhomogeneous Thick Elastic Plate

Dr. A.H. England
Division of Theoretical Mechanics, Nottingham University

In a series of papers commencing in 1988, Rogers and Spencer and their co-authors developed a procedure for deriving exact solutions to the equations of elasticity for materials that are isotropic but are inhomogeneous along a specified direction, so that the elastic constants may be taken as functions of a single space variable. In the case of a thick elastic plate we will suppose the elastic moduli are known functions of the coordinate normal to the plane of the plate, so that laminated plates and functionally-graded plates are covered by this analysis. In the case of a plate with traction-free upper and lower surfaces, England and Spencer (2005) have derived general solutions which may be expressed in terms of four analytic functions of the complex coordinate x + iy in the mid-plane of the plate.These solutions are generalisations of the Kolosov-Muskhelishvili solutions for plane-strain elasticity. Whilst these solutions do not contain enough generality to satisfy the boundary conditions pointwise around the edge of the plate, resultant force and moment conditions or averaged displacements may be specified over the edge of the plate.

These solutions have been extended to cover the case of a pressure field applied to one face of the plate. In general the bending and the in-plane extensional behaviour of the plate is coupled. The intention in this talk is to illustrate these solutions and to derive some stiffness coefficients for general inhomogeneous plates of this type.

Engineering Mechanics of Biologically Inspired Products and Structures

ORGANIZERS:

Ashok Kumar Ghosh, *Department of Mechanical Engineering, New Mexico Tech*

Eric N. Brown, *Los Alamos National Laboratory*

SYMPOSIUM

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Deformation Mechanism of Nacre and Nacre-Inspired Composites

Horacio Espinosa*
Professor
Mechanical Engineering, Northwestern University
espinosa@northwestern.edu

Felix Latoute
Postdoctoral Fellow
Mechanical Engineering, Northwestern University

Jee E. Rim
Postdoctoral Fellow
Mechanical Engineering, Northwestern University

In contrast to man-made materials, nature can produce materials with remarkable structural properties out of relatively weak constituents. Nacre from seashells is a perfect example: mostly made of a fragile ceramic (polygonal calcium carbonate tablets), it exhibits surprisingly high levels of strength and toughness. Features leading to this performance are a very well designed microstructure organized in a hierarchical fashion, and the addition of a small volume fraction of biopolymers [1-3]. The resulting material is stiff and hard yet surprisingly tough, an essential requirement to protect the seashell against predators.

While nacre has been studied extensively, the specific features and mechanisms leading to its remarkable toughness have yet to be fully elucidated [4]. A key to the mechanical performance of nacre is the cohesion and sliding of the ceramic polygonal tablets. We have shown previously through experiments and numerical modeling that microscopic tablet waviness is the key feature generating progressive interlocking of the tablets and hardening at the macroscale [5-6]. With this understanding, it is now possible to design artificial materials that utilize the deformation and hardening mechanism of nacre to result in superior toughness and high strength. A strategy combining experiments and simulations for optimizing material and geometric parameters of such a nacre-inspired composite will be presented.

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Hierarchical Modeling of Gecko Toe Adhesion

Bin Chen*
Mechanical Engineering, McMaster University, Canada
binchen@mcmaster.ca

Peidong Wu
Mechanical Engineering, McMaster University, Canada

Huajian Gao
Engineering Division, Brown University, USA

A hierarchal modeling framework is adopted to investigate adhesion of the microstructures on gecko toe for both attachment and detachment. At the bottom of hierarchy, we show that, a spatula pad can have a large absorption area on to a surface but also a strongly constrained decohesion process zone upon loading, both of which are beneficial to the robust attachment. With different peeling angles, the peel-off force of a spatula pad for attachment can be 10 times larger than that for detachment. At the intermediate level of hierarchy, we show that the fibrillar structure of seta can collect the tiny forces effectively and maintain a stress level similar to that in the spatula pad; in addition, the 10 times difference in peel-off force on a single spatula pad for attachment and detachment is magnified to a 100 times difference in adhesion energy at the level of seta. At the top of hierarchy, gecko toe attachment is modeled as an adhesive pad under displacement controlled pulling, leading to an adhesive force much larger than gecko's body weight, while gecko toe detachment is modeled as a pad under peeling, which incurs a negligible force for detachment. Our work reveals that hierarchical microstructures on gecko's toe can indeed provide gecko with robust adhesion for attachment and reversible adhesion for easy detachment at the same time.

Topology Optimization of Structures Using Hybrid Cellular Automaton: Application to the Design of Periodic Materials

Kumar Vemaganti
Associate Professor
Mechanical Engineering, University of Cincinnati

Raghavender Cheerkapally
Graduate Student
Mechanical Engineering, University of Cincinnati

Many biological structures continually adapt their structure to the external stimulus by the environment. The hybrid cellular automaton (HCA) methodology [1], inspired by the biological process of bone remodeling, integrates local design rules from the cellular automaton framework with a grid-based computational method like finite element analysis. The remodeling or adaptation process is achieved through local communication among the automata (cells of the grid) based on a set of pre-defined rules; this communication leads the structure to an equilibrium state at which point no further remodeling is required.

In this work, we discuss the use of the HCA approach to design periodic materials that have prescribed material properties. This can be formulated as an inverse homogenization problem, where the goal is to design the topology of the structures base cell or unit cell such that the macroscopic properties of the material match the prescribed values. The HCA approach to this problem and the corresponding equilibrium state of the unit cell are described in this talk. Several numerical experiments illustrating the approach and its efficacy are discussed.

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Nonlinear Fracture of Implant Polymers: Polytetrafluoroethylene and Polyethylene

Eric N. Brown*
ADWP, Los Alamos National Laboratory
en_brown@lanl.gov

In vivo fracture and wear have been identified as some of the major problems leading to implant failure. To alleviate this, the selection and optimization of biomaterials have necessitated a balance of trading fracture toughness for wear resistance. One of the most mechanically demanding implants is the total hip replacement (THR), which includes a polymer lining at the sliding interface between the prosthetic femoral head and socket. Early applications utilized polytetrafluoroethylene (PTFE), commonly known as Teflon, for the lining due to its strength and low sliding resistance. Unfortunately, low wear behavior, compounded by tissue reaction with wear debris, has lead to replacement with ultra-high molecular weight polyethylene (UHMWPE). However, PTFE continues to be widely used for implants, including ball-and-socket joint reconstructions such as the temporomandibular joint, ossicular chain reconstructions, and orbital floor reconstructions [1]. In this paper we present a review of the non-linear J-integral fracture behavior of PTFE and PE employing the single-specimen normalization technique [2]. Moreover, we discuss the effect of crystallinity [3] and conformation on fracture [4]. A new neutron diffraction method during far-field loading is presented to enable the in-site measurement of inter-atomic crystalline lattice strains of the crystalline domains of these semi-crystalline polymers [5].

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Effects of a Bio-inspired Interfacial Modification on the Properties of Polymer Matrix Nanocomposites

Lesley Hamming
Department of Materials Science and Engineering, Northwestern University

Phil Messersmith
Department of Biomedical Engineering, Northwestern University

Cate Brinson
Department of Mechanical Engineering, Northwestern University

Marine mussels have the remarkable ability to attach to virtually any organic and inorganic substrate even in a tumultuous aquatic environment. The proteins responsible for their adhesion contain an unusual abundance of the amino acid L-3,4-dihydroxyphenyl-alanine (dopa) [1]. We have capitalized on dopa's role in adhesion by creating its synthetic analog for use in adhering polymer to metal-oxide surfaces [2]. After demonstrating that our adhesion method improved the interfacial shear stress between a metal wire and bulk polymer by 116% [3], we applied our method to polymer nanocomposites, a research area of growing interest to industries looking for a light-weight but strong alternative to metals. Two of the most important variables influencing a nanocomposite's properties include the quality of the interphase and dispersion of the nanoparticles. In order to improve the interfacial adhesion and dispersion, we applied our biomimetic modification to titanium dioxide nanoparticles embedded in poly (methyl methacrylate) and then examined the subsequent structural, mechanical, and thermal properties. Our modified nanocomposites demonstrated shifts in the glass transition temperature (Tg) towards higher temperatures. By contrast, the composites with unmodified nanoparticles led to a shift in Tg towards lower temperatures. We further discovered that better dispersion led to a larger Tg shift by systematically quantifying the distribution of nanoparticles in each composite from scanning electron microscope (SEM) images. As Tg is considered a measure of interfacial interaction in nanocomposites, this work highlights a biomimetic technique for increasing the reinforcement capability of nanoparticles. Interestingly, the mechanical properties of our modified composites have demonstrated stability even after submersion in water for up to 9 months while unmodified composites showed a breakdown in integrity over the same period of time. The superior performance of our biomimetic composites is attributed to the stability of dopa adhesion in water. As medical implants and devices as well as structural components are often subjected to aqueous environments, our technique may lead to increased lifetime and performance of these systems.

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Mechanically Efficient Cellular Microstructures in Plants

Lorna Gibson
Professor
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Natural cellular materials, such as wood, often have exceptional mechanical performance on a weight basis. The properties of wood depend both on the fibre composite nature of the cell wall as well as on the honeycomb-like cellular structure. The mechanical properties of the constituents of wood (cellulose, lignin and hemicellulose) are not themselves particularly unusual: it is the arrangement of those materials which gives rise to the exceptional properties of wood. Plants have a number of strategies for mechanical efficiency. The trunk of a palm has a density gradient, both radially and longitudinally, that concentrates material where the stresses are highest: at the periphery and base of the trunk. Bamboo is tubular, with a density gradient within the cylindrical shell and transverse plates at the nodes. Grassy plant stems have an almost fully dense cylindrical shell supported by a foam-like core. Iris leaves have a sandwich structure, with fibrous ribs running longitudinally on the outer faces separated by a foam-like core of parenchyma cells. Here we review the way in which the cellular microstructure contributes to the mechanical performance of wood, palm, bamboo, grassy stems and iris leaves.

Influence of Weak Anchoring upon the Alignment of Planar Lipid Bilayers with Surface Pretilt

Raffaella De Vita
Department of Engineering Science and Mechanics, Virginia Tech

Iain W. Stewart
Department of Mathematics, University of Strathclyde

Lipid bilayers are being increasingly used in many medical, defense, and engineering applications ranging from biocompatible and biodegradable drug delivery systems [1] to portable and fast biosensors for detecting biological agents. [2]. A rigorous characterization of their mechanical properties, however, remains limited due to the signifcant challenges encountered in experimental investigations such as their poor stability and nanometer size thickness. Therefore, the formulation of reliable mathematical models is essential in making a big leap forward in the development of the next generation of bio-inspired products and structures that include lipid bilayers.

Lipid bilayers have been universally recognized to be smectic A liquid crystals in which molecules possess positional and orientational order, form layered structures, and have axes normal to the layers [3]. In this talk, we will present novel continuum models that describe the efect of weak anchoring upon the alignment of planar lipid bilayers with surface pretilt by accounting for their liquid crystallinity. The models will be derived within a new theoretical continuum framework for smectic A liquid crystals in which the decoupling between the average alignment of lipid molecules and the layer normal is considered [4, 5]. The equilibrium equations for planar lipid bilayers assemblies will be determined by using variational methods and their solutions will be computed by analytical and numerical methods.

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Magnetoelastic MEMS Sensors for Detection of Biological Species

Bart Prorok
Department of Mechanical Engineering, Auburn University

We have devised a sensor scheme that addresses the major issue of the target species diffusing and coming into contact with the sensor platform, a serious concern for many biological sensors. The scheme is aimed a mimicking how the human immune system generates multitudes of antibodies that diffuse throughout the body and attack the infecting species. We employ microfabrication to generate numerous microscale magnetoelastic sensor platforms that are added and mixed with the sample to be interrogated. Like antibodies they diffuse throughout and their shear number ensure quick contact with target species in the sample. Owing to their magnetoelastic properties they can be remotely/wirelessly driven to resonance with a modulated magnetic field and response read with a pick-up coil. By coating their surfaces with antibodies and other specific capture films, target species are captured, which alters the resonant state of the sensors. Frequency shifts are recorded and indicative of the presence of the target. We demonstrate the feasibility of this approach to biological detection. The technique is expected to impact the fields of medical diagnostics, food safety and biological warfare agent detection.

Mechanobiology of Cell-Extracellular Matrix Interactions

ORGANIZERS:

Amy Wagoner Johnson, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Brendan Harley, *Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign*

Taher Saif, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Ning Wang, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

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Quantifying the Effects of Preload and Afterload on Cardiomyocytes Using Forcepost Detector Arrays

James Norman
Mechanical Engineering and Pediatric Cardiology, Stanford University

Chelsey Simmons
Mechanical Engineering, Stanford University

Niveditha Arumugam
Mechanical Engineering, Stanford University

Subhanu Samarajiva
Mechanical Engineering, Stanford University

Rebecca Taylor
Mechanical Engineering, Stanford University

Giovanni Fajardo, M.D.
Pediatric Cardiology, Stanford University

Daniel Bernstein, M.D.
Pediatric Cardiology, Stanford University

Beth Pruitt
Mechanical Engineering, Stanford University

We are developing force post arrays as a high-throughput biomechanical assay platform for quantifying the fully loaded biomechanical function of cardiac myocytes. Isolated cardiomyocytes are allowed to attach to the tops of compliant posts which act as linear springs (F=kd). When a cell contracts, the posts are displaced (d) and the applied force (F) can be determined based on the geometry and material properties of the posts (k). A significant advantage of force post arrays over other technologies is that they allow for high throughput analysis of individual cardiomyocyte biomechanical function. Most importantly, the effects of preload and afterload can be studied independently or simultaneously. Measurements of wildtype mouse left-ventricular cardiomyocyte total force generation, force per cross-sectional area, and work performed agreed well with previously reported studies. We are also able to map subcellular force generation patterns common to healthy cardiomyocytes and examine longitudinal and transverse force patterns independently. Greatest forces were found at the ends of cells in the direction of the long-axis, forces along the short-axis of the cell were gerneally directed outward. Due to the unique elastic properties and tunable processing conditions we are able to independently emulate preload and afterload on cells. Finite element modeling of forceposts under tensile strain was performed to determine affects of strain on the loading conditions of the cell. For an increase in strain up to 10%, the force-displacement characteristics of the device did not change. Therefore, we are able to preload the cells without changing the afterload level. This value is in the range necessary to increase intersarcomeric distance sufficiently to study the Frank-Starling mechanism in single cells. Force posts devices spanning an order of magnitude change in elastic modulus were constructed by varying ratio of polymer to curing agent. Changing the post stiffness in this manner allows for changing the amount of load the cells work against in the heart. This allows us to emulate the effect of afterload on single cells.

Quantifying the Contractile Behavior of Individual Fibroblasts within 3D Collagen Scaffolds

Brendan A. Harley
Department of Chemical and Biomolecular Engineering, University of Illinois

Lorna J. Gibson
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Cell-mediated contraction plays a critical role in many physiological and pathological processes, notably organized contraction during wound healing. Implantation of an appropriately formulated (i.e., mean pore size, chemical composition, degradation rate) three-dimensional scaffold into an in vivo wound site effectively blocks the majority of organized wound contraction and results in induced regeneration rather than scar formation. Improved understanding of cell contraction within three-dimensional constructs therefore represents an important area of study in tissue engineering.

Studies of cell contraction within three-dimensional constructs typically calculate an average contractile force from the gross deformation of a macroscopic substrate by a large cell population. In this study, cellular solids theory has been applied to conventional column buckling relationships in order to quantify the magnitude of individual cell contraction events within a three-dimensional, collagen-glycosaminoglycan (CG) scaffold. This new technique can be used for studying cell mechanics with a wide variety of porous scaffolds that resemble low-density, open-cell foams. It extends previous methods for analyzing cell buckling of two-dimensional substrates to three-dimensional constructs. The mean contractile force (Fc) generated by individual dermal fibroblasts within CG scaffolds was calculated to range between 11 and 41 nN (Fc = 26 ± 13 nN, Mean ± StDev), with an upper bound of cell contractility estimated at 450 nN.

Matrix Mechanics and Cell Traction Regulate Integrin-Adhesion Ligand Bond Formation by Mesenchymal Stem Cells in 3D Micro-environments

Nathaniel Huebsch
Graduate Research Assistant
School of Engineering and Applied Sciences, Harvard University

Praveen Arany
Dental Resident
School of Engineering and Applied Sciences, Harvard University

Angelo Mao
Undergraduate Research Assistant
School of Engineering and Applied Sciences, Harvard University

David J. Mooney
School of Engineering and Applied Sciences, Harvard University

Recent work has shown that the phenotype of a variety of tissue cell types, including mesenchymal cells (MSCs), is affected to the mechanical properties of the extracellular matrix (ECM) [1]. However, the biophysical mechanism behind this observation is incompletely understood. We hypothesize that one important means for cells to sense matrix stiffness is through mechanically-dependent changes in integrin-adhesion ligand bond formation. To test this hypothesis, we assessed RGD bond formation in MSCs encapsulated into 3D alginate hydrogels modified with adhesion peptides (GGGGRGDASSKY) using a non-invasive FRET assay [2,3]. The number of RGD-integrin bonds depended on matrix compliance in a biphasic manner that was independent of the specific type of alginate polymer or crosslinking molecule. A second FRET assay [4], along with live-cell imaging of GFP-tagged alpha-5-integrins, revealed that bond formation correlated with both mechanical reorganization of the matrix by cells and localization of alpha-5-integrins to the cell-matrix interface. Importantly, bond formation, along with intracellular integrin localization and matrix reorganization, was decoupled from matrix mechanics in the presence of drugs that inhibit cell traction forces. The biphasic dependence of integrin-RGD bond number on matrix stiffness found in this 3D study differs from the monotonic dependence of cell adhesion as a function of matrix stiffness observed in 2D studies [5], and likely represents a more physiologically relevant response of cells to ECM stiffness in vivo. This work highlights a role for integrin-mediated signaling and the number of cell-matrix bonds as rational design criteria for selecting both the biological (e.g. the density of adhesion ligands) and biophysical properties of micro-environments used to study and manipulate stem cells in vitro and in vivo.

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Effect of Matrix Structure and Stiffness on Subcellular Viscoelastic Properties of Tumor Cells in 2D and 3D Matrices

Muhammad Zaman
Assistant Professor
Biomedical Engineering, University of Texas at Austin

Erin Baker
Graduate Student
Biomedical Engineering, University of Texas at Austin

Tumors exhibit elevated stiffness compared to normal tissue, and some aspects of tumor cell invasive ability are in part governed by extracellular matrix (ECM) stiffness. Yet neither the relationship between ECM stiffness and intracellular mechanical properties, nor that between intracellular mechanical properties and invasive ability, is well understood. In order to establish these relationships quantitatively, we employ particle-tracking microrheology to investigate the intracellular viscoelastic properties of single cancer cells that are attached to two-dimensional (2D) substrates, as well as those that are embedded within three-dimensional (3D) matrices. While particle-tracking rheological protocols have been established, these techniques have yet to be applied in linking the cytoplasmic mechanical environment of cancer cells to their invasive ability. Specifically, the intracellular mechanical properties of elasticity, viscosity, and compliance of human prostate cancer (PC-3) cells and transformed human breast cancer (MCF-10A) cells of varying invasive ability are extracted from Brownian motions of individual 1.0?m polystyrene spheres that are ballistically delivered to their cytoplasm. Results indicate that the cytoplasmic mechanical environment of PC-3 cells attached to a 2D substrate is non-homogenous, independent of matrix stiffness. Furthermore, the heterogeneously varying intracellular viscoelastic properties show a strong correlation with tumor invasiveness as well as matrix chemistry and mechanical architecture. Finally, our results show that sub-cellular mechanical properties vary significantly between 2D and 3D environments suggesting a quantitative basis for the observed differences in migration of tumor cells cultured in 2D and 3D.

Synthetic Stem Cell Niche for *In Vitro* Spermatogonial Stem Cell Culture

Hyunjoon Kong
Department of Chemical and Biomolecular Engineering, University of Illinois

Cathy Chu
Graduate Student
Department of Chemical and Biomolecular Engineering, University of Illinois

John Schmidt
Graduate Student
Department of Chemical and Biomolecular Engineering, University of Illinois

Kay Carnes
Research Specialist
Department of Veterinary Biosciences, University of Illinois

Zhen Zhang
Postdoctoral Researcher
Department of Veterinary Biosciences, University of Illinois

Marie-Claude Hofmann
Department of Veterinary Biosciences, University of Illinois

Stem cells are increasingly studied for potential use in various therapies including tissue regeneration. Specifically, spermatogonial stem cells (SSCs) are attracting attention due to their potential pluripotency arising from their ability to dedifferentiate into embryonic stem cell-like cells [1]. For their successful therapeutic use, these cells first must be expanded in vitro using an appropriate culture system. We have previously shown that the mechanical stiffness and cell adhesion cues of hydrogel substrates can be engineered to control cell proliferation [2]. Therefore, we hypothesized that a hydrogel with proper biochemical and biomechanical properties may mimic the composition and structure of the native basement membrane onto which SSCs reside, thus allowing us to control SSC proliferation. This hypothesis was examined with a hydrogel containing chemically linked synthetic oligopeptides including the Arg-Gly-Asp sequence (RGD peptides). The RGD peptide density (N_RGD) and the mechanical stiffness of the hydrogel were varied to examine their effects on cell proliferation in both 2D and 3D cultures. Interestingly, cell proliferation in 2D cultures was greatly dependent on N_RGD but minimally influenced by mechanical stiffness. The N_RGD also modulated the number and size of SSC colonies formed in 3D cultures. Overall, the results of this study elucidate an important factor regulating SSC proliferation and also present a bioactive hydrogel that can be used as a 3D synthetic basement membrane. In addition, the results of this study will be broadly useful in controlling the proliferation of various stem cells and expedite the use of stem cells in clinical treatments.

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Effects of EGF-induced Matrix Proteolysis on Tumor Cell Migration in 3D Environments Arise from Increase in Cell Speed and Matrix-Dependent Increase in Directional Persistence

Hyung-Do Kim
Biological Engineering, Massachusetts Institute of Technology

Tiffany W. Guo
Biological Engineering, Massachusetts Institute of Technology

Angela P. Wu
Biological Engineering, Massachusetts Institute of Technology

Frank B. Gertler
Professor
Koch Institute for Integrative Cancer Research, Massachusetts Institute of Technology

Douglas A. Lauffenburger
Professor
Biological Engineering, Massachusetts Institute of Technology

Activation of epidermal growth factor receptor (EGFR) and the resulting enhanced motility play a critical role in tissue invasion by a variety of solid tumor types. In particular, EGFR ligands have been demonstrated to increase tumor invasiveness via induction of matrix metalloproteinases (MMPs). However, the biophysical premise of this effect on the various aspects of cell migration has not been examined in detail. In this study, we quantitatively analyze cell tracks obtained from 3D real-time images of tumor cells in varying concentration of 3D collagen matrices upon EGF stimulation. We find that EGF-induced matrix proteolysis increases cell motility and dispersion, which is mediated by an increase in cell speed and a matrix concentration-dependent increase in directional persistence. Analogous studies of cell migration on 2D substrates show that the cell-intrinsic response to EGF stimulation is to decrease directional persistence. Therefore, EGF-mediated increase in directional persistence in 3D matrices is associated with overcoming matrix confinement effected by cell-extrinsic matrix proteolysis. Modulation of matrix proteolysis activity shows that it indeed correlates with directionally persistent movement. We conclude that the biophysical effect of EGF-induced matrix proteolysis on the increase in 3D cell migration is critically dependent on the extracellular matrix environment.

Bioactive Microgels for Large-Scale Eukaryotic Cell Culture

Hyunjoon Kong
Department ofChemical and Biomolecular Engineering, University of Illinois

John Schmidt
Graduate Student
Department of Chemical and Biomolecular Engineering, University of Illinois

One of the critical components for successfully using stem and progenitor cells in clinical treatments is a large-scale cell culture technology, which regulates the diverse cellular activities (i.e. growth, death, and differentiation) in a sophisticated manner. Currently, dextran and collagen-coated dextran microcarriers are used as the cell adhesion substrates on an industrial scale, because they significantly increase the ratio of the surface area for cell adhesion to the volume of bioreactors. However, currently commercialized microcarriers present several limitations, such as the use of organic solvents in preparation of microcarriers, limited control of biological function, and difficulty in the cell isolation from the microcarriers following the completion of cell culture [1]. Previously, we have demonstrated that chemical and mechanical properties of calcium cross-linked polysaccharide hydrogel modified with oligopeptides containing Arg-Gly-Asp sequence (RGD peptides) is able to regulate proliferation rate and differentiation level of cells adhered to the hydrogel disk surface [2,3]. We hypothesized that processing of these calcium cross-linked alginate hydrogels as microgels would allow us to control the cell proliferation and differentiation on a large scale and readily collect the cells from the microgels through the dissolution of gel matrices in aqueous environment. This hypothesis was examined with RGD peptides-presenting calcium cross-linked alginate microgels with diameters ranging from 300 to 700 m. The density of RGD peptides was varied by mixing unmodified alginate molecules and RGD peptides-presenting alginate molecules at different ratios. The mechanical stiffness of the gel was controlled with the cross-linking density. We tested both bone precursor cells (MC3T3-E1 presoteoblasts) and bone marrow-derived mesenchymal stem cells. We found that the proliferation rate and the differentiation level of the cells were significantly controlled with these material variables on a large scale. In addition, a process to collect the expanded cells through the dissolution of microgel matrices with citric acid did not affect cell viability. Overall, the results of this study present a unique cell culture device, which allows one to control the proliferation rate, differentiation level and cell recovery on a large scale. The results of this study will be widely useful in culturing a broad array of stem and progenitor cells within a bioreactor with limited volume and thus greatly benefit the use of cells in various therapeutic interventions.

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Mechano-chemical Coupling in the Adhesion of Thin Structures to Surfaces with Topography

Richard Springman
Department of Mechanical Engineering, University of Pennsylvania

Dr. John L. Bassani
Department of Mechanical Engineering, University of Pennsylvania

The mechanical and chemical equilibrium fields of adhered cells in both in-vivo and in-vitro micro-environments are coupled through interactions that depend on the local concentrations of certain chemical species (e.g. integrins) and on the local separation of the cell-cell or cell-substrate interface. An adhesive law capturing these dependencies in the presence of mobile species of both strengthening and weakening type is used to study the adhesion of shells to a rigid substrate with surface topography, which is the model system for cell adhesion in 3D micro-environments. The adhesive species, which are confined to the shell surface, are assumed to form an ideal solution with spatially-varying concentrations at equilibrium. Nonlinear shell kinematics accounting for finite rotations of both closed spherical shells and open spherical caps are coupled with the equilibrium equations for axisymmetric deformations and with linearly elastic material response. Surface topography is shown to alter the equilibrium configurations and to determine the distributions of chemical species. Deep and closely spaced surface features result in shell configurations that bridge across the topological features resulting in highly nonuniform species distributions. In addition to understanding in-vivo cell adhesion, which almost always involves 3D surface topography, understanding how surface features affect equilibrium is crucial for the engineering of scaffolds used to support the growth of cells.

The Fly Eye: A Biomechanics Model for Understanding Tissue Morphology

Sascha Hilgenfeldt
Mechanical Science and Engineering, University of Illinois

Ian Gemp
Mechanical Engineering, Northwestern University

Richard Carthew
BMBCB, Northwestern University

Cells in differentiated tissues have to occupy specific positions and take on specific shapes in order to function properly. The complex shapes of epithelial cells in the invertebrate compound eye show a particularly low tolerance for shape deviations. We study the morphology of tissue in the Drosophila retina, which is crucially dependent on the expression of adhesion molecules (cadherins) [1].

We show that not only the overall tissue organization, but the shape of each individual cell can be understood through quantitative biomechanical modeling using minimization of an interfacial energy functional, without explicit reference to active biological processes in the bulk of the cells. The model contains only two free parameters, encoding for the adhesion strengths of Drosophila E- and N-cadherin, and reproduces interfacial angles and lengths to within the experimental accuracy of a few percent [2]. The model is validated through the observation of characteristic morphological changes in mutant ommatidia. These changes are faithfully represented within this approach and yield important insights into the role of spatial and temporal variations of cadherin expression during morphogenesis.

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Substrate Mechanics and Chemistry Modulate the Balance between Endothelial Cell-Cell and Cell-Matrix Adhesion

Cynthia Reinhart-King
Cornell University

While the effects of extracellular matrix chemistry have been well-studied, the role of substrate mechanics has only recently become of an area of intense interest. It is now well-known that substrate mechanics can alter many fundamental cell functions including cell adhesion, migration, contractility and gene expression. Using well-defined deformable polyacrylamide substrates, we have recently found that cells can communicate mechanically through compliant substrates by exerting traction stresses that alter the strain field beneath adjacent cells. Given a substrate that is sufficiently compliant to permit the transmission of a strain field far from the transmitting cell's edge, mechanical communication can increase cell-cell adhesion by drawing cells together and increasing the stability of cell-cell adhesion between communicating cells. On softer substrates, where cells are less spread, cells tend to adhere to each other whereas on stiffer substrates, cells prefer to adhere and migrate on the substrate. We have recently extended these studies to explore the synergistic effects of substrate compliance and chemistry on the balance between cell-cell and cell-matrix adhesion. Our results indicate that decreasing the strength of cell-matrix adhesion by altering substrate mechanics or chemistry increases the stability of cell-cell adhesion. These changes in cell-cell adhesion result in increased endothelial cell aggregation and the formation of cellular networks. Our data underscore the importance of substrate mechanics in mediating the balance between cell-cell and cell-matrix adhesion and help to define material parameters that can enhance tissue formation on well-controlled biomaterial surfaces.

Substrate Elasticity Influences Bone-Like Matrix Deposition in Low-Density Mesenchymal Stem Cell Cultures but Not in Confluent Cultures

Amy Wagoner Johnson*
Assistant Professor
Mechancial Science and Engineering, University of Illinois
ajwj@illinois.edu

Michael Poellmann
Research Assistant
Bioengineering, University of Illinois

Cytoskeletal tension, or prestess, is a key determinant of cell behavior. Substrate elasticity has been shown to affect the differentiation of widely-spaced mesenchymal stem cells through a mechanism dependent on prestress. Differentiation towards an osteoblastic lineage occurs on substrates with elasticity similar to the extracellular matrix in newly-forming bone [1]. However, cells in high-density cultures and in natural tissue maintain prestress through interactions with neighboring cells in addition to the matrix. We investigate the influence of both cell-cell adhesions and cell-matrix adhesions on the stiffness and differentiation of D1 ORL UVA mesenchymal stem cells. Differentiation of cultures kept at low density with mitomycin-c is strongly dependent on substrate elasticity, while confluent cultures are not as affected by the substrate. The elastic modulus of cell cultures is measured with an atomic force microscope and elasticity of mitomycin-treated cultures are compared to that of confluent cell monolayers. We hypothesize that upon reaching confluence, cells maintain a desired prestress through interactions with neighboring cells and with newly-synthesized matrix rather than by interaction with the substrate.

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Model of Force Generation in a Self-Assembling Toroidal Cluster of Cells

Asha Nurse
Graduate Student
Division of Engineering, Brown University

L. B. Freund
Professor of Engineering
Division of Engineering, Brown University

We describe a model of an experiment in which a suspension of human fibroblast cells is placed in a vertical cylindrical chamber of submicron diameter. That mean mass density of the cells is slightly larger than the solvent in which they are suspended. Instead of being the flat end of the cylinder, the bottom of the chamber is contoured to have an axially symmetric conical pillar extending upward. Gradually, the cells fill the annular trough at the base of the pillar and begin to interact with each other, forming a toroidal cluster. Somewhat surprisingly, the cluster will then proceed to climb the pillar against the force of gravity. We presume that the configurational driving force of the described phenomenon arises from cell interactions and we utilize a mathematical model to gain better understanding of the physical effects which account for the force. The system is modeled by a torus on a cone with a known apex angle and with axis of symmetry in the vertical direction. Due to an excess surface energy, the free energy of the system can be reduced by a reduction in surface area of the torus. This configurational force pushes the torus upward on the pillar, against the force of gravity Assuming that the cells on the surface of the cluster rearrange through surface diffusion, we derived ordinary differential equations that describe the evolution of the system. The solution of these equations provides information on the magnitude of the surface energy effect in terms of physical parameters and direct observation of the process in the laboratory.

Composite Diaphragm Inflation: Probing the Mechanobiological Functions of Desmosomes and Intermediate Filament Networks within a Living Normal Human Epidermal Keratinocyte Sheet

John Selby*
Department of Mechanical Science and Engineering, University of Illinois
jcselby@uiuc.edu

Mark A. Shannon
Department of Mechanical Science and Engineering, University of Illinois

Normal human epidermal keratinocytes (NHEKs), like most all nucleated human cells, possess a filamentous cytoskeleton, composed of microfilaments (MFs), microtubules (MTs), and intermediate filaments (IFs). Distinct from connective tissues cells like the dermal fibroblast, NHEKs in vivo are organized as a multicellular epithelium, a tissue construct that contains primarily cells and only scant extracellular matrix material. As they stratify and differentiate outwards towards the stratum corneum, the structural integrity of NHEKs is thought to be maintained through the formation of cell-cell desmosomes that interconnect pancytoplasmic networks of IFs within individual cells. Although IFs and desmosomes have been implicated in the pathology of various blistering skin diseases [1], the biophysical mechanisms by which these cytoskeletal structures help provide the epidermis an innate mechanical resilience are, at present, not fully understood.

In recent work [2-4], we have developed a new methodology for the exploration of keratinocyte mechanobiology, referred to as the technique of composite diaphragm inflation (CDI). Sheets of living NHEKs were reconstituted in vitro on tensed but highly compliant, freestanding polydimethylsiloxane (PDMS) elastomer membranes, 5.0 mm in diameter and 10.0 microns thick. NHEK-PDMS composite diaphragm (CD) specimens were then subjected to a series of quasi static axisymmetric inflation tests to examine the mechanobiological response of the epithelial sheet to physiologically severe deformations (~50% nominal polar biaxial strains). During the initial sequence of inflation tests, NHEK sheets exhibited rheological behaviors that were suggestive of a markedly dissipative viscoelastic-plastic stress response. However, following a period of quiescent culture, NHEK sheets were observed to recover at least 80% of their original ability to store elastic strain energy, evidence of biological adaptation and recovery or restitutio ad integrum. Although far from conclusive, these findings seem to support the idea that integrated networks of IFs may have both structural and mechanosensory functions in epithelial tissues subject to large deformations [5].

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The Thermodynamics and Kinetics of Focal Adhesion Dynamics

Krishna Garikipati
Department of Mechanical Engineering and Michigan Center for Theoretical Physics, University of Michigan

Joseph E. Olberding
Graduate Student and Research Assistant
Department of Biomedical Engineering, University of Michigan

Michael D. Thouless
Departments of Mechanical Engineering, and Materials Science and Engineering, University of Michigan

Ellen M. Arruda
Department of Mechanical Engineering, and Program in Macromolecular Science and Engineering, University of Michigan

The free energy that drives growth, resorption and sliding of focal adhesions includes mechanical and chemical contributions. We have identified a competition among four effects that control focal adhesion dynamics: (1) work done during addition of complexes, (2) the chemical potential inherent to focal adhesions, (3) the elastic free energy associated with deformation of focal adhesions, and (4) work done on a molecular conformational change. A theoretical treatment of focal adhesion dynamics developed in the framework of rate processes driven by hermodynamics demonstrates that the mechanisms governed by these four effects allow focal adhesions to exhibit a rich variety of behavior without the need to introduce special constitutive assumptions. In this treatment, the structural unit of focal adhesions is a complex consisting of a ligand such as fibronectin, an integrin molecule, and associated plaque proteins. The binding and unbinding of these complexes causes focal adhesion growth and resorption, respectively. The reaction-limited case is considered. Our central findings are that growth, resorption and sliding are all predicted by a very simple chemo-mechanical model. Sliding requires symmetry breaking and is achieved via (1) above, (4) promotes symmetric growth, and (2) and (3) cause symmetric desorption. The role of kinetic modulation is also examined.

Measuring the Surface Adhesion of Cancer Cells: A Novel Way to Characterize and Understand Cancer Metastasis

Xin Tang
University of Illinois

Tony Cappa
University of Illinois

Theresa B. Kuhlenschmidt
University of Illinois

Mark S. Kuhlenschmidt
University of Illinois

Taher A. Saif
University of Illinois

Cancer deaths are mostly caused by metastasis of malignant cells, not by the tumor itself [1]. During metastasis cancer cells detach from the primary tumor, spread to different body locations via lymph system or blood circulation, reattach to invade the target organs and form the secondary malignant tumors [2]. It is clear that the adhesivity plays a crucial role throughout the metastasis process. In this project, we hypothesize that cancer cells manage their invasion by changing their surface adhesivity. Here, we develop a novel and a versatile microelectromechanical systems (MEMS) sensor [3] to measure the adhesivity between living cancer cells and a probe. The Silicon sensor consists of a probe with cross section: 5 um x 7.7 um, and 2 flexible cantilever beams with dimension: 2.1 um x 7.7 um x 3 mm. The probe is used to contact the cell and the flexible beams are used to measure the cell force response in the range from nN to uN. The spring constant of the sensor is 14.4 nN/um. The probe approaches the cell horizontally and remains in contact with it for 10 seconds. The probe is then pulled back when the cell force is measured from the deflection of the MEMS, which is measured from optically. Our preliminary results demonstrate that the aggressive HCT-8 cells (from human colon adenocarcinoma) and less aggressive Caco-2 cells (from human colon carcinoma) have significantly higher adhesivity compared to the control MA104 cell (normal monkey kidney cells) does.

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Adhesion Site Dynamics and Cytoskeleton Multi-compartmental Response Revealed by Transient Bead Twisting: Magnetic Twisting Cytometry Revisited

Daniel Isabey
Faculty of Medicine, INSERM

Sophie Féréol
Faculty of Medicine, INSERM

Gabriel Pelle
Faculty of Medicine, INSERM

Redouane Fodil
Faculty of Medicine, INSERM

Bruno Louis
Faculty of Medicine, INSERM

Inserm UMR 841 and University Paris 12, Cell and Respiratory Biomechanics Group, Faculty of Medicine

Magnetic Twisting Cytometry (MTC) is nowadays a well-established micromanipulation technique to measure the mechanical response of living cells for increasing transient loadings [1][2]. MTC basically uses RGD-coated ferromagnetic microbeads which act as small extracellular matrices attached to transmembrane mechanoreceptors of the integrin-type, transmitting to the cytoskeleton a complex 3D-stress through transient torque application [3]. The present approach is based on theoretical considerations issued from protein mechanics [4], MTC experiments performed on various types of living cells and analyzed during transient loading and relaxation with various multi compartmental models [5] [6]. We presently consider that the first few seconds of time response to transient torque advantageously reflect the maturity state of the various types of bead-cell adhesion sites: immature adhesion sites (slip bonds), fully mature adhesion sites (catch bonds) and an intermediate state corresponding to a torque-dependent slip-catch transition. The short term cell response can advantageously be used to characterize the adhesion dynamics which appears cell specific, while the longer term cell response with fully mature adhesion sites permits an improved assessment of viscoelastic properties of cytoskeleton compartments. Overall, the present results confirm the interest of taking into account the role of adhesion site dynamics in the transient cell response and question the meaning of cytoskeleton dynamic compartments.

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Molecular Mechanism of the Multi-power Law Behavior of Living Cells

Farhan Chowdhury
Department of Mechanical Science and Engineering, University of Illinois

Sungsoo Na
Department of Mechanical Science and Engineering, University of Illinois

Olivier Collin
Department of Mechanical Science and Engineering, University of Illinois

Bernard Tay
Department of Mechanical Science and Engineering, University of Illinois

Fang Li
Department of Mechanical Science and Engineering, University of Illinois

Tetsuya Tanaka
Department of Animal Sciences, University of Illinois

Deborah Leckband
Department of Chemical and Biomolecular Engineering, University of Illinois

Ning Wang
Department of Mechanical Science and Engineering, University of Illinois

All living cells show an atypical behavior, unlike traditional materials, in response to varying forcing frequencies. Some have proposed a soft glass rheology model to explain the weak power law of living cells and concluded that cell rheology is timescale free [1-2]. However, a recent report shows that cell rheology depends on the timescale of mechanical loading: a multi-power law behavior of living cells emerges at physiologically-relevant loading frequencies [3]. The molecular mechanism of the multi-power law behavior is not clear. We used molecular dynamics simulations of non-covalent protein-protein interactions [4] to demonstrate that multi-power laws could originate from nonequilibrium to equilibrium transition. These theoretical analyses remarkably predicted rheology from embryonic stem cells (ESCs) to differentiated cells. A weak power law exponent alpha1 emerged in the short time scale (<1 s) whereas a strong power law exponent alpha2 dominated in the long time scale region (>10 s). The ESCs were softer and showed a higher alpha1 than the differentiated cells. By introducing an equilibrium frequency feq, all modeling data and cell experimental data collapsed into two power laws separated by f/feq being unity. These findings suggest that the timescale-dependent rheology in living cells originates from dynamic responses of force-driven transition from nonequilibrium to equilibrium.

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Force Spectroscopy of Primary Alveolar Epithelial Type II Cells

Esra Roan
Research Assistant Professor
Department of Mechanical Engineering, University of Memphis

Catherine Cozad
Department of Biomedical Engineering, University of Memphis

Christopher M. Waters
Professor and Vice Chair
Department of Physiology, University of Tennessee Health Science Center

Lynn Crosby
Postdoctoral Fellow
Department of Physiology, University of Tennessee Health Science Center

The lung alveolar epithelial lining forms a barrier in the lung where inhaled oxygen is diffused into the blood during the breathing cycle. During respiration cells residing on this lining experience significant mechanical loads, which may increase during injury due to overdistention of air-filled regions adjacent to fluid-filled regions. Two types of alveolar epithelial cells form the epithelial lining, type II (AT2) cells and type I (AT1) cells. AT2 cells have been shown to respond to lung injury by differentiating into alveolar epithelial type I (AT1) cells [1]. This indicates a dependence of the AT2 cells' phenotype on their mechanical environment, which is the motivation for the mechanical analysis of AT2 cells. The Atomic Force Microscope (AFM) can be used as an instrument to evaluate the mechanical properties of AT2 cells under physiological conditions [2]. Previously, magnetic twisting cytometry was used to study the properties of AT2 cells [3]. Here, an AFM was used to perform force spectroscopy measurements with conical shaped cantilever probes (stiffness range within 0.05 N/m and 0.12 N/m). The AT2 cells were harvested from Sprague Dawley rats and cultured in Dulbecco's modified Eagle's medium then seeded on glass coverslips and cultured over two days. Force spectroscopy measurements were taken over a scan size of 50 μm by 50 μm at a resolution of 4.55 μm per scan at a probe indentation velocity of 1.03 μm/sec. Using the Hertzian mechanics approach for a conical indenter, the Youngs modulus for the AT2 cells was computed by averaging of all curves. The average Young's modulus for AT2 cells at two days post-harvesting was 815.25 Pa ±246.74Pa. This result is greater than the previously reported Young's modulus of 45 Pa measured using magnetic twisting cytometry (calculated from shear modulus assuming incompressible) [3], which may be attributed to the differences in experimental modalities.

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Micromechanical Modeling of Cell Cytoskeleton

H. Jerry Qi
Department of Mechanical Engineering, University of Colorado

Sitikantha Roy
Postdoctoral Research Associate
Department of Mechanical Engineering, University of Colorado

Semiflexible polymer network, such as cell-cytoskeleton, differ significantly from their flexible counter-part in the deformation energy storage mechanism. As a result, the network elasticity is governed by both enthalpic and entropic variations. In addition, the enthalpic effect shows two predominantly distinct regimes of energy storage mechanism, affine regime and non-affine regime. Recently some computational models, based on finite element analysis of the actual network, such as Mikado Model, were used to demonstrate the basic physics involved in the mechanical deformation of semiflexible network. These models are computationally expensive and it is very difficult, if not impossible to develop a macroscopic constitutive relation based on them. In the present paper, we are proposing a constitutive model (stress-strain relation) for a 2D semiflexible random network. We idealize a semiflexible network through a unit-cell representation, consisting of four semiflexible main chains and four equivalent springs. The unit cell representation captures the actual network's distinct elastic energy storage mechanisms under the externally applied deformation field. The transition from non-affine (bending dominant) to affine (axial stretching dominant) is captured through the change of the relative positions of joints of the four chain, which also correspond to the crosslinking density. The current model provides a model frame to develop efficient continuum constitutive models of cytoskeleton in the future.

A Coarse-Grained Model for Biomembranes

George Lykotrafitis
Postdoctoral Fellow
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Ju Li
Department of Materials Science and Engineering, University of Pennsylvania

Sulin Zhang
Department of Engineering Science and Mechanics, The Pennsylvania State University

Subra Suresh
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Biomembranes play a vital role in the structural integrity and function of cells and their organelles. They are constituted mostly by a wide variety of lipids and protein molecules which form bilayers. Biological membranes are essentially two-dimensional fluids embedded in a three-dimensional space and they resist bending but they cannot sustain in-plane shear deformation whereas the lipids and most of the proteins diffuse freely in the membrane's plane.

Computer models have been intensely used to study aspects of the structural and functional behavior of lipid bilayers at the nanometer scale. Fully atomistic models are mostly limited to the study of a few hundred lipids for a period of a few nanoseconds [1]. In order to bridge the gap between simulations and experiments which probe the structure and dynamics of membranes on longer length and time scales, simplified particle-based coarse-grained models were developed in the past few years [2-5].

We propose a very efficient solvent-free membrane model which represents a group of lipids molecules as one particle with a diameter equivalent to the width of a lipid bilayer. The particles are equipped with an internal director degree of freedom that allows us to define an anisotropic effective pair potential leading to a formation of a two-dimensional fluid sheet. The proposed model greatly improves the attainable maximum length and time scales and it reproduces the essential mechanical features of fluid membranes. The model can be employed in the investigation of the physical behavior of vesicles, for example vesicle adhesion and spontaneous vesicle formation. It can be also used in the modeling of large length and time scale cell functions such as nanoparticle endocytosis.

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Multimodal Perturbation of Intracellular Calcium Using Dorsal Cell Adhesion

Warren Ruder
Graduate Student Researcher
Department of Biomedical Engineering, Carnegie Mellon University

James Antaki
Department of Biomedical Engineering and Computer Science, Carnegie Mellon University

Philip LeDuc
Department of Mechanical and Biomedical Engineering, and Biological Sciences, Carnegie Mellon University

The cell's chemical and mechanical milieu provides a range of stimuli that must be effectively integrated into intracellular signaling events for the regulation of cell function and physiology. Calcium is a ubiquitous messenger responsible for governing cell processes ranging from muscle contraction to gene transcription[1]. To examine calcium response to both purinergic (P2Y) stimulus and mechanical perturbation through mature, dorsal focal adhesions, we cultured NIH 3T3 cells overnight within our quasi-3D (Q3D) culture environment, consisting of ordered polypropylene microscaffolds constructed over coverglass and mounted into an open-bath perfusion chamber. The Q3D system represents a new technology capable of inducing more physiological cell morphology, similar to 3D culture environment, but confining the cell to a single focal plane for imaging. The scaffold encompasses a 3-6 micron gap size, previously shown to allow dorsal cell attachment[2]. We found cells formed more physiological, stellate/dentritic morphologies when attached between the glass and fiber compared with the typical laminar morphology observed with fibroblasts cultured on glass. For calcium imaging, cells were loaded with Fluo-4-AM, and imaged with 150 ms exposures every 5 s. Both 100 microM ATP (using continuous flow perfusion) and 10 micron dorsal-bound fiber shift (using a micromanipulator) were applied as stimuli to measure purinergic and mechanical responses, respectively. Our initial results indicate that cells can frequently produce robust calcium spikes in response to G-protein coupled receptor (GPCR) initiated stimuli, reset their spatiotemporal calcium signal, and subsequently respond to mechanical stimulation (n = 7 cells), providing evidence that the Q3D system allows for the rapid manipulation of chemical milieu as well as the mechanical environment through stretching of mature focal adhesions of stellate fibroblasts cultured in vitro.

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TRPV4 Channels Mediate Mechanical Control of Integrin Activation and Angiogenesis

Charles Thodeti
Department of Vascular Biology/Surgery, Harvard Medical School/Childrens Hospital, Boston

Donald Ingber
Department of Vascular Biology/Pathology/Surgery, Harvard Medical School/Childrens Hospital, Boston

Mechanical forces govern the orientation of vascular endothelial cells and control the direction of capillary outgrowth during angiogenesis; however the mechanotransduction pathway responsible for these responses remains unknown. Here we show that cyclically stretching capillary endothelial (CE) cells adherent to flexible extracellular matrix (ECM) substrates activates mechanosensitive TRPV4 ion channels that, in turn, stimulate phosphatidyl inositol-3-kinase (PI3K)-dependent activation and binding of additional beta1 integrin receptors, which promotes cytoskeletal remodeling and cell reorientation. Inhibition of integrin activation using blocking antibodies and knockdown of TRPV4 channels using specific siRNA suppress cyclic strain-induced CE cell reorientation, and TRPV4 knockdown inhibits angiogenesis in ECM gels. Thus, mechanical forces that physically deform ECM may guide angiogenesis through an 'integrin to integrin' signaling mechanism that is mediated by force-induced activation of mechanically-gated TRPV4 ion channels on the cell surface.

Stress-Induced Direct Src Activation Is Dependent on Microtubule Deformation

Sungsoo Na
Postdoctoral Research Associate
Department of Mechanical Science and Engineering, University of Illinois

Olivier Collin
Postdoctoral Research Associate
Department of Mechanical Science and Engineering, University of Illinois

Farhan Chowdhury
Graduate Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Bernard Tay
Graduate Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Mingxing Ouyang
Postdoctoral Research Associate
Department of Bioengineering, University of Illinois

Yingxiao Wang
Department of Bioengineering, University of Illinois

Ning Wang
Department of Mechanical Science and Engineering, University of Illinois

It is generally believed that similar to soluble ligand-induced signal transduction, mechanotransduction initiates at the local force-membrane interface (e.g., at focal adhesions) by inducing local conformational changes or unfolding of membrane-bound proteins, followed by a cascade of diffusion-based or translocation-based signaling in the cytoplasm. Recent reports demonstrate force-induced dynamic changes in Src activity [1], mechanical extension of the Src family kinase substrate p130Cas [2], and forced unfolding of proteins in living cells [3]. However, all published reports, including past studies with the reporter type of construct extended here [1], were limited in timescale. Therefore, it has not been possible to compare early dynamics of mechanotransduction with that of soluble ligand-induced signal transduction. Using a FRET-based cytosolic Src reporter in a living cell, we quantified changes of Src activities as a local stress via activated integrins was applied. The stress induced rapid (<0.3 s) activation of Src at remote cytoplasmic sites, which depends on the cytoskeletal prestress. In contrast, there was no Src activation within 12 s of soluble epidermal growth factor stimulation. Nanometer scale cytoskeletal deformation analyses revealed that the strong activation sites of Src by stress colocalized with large deformation sites of microtubules. Our findings suggest that microtubules are essential structures for transmitting stresses to activate cytoplasmic proteins by inducing conformational changes.

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Microstructure and Properties of Natural and Synthetic Biomaterials, Biocomposites, and Interfaces

ORGANIZERS:

Amy Wagoner Johnson, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Brendan Harley, *Department of Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign*

SYMPOSIUM I

A Structural Constitutive Model for Electrospun Scaffolds for Soft Tissue Engineering

Michael Sacks
W.K. Whiteford Professor
Bioengineering, University of Pittsburgh

Synthetic scaffolds for cardiovascular tissue engineering applications require mechanical properties comparable to the native tissue for at least the minimum time necessary for the seeded cells to lay down an equivalent supporting matrix. To achieve maximal results in the scaffold design process, it is beneficial to know and control specific scaffold characteristics that may alter the mechanical properties of the scaffolds so that a minimal amount of parameters could be changed to achieve the characteristics of the desired scaffold (i.e for isotropic, moderately anisotropic, or highly anisotropic tissues). One familiar characteristic in electrospun scaffolds is fiber tortuosity, which is analogous to collagen crimp in soft tissues. One can delay the onset of scaffold stiffness by controlling the degree of tortuosity and the fiber angles at which the tortuosity is more (or less) prominent. A constitutive model that incorporates the effects of these scaffold characteristics, and that can predict the response of the scaffold without having to perform time-consuming mechanical tests, would assist in the design of the scaffold and allow for more expediently-designed and predictable custom-tailored scaffolds. In this study, we extended our previous research with electrospun poly ester (urethane) urea (ePEUUs) scaffolds to incorporate the effects of fiber tortuosity on the mechanical response of the scaffolds. We also developed a constitutive model that is dependent not only on fiber angle but also on the fiber tortuosity with respect to fiber angle. The methods used to develop the ePEUU scaffolds have previously been reported [1]. Biaxial testing was performed on the ePEUUs to determine the mechanical properties of the scaffolds. The procedures for biaxial testing have been previously reported [1]. To determine the degree of alignment for the scaffolds, SEM images were obtained for the various spin speeds and analyzed using a custom image analysis software routine written in MATLAB. Several images were taken for each spin speed and then analyzed, with the resulting orientation data then being combined to determine the overall fiber orientation for the specimen. Tortuosity measures were performed on the SEM images of all unstrained scaffolds by tracking a fiber for the viewable length of the fiber. Tortuosity was calculated by dividing the full length of the fiber by the end-to-end distance of the fiber. To better understand the change in tortuosity as the scaffolds undergo deformations, a stage was designed that allowed the scaffold to be stretched and imaged using SEM. The PEUU effective fiber stress-strain properties were determined from the mechanical data using, where Sf is the 2nd Piola-Kirchhoff fiber stress, K is the fiber elastic modulus and D(x,theta) is the statistical distribution accounting for the fiber recruitment. D(e,theta) is a function of the fiber strain e and orientation theta, with the strain itself a function of fiber angle, since it was found that tortuosity varies with angle as the mandrel speed increases. The structural and mechanical data were then combined to determine the Lagrangian membrane stresses. Using the structural data, R(theta), and a single equibiaxial test for the determination of the fiber stress-strain response, the model allows one to predict the complete biaxial mechanical response of the scaffold.

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Constitutive and Fracture Behavior of a Soft Biogel, Agarose

H.J. Kwon*
Postdoc
Division of Engineering and Applied Science, California Institute of Technology
hkwon@caltech.edu

C. Kovalchick
Graduate Student
Division of Engineering and Applied Science, California Institute of Technology

G. Ravichandran
Professor
Division of Engineering and Applied Science, California Institute of Technology

Agarose gels are excellent model biomaterials because of their structure having appropriate range of pore diameters. They are also widely used for cultivating micro-organisms such as cells for investigating cell-matrix interactions. However, the mechanical properties, especially under tension, have been poorly understood, which is partly attributed to the difficulty in measuring deformation. Very little is known concerning their fracture properties including failure strain or fracture toughness. This study has adopted digital image correlation (DIC) based on fast normalized cross-correlation algorithm to measure the deformation in the agarose gel in their hydrated condition. Since the water contained in the mesh of channels in the supercoiled structure is extravasated when the gel is deformed, speckle pattern necessary for performing DIC is hard to generate. In this study, a new surface modification technique was used to create a speckle pattern and was successfully used to measure the in-plane deformation fields and strain variations. By combining the loads measured by the load cell and the strains obtained using DIC, stress-strain relationships for various concentrations of agarose and loading rates have been determined. By considering the different resistance mechanisms involved in the deformation, a constitutive model has been proposed, and stress-strain curves predicted by the model were compared with model predictions, which show excellent agreement. To verify the measured stress-strain relationships and the constitutive equation, FEM simulations have been performed and the load-displacement curve from the simulations have been compared with the experimental curve, which also shows good agreement. The visco-elastic behavior of the agaraose gels has been determined through relaxation experiments and verified using tests at different strain rates. This study also applied DIC technique to Single-Edge-Notched-Tension (SENT) specimen to evaluate the fracture toughness (JIC) of Agarose. The measured value for 2% agarose gel is around 25 J/m^2 and is path independent. For comparison purpose, the Essential Work of Fracture (EWF) concept has been extended to visco-elastic fracture in which stress relaxation occurs around the crack tip. The measured fracture toughness using the EWF concept is in reasonable agreement with the JIC value. Key Words: Agarose, DIC, fracture toughness

Structure-Property Relationship of Single Electrospun Nanofibers

Chwee Teck Lim*
Division of Bioengineering and Department of Mechanical Engineering, National University of Singapore
ctlim@nus.edu.sg

Nanoscale biomaterials such as nanofibers have been extensively used in biomedical applications including tissue engineering, molecular filters and controlled drug delivery [1]. As these nanofibers are often subject to physical stresses during use, there is a need to ensure their structural integrity remains intact and that they do not fail.

Mechanical characerization of a single nanofiber has not been widely performed due to its small size [2]. However, such tests are important as the structural makeup and mechanical properties are found to vary significantly for nanofibers with diameters ranging from tens to hundreds of nanometers. These tests aim to help us better understand the structure-property relationship at the nanoscale. Here, we present tensile tests of single polymer nanofibers [3-5] with varying diameters performed under a scanning electron microscope where the deformation and failure modes of the nanofiber were observed. We also performed atomic force microscopy of a nanofiber undergoing stretching from elastic to plastic deformation and eventually to failure. Nanofibers are observed to consist of both crystalline and amorphous states and the amount of crystallinity will greatly affect the tensile strength of the nanofiber. Also, there was significant nanostructural rearrangement and fragmentation of the crystallites in the nanofiber during stretching. These results will help us to better relate the nanomechanical properties to the nanostructural rearrangement and makeup of the nanofibers.

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Modeling Agarose-Nanocomposite Biomaterials for Tissue Engineering Applications

Kumar Vemaganti
Associate Professor
Mechanical Engineering, University of Cincinnati

Nilesh Billade
Graduate Research Assistant
Mechanical Engineering, University of Cincinnati

Shawn Hunter
Research Director
Community Tissue Services

Currently used biomaterials for making tissue engineering scaffolds are considerably weaker than the native tissue and cannot withstand the mechanical stimuli during culture and the physiological loads in vivo. Recent developments in the nanotechnology world offer promising new materials for use in tissue scaffolds. Carbon nanomaterials, such as carbon nanotubes (CNTs) and carbon nanofibers (CNFs), are known to enhance the mechanical properties of various engineering materials. However, their applications in tissue engineering are largely unexplored, particularly for the purpose of augmenting the stiffness of the bio-scaffolds. It is also of primary importance to ascertain their biocompatibility.

This work focuses on the biocompatibility, mechanical characterization and computational modeling of agarose hydrogel scaffolds reinforced with CNFs. Biocompatibility studies are performed using cell viability tests and MTT assays. Uniaxial unconfined compression stress relaxation tests are performed on cylindrical samples of agarose gel (2% wt/vol) with 0%, 0.2% and 2.0% CNFs to determine their equilibrium response. Compressive strains are applied in increments of 5% strain up to 50% strain, followed by unloading in steps of 5% strain. The lateral expansion of the samples is measured optically by taking photographs at each equilibrium step. Results show increases in the initial shear and bulk moduli of 52.9% and 85.5% respectively for 0.2% CNF concentration, and 86.8% and 164.5% for 2.0% CNF concentration compared to the control case. It is also observed from the unloading data that the specimens display plasticity. We describe these findings and discuss the development of macro-scale computational models of these composite biomaterials. We also discuss an approach for the correction of the buoyancy force variation during the mechanical tests.

Saw-Tooth Behavior of Bio-macromolecules

Ying Wang
Mechanical Engineering, University of Florida

Youping Chen
Professor
Mechanical Engineering, University of Florida

Natural materials, like bone and abalone shell, are renowned for their strength and toughness. Both bone and shell are nanocomposite of mineral crystals and organic matrix. The abalone shell, a composite of calcium carbonate plates sandwiched between organic material, is 3,000 times more fracture resistant than a single crystal of the pure mineral. Despite centuries of work, the molecular basis of their toughness and strength remains largely a mystery. Previously, the origin of the toughness was attributed to the contribution of crystal component, explained by "microcrack" method (bone), Nano-asperity and mineral bridge model (shell). But after the atomic force microscope (AFM) pulling experiments done on the natural biomacromolecules of bone and nacre (P. K. Hansma et. al. 1999 and 2001) which exhibit so called "saw-tooth" force extension curves, it is believe that the key to bone and shell's fracture resistance resides in the polymer part. To verify this point, we present molecular dynamic simulation of collagen, lustrin A and poly-acrylic acid (PAA), which inside the bone, abalone shell and bio-mimetic materials, respectively. The force-extension curves of collagen and lustrin A show the "saw-tooth" like behavior though with slight difference. In contrast, PAA does not show the same kind of behavior. Those simulated phenomena can provide some insight about the molecular mechanism of the AFM experiments and further the toughness of natural bio-minerals.

Correlation between Atomic Force Microscope-Based Experiments and Atomistic Simulations-Based Deformation Analyses of Bone Tissue

Vikas Tomar
Department of Aerospace and Mechanical Engineering, University of Notre Dame

Ming Gan
Department of Aerospace and Mechanical Engineering, University of Notre Dame

Albert Cerrone
Department of Aerospace and Mechanical Engineering, University of Notre Dame

Devendra K. Dubey
Department of Aerospace and Mechanical Engineering, University of Notre Dame

Bone tissue is a hierarchical nanocomposite material system consisting primarily of organic (type I and II collagen and non-collagenous tissue) and inorganic (primarily calcium hydroxyapatite (HAP)) phases. It has been shown that fundamental to the strength of bone tissue are two factors: (1) the way the organic and the inorganic phases interact with each other, and (2) the way the structure of bone tissue is hierarchically organized. The focus of the reported analyses is on analyzing the above two issues using atomistic simulations based on equilibrium and non-equilibrium molecular dynamics (MD) and experiments based on atomic force microscope (AFM). Atomic force microscope is used for nanoindentation based modulus measurements for bovine tibial trabecular bone samples.

AFM based experimental measurements are correlated to the tensile, shear, and compressive deformation molecular dynamics (MD) simulations of type-I collagen (COL), HAP, and COL-HAP interfacial supercells using the NAMD package (UIUC). Besides obvious insights into the nanomechanics of COL and HAP, the analyses report the atomistic basis of the strengthening mechanism in bone. It has been well established that biological tissue show significant change in stability and entropic properties as a function of chemical environment. To investigate this issue, our simulations also report nanomechanics of COL-HA composites in three different chemical environments: vacuum, water, and calcinated water.

Geometric Confinement Governs the Rupture Strength of H-bond Assemblies at a Critical Length Scale

Markus J. Buehler
Esther and Harold E. Edgerton Assistant Professor
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Sinan Keten
Graduate Student
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

The ultrastructure of protein materials such as spider silk, muscle tissue or amyloid fibers in natural adhesives consists primarily of beta-sheets structures, composed of hierarchical assemblies of H-bonds. These H-bond assemblies form the most fundamental interfaces in these protein materials, and therefore control their macroscopic properties. Despite the weakness of H-bond interactions—intermolecular bonds 100 to 1,000 times weaker than those in ceramics or metals—these materials combine exceptional strength, robustness and resilience. We discover that the rupture strength of H-bond assemblies is governed by geometric confinement effects, suggesting that clusters of at most 3-4 H-bonds break concurrently, even under uniform shear loading of a much larger number of H-bonds. This universally valid result leads to an intrinsic strength limitation that suggests that shorter strands with less H-bonds achieve the highest shear strength. We present a quantitative analysis of our predictions with experimental results, illustrating excellent agreement of the predicted strength values with a large range of experimental data. Our results further explain recent experimental proteomics data, suggesting a correlation between the shear strength and the prevalence of beta-strand lengths in biology. We also compare our results with the characteristic dimensions of beta-helical and alpha-helical protein domains and illustrate that similar confinement effects may be the key to explain their characteristic structures. Our hypotheses are confirmed by direct large-scale full-atomistic MD simulation studies of beta-sheet structures in explicit solvent. We explain how the intrinsic strength limitation of H-bonds is overcome by the formation of a nanocomposite structure of H-bond clusters, thereby enabling the formation larger, much stronger beta-sheet structures. Our study illustrates how the formation of such hierarchical structures can lead to a manifold increase of the shear strength, while increasing their ability to undergo large deformation, explaining some of the characteristic properties of spider silk.

Utilization of Atomic Force Microscopy to Study Ligand-Receptor Binding of Immune System Molecules

Irene Chang
Graduate Student
Department of Engineering, Massachusetts Institute of Technology

Jianzhu Chen
Department of Biology, Massachusetts Institute of Technology

Subra Suresh
Dean of Engineering
Department of EngineeringMassachusetts Institute of Technology

Atomic Force Microscopy (AFM) is an extremely versatile technique that is widely used by researchers across different disciplines. The high positional precision and force resolution this technique offers open up new possibilities of applying it to studying delicate biological phenomena such as ligand-receptor binding. In this work, AFM is used to investigate the binding forces of receptors on T cells in the immune system to their ligands, peptide-conjugated major histocompatibility complexes (MHCs). Specifically, the interaction strengths of T cell receptors (TCRs) for self-peptides/MHCs are measured. Self-peptides are important immune system components that are required for 1) selecting thymocytes during T cell maturation, and 2) survival of naïve T cells and maintenance of biological functions of memory T cells in the periphery.

Binding strengths of receptor-ligand pairs are traditionally characterized by their equilibrium dissociation constants, or "affinities", which can be found using methodologies such as surface plasmon resonance and equilibrium dialysis. However, these approaches cannot directly determine the interaction force but require fitting of experimental data to mathematical models. More importantly, many self-peptides exhibit dissociation rates that are too high for their affinities to be reliably determined using the aforementioned methods.

This work looks at the interaction of TCRs of the 2C system and class I MHCs of the type H2-Kb. Soluble 2C TCRs and peptide-conjugated H2-Kb molecules are attached to functionalized AFM probes and glass substrates via heterobifunctional PEG tethers. Self-peptides that induce a range of selection outcomes in T cell maturation and functional studies are used. Force-distance curves are collected, from which the interaction forces between the receptors and ligands can be determined. Correlation of these force values to affinities is attempted based on the Bell model for receptor-ligand unbinding. This involves collecting force-distance curves with loading rates that encompass several orders of magnitude.

Theory of Swimming Filaments in Viscoelastic Media

Henry Fu
Postdoctoral Research Associate
Engineering, Brown University

Thomas Powers
Professor
Engineering, Brown University

Charles Wolgemuth
Professor
Cell Biology, University of Connecticut Health Center

The swimming of microorganisms in Newtonian fluids has been, and still remains, an active area of research. However, in many cases the natural environment which microorganisms move through are non-Newtonian fluids or even gels. For example, mammalian sperm swim through viscoelastic mucus in the female reproductive tract. In this work we focus on the swimming of filaments through viscoelastic fluids. First, the forces exerted by a viscoelastic medium in response to the swimmers motion are different from those exerted by a Newtonian fluid. The swimming shapes and speeds of flexible swimmers such as sperm result from an interplay between hydrodynamic forces and internal mechanical forces. The flagellum of a sperm cell consists of a bundle of microtubules, and is actively bent along its length by dynein motors which slide the microtubules past one another. We use a simple model consisting of two sliding filaments to describe the beating patterns which are observed in sperm flagella beating in highly viscous and viscoelastic media. We find that the swimming speed of flexible swimmers is affected both by changes to the shapes of beating patterns and nonlinear corrections arising in nonlinearly viscoelastic fluids. Second, the time-reversibility of the Stokes flow equations for low Reynolds number constrains what types of swimming motions are effective in Newtonian fluids (Purcells "Scallop theorem"). We describe how this is altered in nonlinearly viscoelastic fluids. We find that reciprocal motions with forward and backward strokes that move at different rates provides an example of a swimming strategy that is effective in nonlinearly viscoelastic fluids but not in Newtonian fluids.

Organ-Level Biomechanical Analysis of Blunt Liver Injury: Dynamic Impact Experiments on Perfused *Ex Vivo* Porcine Livers

Jessica Sparks
Biomedical Engineering, Wake Forest University School of Medicine

Jason Stammen
NHTSA Vehicle Research and Test Center

Rodney Herriott
Transportation Research Center Inc.

John Bolte IV
Injury Biomechanics Research Laboratory, The Ohio State University

Rapid increases in internal fluid pressure have been proposed as the primary mechanism of "viscous" liver injury, which is characterized by capsule lacerations or parenchymal disruption from excessive tensile or shear strains at high loading rates [1]. This form of injury is typical of liver trauma due to motor vehicle collisions. Pressure-based liver injury tolerance values could be used to evaluate liver injury risk in finite element simulations of abdominal impact events [2] and to facilitate the design of a crash dummy abdomen which assesses solid organ injury risk; however, the relation between internal pressure and organ-level liver injury is not well understood. Study objectives were (1) to develop an experimental technique to produce realistic viscous injury patterns in impacts to perfused ex vivo porcine livers; (2) to validate the technique through comparison of experimentally induced injuries with liver injury cases from the CIREN (Crash Injury Research Engineering Network) database; and (3) to quantify the relationship between impact-induced internal pressures and injury risk in ex vivo porcine livers. Excised porcine livers (n = 19) were instrumented with pressure sensors in the hepatic veins and perfused with normal saline at physiological temperature and pressures. A drop tower was used to apply blunt impact at varying velocities (3-6 m/s). Injury severity scores were assigned according to the Abbreviated Injury Scale (AIS) [3]. The relationship between peak vascular pressure and AIS score was analyzed using logistic regression. The porcine model successfully reproduced viscous liver injury, as evidenced by the remarkable similarity of injury patterns between the porcine model and liver trauma documented in CIREN cases (shallow capsular lacerations, deep lacerations, stellate lacerations, and parenchymal disruption). Peak pressure was a significant predictor of serious (AIS 3 or higher) liver injury ($p<.001$, pseudo-R square=.70). A pressure of 130 kPa (975 mmHg) was associated with 50% probability of serious liver injury in the porcine model. The results of this study support internal pressure as an indicator of liver injury risk in motor vehicle crash scenarios.

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Two Different Pathways of Abscission Stage of Cytokinesis in Bovine Pulmonary Arterial Endothelial Cells

Tawhid Ezaz
Graduate Student
Department of Mechanical Science & Engineering, University of Illinois

Huseyin Sehitoglu
Professor
Department of Mechanical Scrience & Engineering, University of Illinois

We have studied the spatial and temporal distribution of traction force of endothelial cells during the terminal stage of cytokinesis. Traction force and prestress of the cell were used as parameters to differentiate the discrete pathways the cells take during this period. This distribution of mechanical forces shows two different patterns during the abscission which indicates the dissimilarity in the underlying mechanism of the breakage of the midbody. Our results show there is a definite decreasing of traction forces of the cells when the midbody is broken by vesicle transfusion and traction force exerted by the daughter actually increases first during the separation which tears the midbody.

Biorheology of Healthy and Diseased Human Red Blood Cells

David Quinn
Mechanical Engineering, Masschusetts Institute of Technology

Sophie Wong
Biological Engineering, Masschusetts Institute of Technology

Subra Suresh
Professor
Materials Science and Engineering, Massachusetts Institute of Technology

Hereditary hemolytic disorders and foreign organisms can introduce changes to the spectrin molecular network and membrane of human red blood cells. These structural changes can, in turn, lead to altered cell shape, deformability, cytoadherence and rheology. This work aims to experimentally investigate these connections among structure, mechanics, and disease states. Specifically, we examine quantitative experimental measurements of cell deformation and rheology by recourse to optical tweezers and compare these measurements to similar measurements in the literature and in collaborative efforts using magnetic twisting cytometry (MTC) and molecular force spectroscopy. The flow behavior of healthy and diseased cells is then quantified with the aid of microfluidic channels fabricated to provide in vitro assays of capillaries in microcirculation. Both experimental techniques are performed at physiologically relevant temperatures. These experimental results for two diseases systems, plasmodium falciparum malaria and sickle cell anemia, illustrate strong connections between mechanics and disease pathology. The experimental measurements are also accompanied by detailed computational simulations, at the continuum and meso-scale levels, of cell shape, viscoelastic deformation, relaxation, and dynamics of flow through microchannels.

Cartilage Tissue Engineering on Fibrous Chitosan Scaffolds Produced by a Replica Molding Technique

Guillaume R. Ragetly
Veterinary Clinical Medicine, University of Illinois

Dominique Griffon
Associate Professor
Veterinary Clinical Medicine, University of Illinois

Brian Cunningham
Associate Professor
Electrical and Computer Engineering, University of Illinois

Gregory Slavic
University of Illinois

The biocompatibility of chitosan and its structure similarity with glycosaminoglycans make it particularly attractive as a scaffold for cartilage engineering [1]. Chitosan may be molded into fibrous scaffolds that would simulate the structural characteristics of the extracellular matrix of cartilage and promote chondrocyte functions [2]. The objectives of this study were to produce chitosan fibers varying in diameter and evaluate the potential of chitosan fibrous scaffolds for cartilage engineering.

A novel replica molding technique was developed to produce non-woven chitosan scaffolds composed of fibers measuring 4 μm, 13 μm, and 22 μm in diameter. A polyglycolic acid mesh (PGA, 13 μm diameter fibers) served as a reference group. Five million porcine chondrocytes were seeded on each of 20 scaffolds per group. Seeding controls were analyzed after 48 hours via scanning electron microscopy (SEM), DNA and glycosaminoglycan (GAG) quantifications. Constructs were cultured for 21 days prior to confocal microscopy, SEM, histology and quantitive analysis (weight, water, DNA, GAG and collagen II contents). Parametric data was compared between groups ($p=0.05$) with ANOVA and Tukey's studentized range test.

Chondrocytes maintained their phenotypic appearance and a viability above 85 % in all constructs throughout the study. After seeding, the DNA content was greater in PGA constructs and lower in chitosan constructs composed of the smallest fibers. After 3 weeks of culture, the DNA content did not differ between chitosan constructs but was greater in PGA constructs. The PGA constructs had the lowest GAG/DNA ratio (19.4 ± 3.1) and Collagen II/DNA ratio (7.5 ± 3.5) compared to chitosan scaffolds (range from 27.3 to 35.8 for the GAG/DNA and 101.4 to 110.8 for the Collagen II/DNA ratio). Although the difference was not statistically significant, the largest increase in dry weight was obtained when chondrocytes were cultured on the smallest chitosan fibers (330 ± 129) while the lowest value was obtained with the PGA mesh (250 ± 159).

Chondrocytes appear to attach preferentially to PGA than chitosan fibers, resulting in a greater cellularity of constructs produced on PGA. However, matrix production appears improved in chitosan constructs, especially when chondrocytes were cultured on smaller fibers. The differences between PGA and chitosan are more likely to result from the chemical composition rather than structural characteristics of the scaffolds. Although chitosan appears to promote matrix formation, further studies should be aimed at improving the attachment of chondrocytes.

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Mechanical Property and Biocompatibility of Poly(diol citrate) Micro- and Nano-composites for Bone Tissue Engineering

Hongjin Qiu*
Research Associate
Department of Biomedical Engineering, Northwestern University
h-qiu@northwestern.edu

Pradeep Kodali
Residency
Department of Orthopedic Surgery, Northwestern Memorial Hospital

Jason Koh
Department of Orthopedic Surgery, Northwestern Memorial Hospital

Guillermo A, Ameer
Department of Biomedical Engineering, Northwestern University

There is a significant demand for the development of bone substitutes that are bioactive and exhibit material properties that are comparable to those of natural, healthy bone [1]. In this study, POC composites containing hydroxyapatite (HA) nanoparticles or microparticles were developed and mechanical properties of bending and compression strength and modulus as well as tissue response were characterized. It was hypothesized that the composite with nanoparticles would elicit a physiological response that was different from that of its micro-HA composite counterpart. The feasibility, mechanical property and the effect of size and content of HA particles on the mechanical properties and biocompatibility were evaluated. Biocompatibility was assessed by implanting the composite in an osteochondral defect in the rabbit femur bone and evaluating the tissue by histological and histomorphometric analysis via H&E, Masson Goldner Trichrome, and von Kossa stains after 6 weeks of implantation. The nanocomposites with 60 wt. % HA have the highest bending modulus, compression modulus, and compression strength (Eb=322+/-19 MPa, Ec=328+/-20 MPa, Sc+47+/-4 MPa), suitable for the fabrication of potentially osteoconductive interference screws. Except for bending strength, the mechanical properties (strength and modulus) increased with increasing HA percentage whether nano or micro HA particles were used. All implants demonstrated favorable integration with surrounded tissue with no signs of inflammation. Both nanocomposites and microcomposites exhibited active bone remodeling and the nanocomposite induced more active bone formation at the interface relative to the microcomposite, which was affected by the particle size and HA content in the composites.

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Hydroxyapatite Scaffolds with Multiscale Porosity

Amy Wagoner Johnson
Department of Mechanical Science and Engineering, University of Illinois

Samantha Polak
Research Assistant
Department of Bioengineering, University of Illinois

Sheeny Lan
Research Assistant
Department of Materials Science and Engineering, University of Illinois

Shanna Wilson
Research Assistant
Department of Animal Sciences, University of Illinois

Matthew B. Wheeler
Department of Animal Sciences, University of Illinois

Sherrie Clark
Department of Veterinary Clinical Medicine, University of Illinois

Porosity is known to influence bone scaffold permeability and mechanical properties, as well as cell function and the type and extent of tissue ingrowth. There is general agreement that pore sizes or connections greater than 100 μm must be present to allow for growth of mineralized tissue. Pores of this size allow for cellular and vascular invasion, which are required for tissue growth and viability. More recently, research has shown that scaffolds containing a combination of macroporosity (typically defined as pore sizes >50 μm) and microporosity (pore sizes <10 μm), or multi-scale porosity (MSP), can further promote bone ingrowth.

Our work showed that bone growth in to macroporous hydroxyapatite scaffolds that also contained microporosity, was significantly greater as compared to those containing only macroporosity after 8 weeks in the lattisimus dorsi muscle of pigs[1]. Scaffolds with only macroporosity contained no bone. Further, scaffolds with MSP showed a transition in mechanical properties from brittle to bone-like after implantation.

Here we will present an extension of the intramuscular study described and show the evolution of bone growth in scaffolds implanted in porcine mandibles. Scaffolds containing MSP showed a faster rate of healing, or significantly more bone ingrowth, at 3 weeks as compared to those with only macroporosity. At 24 weeks, the volume of ingrown bone was comparable. Histological data showed evidence of organic material in the micropores after in vivo implantation, particularly in regions immediately adjacent to ingrown bone. The organic material, ingrown bone, and HA scaffold create an interconnected composite structure on both the macro- and micro- length scales, which could potentially result in significantly improved in vivo properties, such as toughness, and extend the clinical use of HA scaffolds to large and load-bearing defects. This, in turn, could improve the quality of life for millions who would receive bone grafts, or for whom grafts have been unsuccessful, and significantly decrease health care costs associated with grafting procedures.

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Scaffold and Growth Factors Induced Regeneration in Critical Size Limb Bone Segmental Defects

Iwona Jasiuk
Department of Mechanical Science and Engineering, University of Illinois

Liang Feng
PhD Student
Department of Mechanical Science and Engineering, University of Illinois

Holly Nye
Research Scientist
Department of Cell and Developmental Biology, University of Illinois

Derek Milner
Department of Cell and Developmental Biology, University of Illinois

Chunguang Xia
Department of Mechanical Science and Engineering, University of Illinois

Patrick Redwood
Department of Cell and Developmental Biology, University of Illinois

Jo Ann Cameron
Department of Cell and Developmental Biology, University of Illinois

Nick Fang
Department of Mechanical Science and Engineering, University of Illinois

We focus on a medically important problem of large bone wound healing by regeneration. More specifically, we developed a small animal in vivo load bearing model to study the effect of an artificial biocompatible polymer scaffold on regeneration of long bone segmental defects of critical size in adult Xenopus laevis frog hind limbs. One bone of the dual skeletal element tarsus bone was extirpated, and a scaffold of comparable size was implanted in situ. The skin adjacent to the intramuscular incision and scaffold was sutured and the limb was permitted to heal. The scaffolds were made of 1,6 hexanediol diacrylate (HDDA) using an innovative 3D microfabrication technology, Projection Micro Sterelithography (PμSL). The process is able to precisely and locally introduce the porosity into the scaffolds. After 6 weeks the limbs were harvested and processed for histological observation. Macrophages and lymphocytes invaded the scaffolds and no cartilage or bone formation was observed. The area previously occupied by the extirpated tarsus was filled with connective scar tissue. In contrast, a second set of scaffolds was treated with VEGF (Vascular Endothelial Growth Factor) and BMP4 (Bone Morphogenetic Protein 4) prior to implanting into the extirpated tarsus bone site. The area previously occupied by scaffold was completely filled with cartilage. Additionally, blood vessels had invaded the cartilage and bone was forming adjacent to the blood vessels. Our model sets a framework for studying and screening scaffold and growth factor combinations known to be important in bone repair by regeneration.

Bioengineered Gelatin Microspheres for Growth Factor Delivery: Improving *Xenopus laevis* Hind Limb Regeneration

Holly Nye
Research Scientist
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Derek Milner
Research Scientist
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Bingbing Li
Postdoctoral Associate
University of Illinois

Nandini Rao
Postdoctoral Associate
University of Illinois

Paul Miller
Graduate Student
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Kenneth Ringwald
Laboratory Technician
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Patrick Redwood
Laboratory Technician
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Jo Ann Cameron
Associate Professor
Cell and Developmental Biology, University of Illinois, Institute for Genomic Biology

Xenopus laevis tadpole hind limbs lose the ability to express developmentally regulated genes and to regenerate amputated limbs with increasing tadpole age. Tadpoles with fully formed limbs and significantly ossified skeletal elements are regeneration-deficient and are a good model for rapidly screening regeneration improvement techniques. Our hypothesis is that ectopic application of the protein forms of these genes, delivered by bioengineered materials, will improve tadpole hind limb regeneration. We first determined that untreated mid-tarsus amputations regenerate non-functional cartilage spikes or stumps in 95% of samples. Gelatin microspheres prepared using the emulsion solvent displacement method were soaked singly and in combination in commercially available protein solutions of Sonic Hedgehog (SHH) and Fibroblast Growth Factor 10 (FGF10). These were microinjected into amputated hind limb stumps 5 days after amputation, or injected 5 days after amputation with a second injection 12 days after amputation. Injection of either SHH or FGF10 microspheres modestly improved regeneration quality, but single and double injection of the SHH + FGF10 microspheres had the most significant beneficial effect. Regeneration of skeletal elements and muscle following mid-tarsus amputation was increased more than three-fold, compared to untreated amputations. This animal model, coupled with the use of a microsphere-based protein delivery system, provides the necessary research tools for scaling potential regeneration therapies to large animal models and preclinical trials for human digit regeneration.

Mathematical Modeling of Cortical Bone Adaptation in Rat Ulna

Iwona Jasiuk
Professor
Department of Mechanical Science & Engineering, University of Illinois

Natarajan Chennimalai Kumar
Graduate Research Assistant
Department of Mechanical Science & Engineering, University of Illinois

Jonathan A. Dantzig
Professor
Department of Mechanical Science & Engineering, University of Illinois

Charles H. Turner
Professor
Department of Orthopedic Surgery, Indiana University School of Medicine

Bone remodeling (or adaptation) is a complex biological process through which bone is formed or resorbed, depending on biochemical stimuli, such as hormones and cytokines, and mechanical stimuli. Experimental studies of Warden and Turner [1] and Robling et al [2] on rat ulna established that cortical bone remodeling depends on the applied load, the frequency of loading and time between bouts of loading. We introduce an evolution model to describe the dependence of the rate of shape change in cortical bone on the applied mechanical stimulus. This mathematical model is implemented using a poroelastic formulation and the finite element method in the commercial code ABAQUS. We generate the finite element meshes from micro-CT images of the rat ulna, using Hypermesh, a commercial meshing program. The shape change in the rat ulna due to growth/resorption process is effected by moving the position of the surface nodes of the finite element model systematically, according to the evolution model. The entire mesh is then updated based on the movement of the surface nodes. We present numerical results obtained from the coupled poroelastic finite element simulations and the evolution model. These results are compared with the experimental observations of Warden and Turner [1] and Robling et al [2], to gain insight into the mechanical stimuli that govern the process of cortical bone adaptation.

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Assessment of Plasticity in Bovine Cortical Bone during Crack Growth

Denis Torres
Research Assistant
School of Mechanical Engineering, Purdue University

Thomas Siegmund
School of Mechanical Engineering, Purdue University

Tamim Diab
Department of Anatomy and Cell Biology, Indiana University

David Burr
Department of Anatomy and Cell Biology, Indiana University

Background: Bone is a composite material that exhibits several toughening mechanisms along different length scales. In addition to the energy spent on the formation of new crack surfaces, multiple studies have shown that crack bridging, crack deflection and potentially plastic dissipation mechanisms can contribute to bone fracture toughness. The term "plasticity" is used to capture any form of irreversible deformation in the bulk bone. The degree into which these mechanisms are present is a combined function of the loading history and tissue matrix properties.

Recently, NLEFM models have been shown to accurately predict macroscopic load-displacement curves from crack growth experiments. As a result, these cohesive zone laws have been proposed as the relevant material property related to toughness. However, these models do not yet take into account microstructural details and would not predict residual or plastic deformation.

Hypothesis: Plastic dissipation mechanisms are responsible for the observed non-linear response in crack growth experiments. The influence of these mechanisms can be quantified by comparing LEFM and NLEFM predictions of the non-linear behavior during partial unloading. It is proposed that quantitative fractography profile analysis is also a measure of plasticity.

Materials and Methods: Notched cortical bovine (cow) bone beams (2.0 mm x 1.5mm) in dehydrated and wet states were loaded to fracture in a three-point bending configuration. The compliance history and the Crack Mouth Opening Displacement (CMOD) were recorded in order to estimate crack extension as a function of applied displacement. Following mechanical testing, the specimens were then analyzed using an Olympus SZX 12 optical stereo microscope and MeX 3D digital quantitative fractography software to reconstruct the fracture process and to measure surface roughness. A Cohesive Zone FEM was developed using ABAQUS 6.2 simulation package. This model accounts for friction and realistic contact boundary conditions.

Preliminary Results: Load vs. load line displacement data show clear non-linear unloading behavior and residual strains indicative of dissipative behavior. The influence of friction on dissipation was filtered. As a result the progression of bulk dissipation as a function of crack extension was obtained by comparing the NLEFM solution to the experimental data. A potential correlation between fracture surface roughness and water content was observed.

Further work will investigate if any fracture surfaces mismatch is present. If observed, this mismatch could be correlated to plastic dissipation occurring during crack extension.

Physical Imaging for Human Cortical Bone Crack Growth

Elisa Budyn
Department of Mechanical Engineering, University of Illinois at Chicago

Thierry Hoc
Department of Material Science, Ecole Centrale Paris

Julien Jonvaux
PhD Student
Department of Mechanical Engineering, University of Illinois at Chicago

A preliminary model that replicates tensional experiments in Haversian cortical bone and provides valuable information on three scales is presented. The model provides the fracture strength and the global response at the material scale, the stress-strain fields at the microscopic level and the crack profiles at the micron scale. The model creates a constitutive law at the material scale and emphasizes the influence of the microstructure on bone failure and fracture risk assessment. The model incorporates pathological modifications of the morphology and/or the mechanics of the tissue and measures their possible alteration of the microstructure integrity, in particular concerning the fracture properties that are not detectable by conventional clinical tools. The model proposes a new procedure to investigate such properties and diagnose pathologies.

Damage and Energy Dissipation in Trabecular Bone

Glen L. Niebur
Assistant Professor
Mechanical Engineering, University of Notre Dame

Rachel C. Paietta
Research Assistant
Mechanical Engineering, University of Notre Dame

Jacqueline G. Garrison
Graduate Student
Mechanical Engineering, Bioengineering Program, University of Notre Dame

Osteoporosis is a disease characterized by decreased bone density and deterioration of trabecular microarchitecture leading to skeletal fragility. The increased fracture risk of osteoporotic patients cannot be completely described by changes in bone mineral density alone [1]. Bone quality, including microdamage burden, material properties, and microarchitecture may also be a factor in fracture risk [2]. The goal of this study was to assess the relationship between trabecular architecture and microcracking during compressive failure in order to identify architectural parameters associated with microdamage and energy dissipation in trabecular bone.

Bovine tibial trabecular bone samples were studied using high-resolution imaging and mechanical testing. The microarchitecture and relative density were quantified from micro-computed tomography scans at 20 micron resolution. Specimens were then compressed along their principal mechanical axes to 7.5% strain to measure the mechanical properties. Microdamage and microfractures were stained with fluorochromes and quantified by microscopy.

The number of microcracks increased with increasing structure model index (SMI)—a measure of plate- vs. rod-like morphology—($p < 0.002$), and with increasing slenderness ratio ($p < 0.015$). There was also a trend toward a negative correlation between the number of microcracks and energy to failure ($p < 0.08$).

Microcracking is a mechanism of energy dissipation in solids. However, in porous solids, elastic and plastic strut deformation may provide greater energy dissipation. Hence, a tendency to form microcracks decreased the energy absorption during compressive loading. The relationships between microcrack density and architecture indicate that wall and strut buckling, consistent with more slender, rod-like struts, lead to microdamage formation. Taken together, the results indicate that trabecular architecture is a determinant of both energy dissipation and microcracking, providing new insight into fracture risk in osteoporosis.

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Transmenopausal Changes in the Intrinsic Material Properties of Trabecular Bone Using Nanoindentation

Benjamin J. Polly
Graduate Student
Engineering Mechanics, University of Nebraska, Lincoln

Mohammed P. Akhter
Director, Biomechanics Lab, Associate Professor
Osteoporosis Research Center, Creighton University

Joseph A. Turner
Professor
Engineering Mechanics, University of Nebraska, Lincoln

Post-menopausal osteoporosis in elderly women is characterized by an increase in bone fragility and risk of fracture. In addition to the previously documented transmenopausal decline in three-dimensional trabecular bone architecture, changes in intrinsic material properties (local stiffness and hardness) may also contribute to increased bone fragility. Nanoindentation was used to determine the transmenopausal changes of intrinsic properties in trabecular bone. Paired transilial biopsy specimens were used from a previously reported study in which bone biopsies were obtained from women on entry (pre-menopausal and >age 46), and at 12 months past the last menstrual period. Elastic and viscoelastic material properties were measured using the quasi-static and dynamic nanoindentation techniques, respectively. This work represents an ongoing collaboration between the University of Nebraska-Lincoln and the Osteoporosis Research Center at Creighton University.

Microstructure and Mechanical Properties of Mineralized Collagen-GAG Scaffolds for Bone Regeneration

Lorna Gibson
Professor
Materials Science and Engineering, Massachusetts Institute of Technology

Biraja Kanungo
Graduate Student
Materials Science and Engineering, Massachusetts Institute of Technology

Mineralized collagen-glycosaminoglycan scaffolds for bone regeneration have previously been fabricated by freeze-drying a slurry containing a triple co-precipitate of calcium phosphate mineral, type I collagen and glycosaminoglycan (GAG) [1]. Typical scaffolds made using this technique are 50 wt% mineral and have a density of 0.063±0.0015 g/cc, a relative density of 0.038±0.001, and a pore size of roughly 200 microns. The Youngs modulus and compressive strength of the scaffold are typically 1.00±0.27 MPa and 102±9.03 kPa. Previous attempts to increase the mechanical properties of the scaffold by increasing the mineral content led to scaffolds with lower mechanical properties due to the presence of defects [2]. Additional attempts to increase the mechanical properties by increasing the volume fraction of the components of the slurry have not been successful due to the difficulty in mixing the viscous slurry at higher volume fractions of the mineral, collagen and GAG.

Recently, we have developed a new technique for increasing the relative density of the scaffold that has led to improved mechanical properties. Here, we describe the microstructure (relative density, pore size, homogeneity) and compressive stress strain response (Youngs modulus, compressive strength) of mineralized collagen-GAG scaffolds with relative densities up to 0.164±0.027. We find that the Youngs modulus and compressive strength of the scaffolds made using this technique can be increased to 4.8±0.18 MPa and 655±50 kPa.

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Mechanics and Surgical Strategies for Tendon-to-Bone Repair

Guy M. Genin
Department of Mechanical, Aerospace, and Structural Engineering, Washington University

Youngjune Yoon
Postdoctoral Fellow
Department of Orthopedic Surgery, Washington University School of Medicine

Alistair J. Kent
Washington University School of Medicine

Brigitte Wopenka
Senior Scientist
Department of Earth and Planetary Sciences, Washington University

Jill D. Pasteris
Department of Earth and Planetary Sciences, Washington University

Victor Birman
Professor
Department of Mechanical Engineering, Missouri University of Science and Technology

Rosalina Das
Department of Orthopedic Surgery, Washington University School of Medicine

Stavros Thomopoulos
Department of Orthopedic Surgery, Washington University School of Medicine

Attachment of tendon to bone is an engineering feat: a millimeter-sized transitional organ called the tendon-to-bone insertion achieves a structural connection between tissues with a modulus mismatch of a factor of nearly 50. Reattachment of tendon to bone is a persistent surgical challenge. The transitional organ is not regenerated during healing, and surgical reattachment ends in a recurrence of rotator cuff tears of more than 90% in some populations. Our hypothesis is that these high failure rates are due to surgical procedures that do not account for interfacial stress concentrations. Our long-term goal is the development of grafts and surgical strategies that lead to reduced stress concentrations at the healed tendon-to-bone interface.

We have characterized structure-function relationships in the healthy tendon-to-bone insertion and found that gradations in mineral content and collagen fiber orientation combine to give the healthy tendon-to-bone transition a characteristic functional grading in mechanical properties. Results support a new organ-level physiological model of continuous tissue transition from tendon to bone. Brielfy, we observed through Raman microprobe spectroscopy a linear increase in mineral accumulation on collagen fibers that provide significant stiffening of the partially mineralized fibers above the percolation threshold. Increasing dispersion in the orientation distribution of collagen fibers from tendon to bone is a second major determinant of tissue stiffness. The combination of these two factors results in the previously reported, non-monotonic variation of stiffness over the length of the tendon-to-bone insertion, and describes how tendon-to-bone attachment is achieved in nature through a functionally graded material composition.

We will present experimental observations and mechanical models that describe how the healthy tendon-to-bone insertion transfers mechanical loads from tendon to bone, and present preliminary results of our efforts to develop surgical grafts that imbue the healing tendon-to-bone insertion with improved toughness.

Nanomechanical Property Dependence on Crystallinity in Modern and Fossilized Bone Tissues

Sara Olesiak
Graduate Research Assistant
Department of Mechanical Engineering, University of Colorado

Matthew Sponheimer
Associate Professor
Department of Anthropology, University of Colorado

Jaelyn J. Eberle
Assistant Professor
CU Museum and Department of Geological Sciences, University of Colorado

Michelle L. Oyen
Lecturer
Department of Engineering, University of Cambridge

Virginia L. Ferguson
Assistant Professor
Department of Mechanical Engineering, University of Colorado

Fossilized bone provides a unique model to explore nanomechanical properties of mineralized tissues as complex heterogeneous composite materials. The mechanical response of bio-mineralized tissues varies even at the smallest scale, where large-scale porosity and structural variation are not factors, yet other heterogeneities such as changes in mineral composition or crystallinity must contribute. The process of fossilization creates a heterogeneous geo-bio-mineralized material where variations in the mineral phase can include uptake of foreign minerals, variations in crystallinity, and dissolution or re-precipitation of authentic mineral. In modern bone, the effect of heterogeneities in crystallinity on mechanical properties is widely unknown; further, no nanomechanical properties of fossilized bone have been published. To establish the nanomechanical dependence on crystallinity, a series of bone samples, ranging from modern to 50 million years old (Ma), were investigated using nanoindentation and x-ray diffraction (XRD). Nanoindentation, performed in both longitudinal and transverse directions, revealed preservation of bone's natural anisotropy in fossilized bone. As in modern bone, the longitudinal values remained (2 to 62%) greater than transverse values. The elastic modulus values varied from 24 GPa in modern bone to 98 GPa in 50 Ma fossilized bone samples and generally increased with geologic age ($R^2 = 0.89$, $p < 0.001$). Using XRD, significant peak narrowing that occurred with increasing sample age indicated an increase in crystallinity. The nanoindentation modulus was highly dependent on the crystallinity of the sample ($R^2 = 0.65$, $p < 0.0001$), indicating that the size and perfection of the hydroxyapatite crystals has a direct effect on the material level mechanical properties of the bone. These novel data provides insight into the relationship of crystallinity and nanomechanical heterogeneities seen in bone. Understanding the interplay between structure and function of these materials will help to further explore the mechanical response of mineralized tissues and can led to the development of better biomimetic materials.

The Effects of Diets Containing 15% and 30% of Energy from Protein on Mechanical Strength of the Femur in Rats

Matthew Thorpe
Research Assistant
Division of Nutritional Sciences, University of Illinois

Rudy Valentine
Research Assistant
Department of Kinesiology and Community Health, University of Illinois

Amy Wagoner Johnson
Department of Mechanical Science and Engineering, University of Illinois

Ellen Evans
Department of Kinesiology and Community Health, University of Illinois

Donald Layman
Department of Food Science and Human Nutrition, University of Illinois

The effect of higher protein diets on bone health remains controversial. Additional dietary protein increases urinary calcium, posing a theoretical risk to bone strength [1]. However, recent work indicates these calcium losses do not originate from bone, but from improved absorption of dietary calcium [2]. Epidemiological evidence [3] and limited data from clinical trials suggest additional protein may be beneficial to bone health [4], however the independent effects of protein and other nutrients such as calcium and vitamin D are difficult to ascertain in free-living human subjects.

To test the role of higher protein diets in bone physiology in a highly controlled setting, 48 female Sprague-Dawley rats were randomized to isoenergetic diets matched in micronutrient content and providing either 30% of energy from protein and 40% from carbohydrate (PRO diet), or providing 15% of energy from protein and 55% from carbohydrate (CARB diet).

Rats were euthanized after 20 weeks, and the right femora were excised, cleansed of soft tissue, wrapped in gauze, soaked in a physiological phosphate buffer solution and frozen at -80 degrees C. At the time of testing, femora were thawed 3 hours at room temperature, imaged using dual x-ray absorptiometry, and underwent 3-point bend testing to determine work to failure, ultimate force and approximate stiffness [5]. Bone mineral density and mechanical strength parameters will be presented and their relevance to the protein—bone question discussed.

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Dependence of the Mechanical Properties of Sintered Hydroxyapatite on the Sintering Temperature

Igor Sevostianov
Associate Professor
Mechanical and Aerospace Engineering, New Mexico State University

Oleg Prokopiev
Mechanical and Aerospace Engineering,
New Mexico State University

We discuss the dependence of microstructure and mechanical properties of sintered hydroxyapatite on the temperature of sintering. Hydroxyapatite powder was prepared by the precipitation method and its purity and crystallinity were evaluated via XRD. A set of specimens was produced from this powder and sintered in conventional furnace at temperatures ranging from 1140 to 1340 °C. Elastic moduli of the specimens have been measured ultrasonically; compression strengths—on the Instron testing machine. Information about the microstructure has been derived from the measured elastic moduli and then verified by analysis of photomicrographs of shatters. It is observed that the average shape of pores transforms from strongly oblate to round at higher sintering temperatures. This transformation leads, in particular, to increased strength of the material since the stress concentration near pores is reduced.

Multiscale Modeling in Biological Problems

ORGANIZERS:

Yuliya Gorb, *Department of Mathematics, Texas A&M University*

Leonid Berlyand, *Department of Mathematics, Pennsylvania State University*

Jay R. Walton, *Department of Mathematics, Texas A&M University*

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Understanding *In Vivo* and *In Vitro* Cell Matrix Interactions through Multiscale Modeling and Simulations

Muhammad Zaman
Assistant Professor
Biomedical Engineering, University of Texas at Austin

Cells reside in a complex, dynamic and heterogeneous environment known as the extra-cellular matrix. Interactions with the extra-cellular matrix regulate fundamental cellular processes such as signaling, adhesion, migration and affect sub-cellular mechano-chemical architecture. Alterations in cell-matrix interactions can result in a variety of life threatening consequences including cancer, neurological disorders and bone defects. Our current understanding of cell matrix interactions is primarily derived from experimental studies and the theoretical efforts have focused mainly on the continuum level. While a number of these studies have some predictive power and have shown reasonable agreements with experiments, a majority of these models are qualitative and have ignored the molecular basis of cell-matrix interactions. As a result traditional cell-matrix interaction models are unable to capture the underlying multi-scale biophysics or the thermodynamics of the processes that allow the cells to live and function in a dynamic and complex environment. Using multi-scale algorithms rooted in fundamentals of thermodynamics, non-equilibrium statistical mechanics and probability theory, we develop a bottoms up approach to quantify cell-matrix interactions including adhesion and migration in 2D and 3D environments. Our integrated models synthesize information from long-time molecular dynamics simulations of integrins at the cell surface, incorporate key events into diffusion of receptors on the lipid bilayer and quantify the mechanical and chemical interactions between receptors and ligands at the cell and the tissue level, all within a single modeling framework. Our results not only show good agreement with existing experimental studies but also make a number of predictions to analyze and quantify cell matrix interactions during cancer invasion and metastasis.

A Multiscale Approach to Modeling the Human Respiratory and Circulatory Systems

Anne Staples
Postdoctoral Researcher
Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory

Elaine Oran
Senior Scientist
Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory

Jay Boris
Senior Scientist
Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory

Carolyn Kaplan
Scientist
Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory

There are now a number of extremely detailed models of components of the respiratory and circulatory systems; for example, Peskin and McQueen's model of the human heart [1] and Sznitman et al.'s detailed computational model of alveolar flow in the lungs [2]. These models compute 3D flows with expanding walls and model the fluid-structure interactions in those flows. What prevents simply joining models like these together to form a unified model of the respiratory or circulatory system is, on one hand, the lack of a consistent computational framework for integrating these disparate models, and, on the other hand, the complexity and computational cost of the resulting model. Even for just the respiratory system, a fully detailed three-dimensional model of the entire system that modeled all of the fluid-structure interactions, chemical and physical reactions, and the flow through every branch of the bronchial tree down to the flow through the alveoli would require large computational times to simulate a few second of this model system's behavior.

We are in the process of compiling a precise, consistent, and globally comprehensive description of the human body as a complex network of multiscale multiphysics computational models of physiological systems and their couplings.

We are now beginning to develop a low-order fast (our goal is faster than real time) multiscale computational model of the coupled respiratory and circulatory systems in the human body. This will be based on a quasi-1D fluid dynamics macroscopic model for each system separately with integrated higher-dimensional, more detailed models that can be invoked at appropriate times.

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Dependence of the Vibrational Frequency Spectrum of a Nonlinear Residually Stressed Elastic Body on Material Properties, Geometry, and Residual Stress

Yuliya Gorb
Department of Mathematics, Texas A&M University

Jay R. Walton
Department of Mathematics, Texas A&M University

Our work is on the modeling and analysis of the high frequency vibrational response of nonlinear elastic bodies subjected to large deformations and residual stresses. The problem derives from modeling the use of an ultrasound catheter to interrogate in-vivo atherosclerotic plaques in large arteries.

Given the theoretical and practical difficulties of determining the residual stress in healthy arteries, it is even more daunting to model and measure it in arteries with a significant atherosclerotic plaque burden. The difficulty in determining the residual stress is a central motivation for an aspect of the study that addresses the question of how much detail of the residual stress is necessary in order to distinguish key tissue types via ultrasound techniques.

Experimental and Theoretical Studies of Ultimate Strength of Cortical Bone

Iwona Jasiuk
University of Illinois

Liang Feng
PhD Student
University of Illinois

Research on bone fracture has lead to the growing attention to use micromechanics and finite element models for prediction of mechanical properties of cortical bone. While the ultimate strength is more important than the modulus because it is closely related to the fracture of bone, there are only a few models developed to predict the bone strength [1] compared with the models for elastic modulus [2-5]. The purpose of this study is to use experimental methods to characterize swine femoral cortical bone and develop a multiscale theoretical model to predict the ultimate strength of the tissue. In this study, the structure and porosity at the nano-scale level are measured by transmission electron microscopy (TEM) and Fourier transform infrared microscopy (FTIR) is used to obtain chemical composition information such as collagen: mineral ratio. Nanoindentation is also employed to measure the local mechanical properties. At the higher level, micro-CT and scanning electron microscopy (SEM) are used to obtain information such as bone types (lamellar, woven bone or osteon bone), porosity, osteon volume fraction. The mechanical properties are measured by using tensile testing. The samples after tensile testing are also examined by SEM to study the failure mechanisms. These experimental data serve as the inputs for the multiscale micromechanics model to predict the ultimate strength. Furthermore, the computed theoretical values are compared with the results from the tensile testing to validate the model.

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Flocculating Infectious Bacteria: Smoluchowski and Sepsis

David Bortz
Assistant Professor
Applied Mathematics, University of Colorado

John Younger
Associate Professor
Emergency Medicine, University of Michigan

Klebsiella pneumoniae and *Staphylococcus epidermidis* are the most common causes of intravascular catheter infections, potentially leading to bacteremia. These bloodstream infections dramatically increase the mortality of illnesses and often serve as an engine for sepsis. Our current model for the dynamics of the size-structured population of aggregates in a flowing system is based on the Smoluchowski coagulation equations, which we are using to study properties of these flocculating bacteria.

In this talk, I will discuss the progress of several investigations into properties of our model equations as well as the comparison with data [1]. In particular, I will focus on the derivation of an alternative fragmentation kernel in laminar flow as well as the post-fragmentation aggregate size distribution.

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Fluid-Structure Interaction and Transport in Blood Flow

Suncica Canic
Department of Mathematics, University of Houston

The focus of this talk will be on the analysis and computation of fluid-structure interaction in blood flow. Understanding solutions to moving-boundary problems describing fluid-structure interaction between blood flow and arterial walls is important in understanding the mechanisms leading to various complications in cardiovascular function. Although fascinating progress has been made in some areas of modeling and simulation of the human cardiovascular system

many of the basic difficulties remain open and will continue to present major challenges in the years to come.

The speaker will give an overview of the main problems and difficulties associated with the study of fluid-structure interaction in blood flow. Recent results in the analysis of solutions to

the benchmark problem in blood flow, obtained by the group at the University of Houston, will be summarized and recent developments in the numerical algorithm design will be mentioned.

Applications involving certain cardiovascular applications will be shown, including the problem of transport of nanoparticles for cancer derug delivery.

Colalborators:

Dr. Z. Krajcer and Dr. D. Rosenstrauch (Texas Heart Institute),

Dr. C. Hartley (Baylor College of Medicine), Prof. R. Glowinski, Prof. T.W. Pan,

Prof. G. Guidoboni (University of Houston), Prof. A. Mikelic (University of Lyon 1, FR),

Prof. J. Tambaca (University of Zagreb, CRO), Prof. F. Marpeau (University of Houston)

Mechanics of Microtubules Buckling Supported by Cytoplasm

Hanqing Jiang
Assistant Professor
Mechanical and Aerospace Engineering, Arizona State University

Jiaping Zhang
Graduate Student
Mechanical and Aerospace Engineering, Arizona State University

The cytoskeleton provides the mechanical scaffold and maintains the integrity of cells. It is usually believed that one type of cytoskeleton biopolymer, microtubules, bear compressive force. In vitro experiments found that isolated microtubules may form an Euler buckling pattern with a long wavelength for very small compressive force. This, however, does not agree with in vivo experiments where microtubules buckle with short-wavelength. In order to understand the structural role of microtubules in vivo, we developed mechanics models that study microtubule buckling supported by cytoplasm. The microtubule is modeled as a linearly elastic cylindrical tube while the cytoplasm is characterized by different type of materials, namely viscous, elastic, or viscoelastic material. The dynamic evolution equations, the fastest growth rate, the critical wavelength and compressive force, as well as equilibrium buckling configurations are obtained. The ability for a cell to sustain compressive force does not solely rely on microtubules, but is also supported by the elasticity of cytoplasm. With the support of the cytoplasm, an individual microtubule can sustain a compressive force on the order of 100 pN. The relatively stiff microtubules and compliant cytoplasm are combined to provide a scaffold for compressive force.

Modeling of Bone at Nanostructural Level

Iwona M. Jasiuk
Department ofMechanical Science and Engineering, University of Illinois

Elham Hamed*
PhD Candidate
Department of Mechanical Science and Engineering, University of Illinois
ehamed2@uiuc.edu

Bone is an excellent structural material owing to its high strength, stiffness, fracture toughness and low weight. These superior properties are due in part to the hierarchical structure of bone ranging from molecular to macroscopic levels [1]. However, it is not clear how the mechanical properties of the various microstructures at different length scales affect the overall behavior of bone. Such understanding is essential in orthopedics for designing optimum implant materials and for investigating the effect of bone diseases, like osteoporosis, and their treatments on bone properties. Furthermore, it would serve as a guide for engineers to design superior synthetic bio-inspired materials for a wide range of engineering applications.

At nanostructral level bone is a multi-phase composite material consisting of collagen Type I molecules (tropocollagen), hydroxyapatite mineral crystals (HAP), water, and non-collagenous proteins. This nano-composite structure serves as a primary building block of bone. Thus, its mechanical and physical characterization is crucial for understanding of bone's structure-property relationship. Many continuum-based analytical and finite element (FE) models have been proposed to predict the mechanics of bone at the nanostructural level [2, 3]. These studies provided general insights into the bone's response at nano scale; however, the molecular level phenomena were not accounted for. They include the interaction and bonding/interphase between collagen molecules and minerals, the location and effect of collagen cross-links, the role of non-collagenous proteins, and the influence of water and its solved ions. These can be captured by using atomistic simulations especially molecular dynamics (MD) [4, 5]. In this research we employed MD to understand the bonding between collagen and HAP and also the effect of water and its impurities on the mechanical properties of collagen-mineral block. To this end, calcinated and saline water as well as water including bisphosphonates were considered in the modeling. The information obtained from MD simulation was used as inputs for FEM models to obtain an overall picture of the bone behavior at the nanostructural level in the presence of its all components.

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Effective Viscosity of Dilute Bacterial Suspensions: A Two-Dimensional Model

Leonid Berlyand
Mathematics and and Materials Research Institute, Pennsylvania State University

B. Haines
Pennsylvania State University

I. Aronson
Pennsylvania State University

D. Karpeeev
Pennsylvania State University

A mathematical model of active suspensions of self-propelled bacteria (swimmers) in the framework of two-dimensional (2D) Stokesean hydrodynamics is proposed. A formula is obtained for the effective viscosity of such suspensions in the limit of small concentrations. This formula includes the two terms that are found in the 2D version of Einsteins classical result for passive suspensions. To this, the main result of the paper is added, an additional term due to self-propulsion which depends on the physical and geometric properties of the active suspension. This term explains the experimental observation of a decrease in effective viscosity in active suspensions.

Modeling the Growth of an Atherosclerotic Lesion

Jay Walton
Department of Mathematics, Texas A&M University

In a series of recent papers, we have been modeling atherogenesis, the earliest phase of atherosclerosis, as an inflammatory instability [1], [2]. In the early phase of the disease, there is minimal apparent damage to the arterial wall or luminal encroachment. Conventional views of atherosclerosis pictured lesion growth as occurring via intimal enlargement into the lumen with negligible overall enlargement of the vessel. It is now well accepted that this conventional view is incorrect and that initial lesion growth occurs through outward distention of the vessel wall with minimal luminal encroachment. Outward thickening of the vessel wall eventually ceases and additional lesion growth occurs into the lumen.

The primary process causing the distention of the arterial wall during the early phases of lesion growth is conjectured to be the breakdown of elastin by elastase production occurring as a byproduct of the inflammatory processes central to the disease. The breakdown of elastin compromises the structural integrity of the medial layer resulting in expansion of the vessel wall. In the model discussed in this talk, account is taken of the inflammatory processes leading to foam cell production, a principal component of an atherosclerotic lesion, and the resulting mechanical growth and remodeling of the arterial wall, first primarily through outward distention promoted by elastin degradation weakening the medial stiffness and progressively via luminal encroachment. An important ingredient in the model involves the role played by the vasa vasorum as a source mechanism feeding the inflammatory processes necessary for disease progression.

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Thermodynamically Consistent Hierarchical Multiscale Constitutive Modeling of Glassy Polymer Materials

Gregory Odegard
Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University

Pavan Valavala
Graduate Research Assistant
Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University

Elias Aifantis
College of Engineering, Michigan Technological University

Polymer-based composite and nanocomposite materials have the potential to provide significant increases in specific stiffness and specific strength relative to current materials used for many engineering structural applications. To facilitate the design and development of polymer nanocomposite materials, structure-property relationships must be established that predict the bulk mechanical response of these materials as a function of the molecular- and micro-structure.

Many multiscale modeling techniques have been developed to predict the mechanical properties of thermoplastic polymers based on the molecular structure and behavior. However, all of these techniques are limited in terms of their treatment of time-dependent deformations, molecular behavior detail, applicability to large deformations, and/or spatial distributions of conformations of polymer chains (microstates). The proper incorporation of these issues into a multi-scale framework may provide efficient and accurate tools for establishing structure-property relationships of polymer-based materials.

The objective of this research is to establish an approach for incorporating the above-listed issues for multiscale modeling of thermoplastic polymer materials. The modeling of amorphous, time-dependent materials subjected to large deformations will be addressed first, followed by the development of a micromechanics approach for incorporating the statistics-based distribution of microstates. Results from this modeling for specific polymers systems are briefly discussed.

A Concurrent Atomistic and Continuum Model and Its Application in Biological Materials

Youping Chen
Department of Mechanical and Aerospace Engineering, University of Florida

Liming Xiong
Department of Mechanical and Aerospace Engineering, University of Florida

From a mechanical viewpoint, perhaps the most distinguishing feature of biological materials from synthetic materials is the structural hierarchy. It is widely believed that the rare combination of mechanical properties, i.e., the simultaneously high strength, stiffness and toughness, of many structural biological materials arises from precise hierarchical organization over a large range of length scales.

This paper will present the formulation of a field representation of classical atomic-level N-body dynamics, will demonstrate that the new field theory is equivalent to a fully atomistic model at the atomic scale and can be reduced to classical continuum mechanics at the macroscopic scale. This will enable concurrent atomic and continuum simulation of materials within a single theoretical framework. Application of the formulated field theory in modeling and simulation of dislocation, phase transformation, fracture and failure of biomimetic materials will be presented. Potential applications in understanding hierarchically-structured biological materials will be discussed.

Orthopedic Bioengineering—Nano to Device Level

ORGANIZERS:

Tarun Goswami, *Department of Biomedical, Industrial and Human Factors, Wright State University*

Orhun K. Muratoglu, *Massachusetts General Hospital*

Debjyoti Banerjee, *Department of Mechanical Engineering, Texas A&M University*

SYMPOSIUM
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A Biomechanical Evaluation of Cadaveric Femurs after Bone Graft Harvesting with the Reamer/Irrigator/Aspirator

Ryan Finnan, MD*
Orthopedic Surgery and Sports Medicine, Wright State University
finnanr@hotmail.com

Michael Prayson, MD
Orthopedic Surgery and Sports Medicine, Wright State University

Tarun Goswami
Biomedical, Industrial and Human Factors Engineering, Wright State University

Danielle Miller
Biomedical, Industrial and Human Factors Engineering, Wright State University

The mechanical behavior of cadaveric femurs after IM reaming using the Reamer-Irrigator-Aspirator (RIA) for autogenous bone graft harvest has not been described. We hypothesized that reamed femurs, regardless of starting point, would adequately withstand cyclic loading simulating postoperative ambulation. Twenty-one cadaveric pairs were randomly assigned to 1 of 3 groups based on starting point: group 1 (trochanteric), group 2 (piriformis fossa), and group 3 (retrograde). Each femur underwent DEXA scanning and radiographs. Each test femur was reamed to 15mm using the RIA, with the contralateral femur serving as the control. The specimens were loaded to 1400N of axial compression with 2° simultaneous torsion for 10,000 cycles. If the femur survived cyclic loading, it was then loaded to failure in axial compression. Comparisons regarding survival of cyclic loading were made using Fisher's Exact Test. No differences were seen between groups regarding age, sex, and T-score. The mean T-score for the femurs was –2.531 ± 1.372. Overall, 18 of 21 (86%) test femurs and 20 of 21 (95%) control femurs withstood cyclic loading ($p = 0.606$). Statistical significance was not reached for the 3 pairwise comparisons between test groups. The femurs failed in patterns consistent with simple pertrochanteric, basicervical, midcervical, or subcapital fractures. IM reaming for bone graft harvest using the RIA without subsequent IM stabilization did not significantly degrade the mechanical behavior of cadaveric femurs in simulated ambulation regardless of reamer starting point. It appears safe to allow weightbearing on a reamed, unstabilized femur after bone graft harvesting using the RIA.

Biomechanical Analysis of a New Locked Plating System for the Proximal Humerus

Ross Schumer MD
Department of Orthopedic Surgery, Wright State University
rossaf44@yahoo.com

Michael Prayson, MD
Department of Orthopedic Surgery, Wright State University

Manny Konstantakos, MD
Department of Orthopedic Surgery, Wright State University

Locking plates have emerged as the implant of choice for stabilization of proximal humerus fractures. There is little support in the literature for use of locked threaded screws versus locked non-threaded pegs. This study evaluates the biomechanical properties of a proximal humerus locked plating system with comparison of smooth pegs and threaded screws for humeral head fixation. Fifteen pairs of fresh frozen cadaveric humeri were randomized to have a surgical neck gap osteotomy (1 cm) stabilized with a locked plate using either threaded screws (n=7) or smooth pegs (n=8). The contralateral humerus was left intact and served as a control. Each specimen was tested with simultaneous cyclic axial compression (40 Nm) and torsion (both ±2Nm and ±5Nm). All specimens were then loaded to failure. Inter-fragmentary motion and load-displacement curves were analyzed to identify any difference between groups. There were no differences between groups in age and bone mineral density. There was a significant difference when comparing the test specimens to their paired control ($p < .001$). Yet no significant differences were noted between the smooth pegs and threaded screws. Average axial load to failure was 3119 N for the control group compared to 1314 N and 1305 N for the peg and screw groups, respectively ($p < .001$). There is no biomechanical difference between the use of smooth pegs and threaded screws for humeral head fixation in an unstable 2-part proximal humerus fracture model.

Dynamic Modeling of Pneumatic Muscle Actuators for Physical Therapy Applications

Jennifer Serres*
Department of Biomedical, Industrial and Human Factors Engineering, Wright State University
serres.3@wright.edu

David B. Reynolds
Department of Biomedical, Industrial and Human Factors Engineering, Wright State University

Chandler A. Phillips
Department of Biomedical, Industrial and Human Factors Engineering, Wright State University

Industrial pneumatic muscle actuators (PMA) offer significant advantages over traditional sources of actuation: greater power-to-weight and power-to-volume ratios.[1] These performance benefits combined with the inherently safe operation behavior make them prime candidates for physical therapy (PT) devices. However, accurate control of a PMA is challenging to achieve due to the nonlinearities associated with the pressure induced bladder expansion. A three-element phenomenological model has been applied to a commercially available industrial PMA.[2] This model is a parallel configuration of a contracting, damping and spring element. The spring coefficient (K), damping coefficient (B) and contractile coefficient (Fce) have all been characterized and are pressure dependent. Empirical data was collected from a dynamic test station utilizing an industrial (fluidic muscle) actuator. These parameter characterization profiles are applicable in control schemes for PMA use in PT devices. As an assistive component, the PMA would act as an agonist helping the human complete a desired task. As a resistive component, the PMA would act as an antagonist and would provide resistance for a targeted muscle group to work against. The dynamic test station provides a method to demonstration each of these concepts.

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Intervertebral Disc Replacement Devices

Kara Muckley
Graduate Research Assistant
Department of Biomedical, Human Factors, and Industrial Systems Engineering, Wright State University

Tarun Goswami
Associate Professor
Department of Biomedical, Human Factors, and Industrial Systems Engineering; Department of Orthopedic Surgery and Sports Medicine, Wright State University

The intervertebral disc acts as a cushion between each vertebra, allowing the spine to transfer loads and motion properly. Disc problems may develop including degenerative disc disease, herniated discs, and injuries from trauma. Reduced movement and pain is associated with these problems because collapse, spontaneous or post-traumatic tears, and fibrosis of the disc may cause pressure on surrounding nerves. Increased loading or a shift in the way loads are distributed on the vertebrae may also occur, causing irritation and pain as well as abnormal bone growth. When nonsurgical methods are ineffective at treating these disorders, surgical alternatives include fusion and disc replacement. Disc replacement is advantageous over surgical procedures such as fusion because it provides better joint mobility, shorter surgery time, shorter recovery time and, potentially, a decreased chance of adjacent level degeneration. There are many disc replacement devices in different stages of development. This presentation will summarize information available on disc replacement devices, including materials used, basic design characteristics, and regulatory status. The devices will be categorized according to the region of the spine in which they are used, their allowable movement, and their center of rotation location. A review of biomechanical evaluations performed on particular devices will also be presented.

Biomechanics of a Single- and Dual-Threaded Pitch Design for Pedicle Screws

Antonio Valdevit
Department of BME, Stevens Institute of Technology

Manuel Pinto
Twin Cities Spine Center

Joeseph Turner
Research and Developement, Medtronic

Introduction: Pedicle screws have been designed with a single pitch thread and are conventionally optimized for insertion within either the cortical or cancellous bone. However, screw insertion usually results in the shaft residing in both cortical and cancellous bone. The hypothesis for this study was that a dual-threaded pedicle screw would exhibit superior mechanical characteristics to a single-threaded design.

Materials and Methods: A dual-threaded (DT) and single-threaded (ST) screw was inserted into the pedicles of bovine vertebral bodies in a randomized fashion. Insertion torques and extraction torques were measured for 6 bilateral. Six vertebral bodies were assigned to static tensile testing, resulting in perpendicular pull-out of the screw with respect to the screw insertion axis. Twelve additional vertebral bodies were subjected to toggle fatigue in a similar configuration to the static test. Static tests were conducted at 25 mm/min with data acquisition at 20 Hz. Toggle testing consisted of sinusoidal loading between –340N and +340N to 2600 cycles at 0.5 Hz. Fatigue load and displacement data was collected at 100-cycle intervals. For insertion, extraction, and static testing, a paired t-test was used to infer statistical differences in mechanical performance between the two screw designs. For toggle fatigue tests, the total deflection at each 100-cycle interval was computed for each screw type and subsequently averaged. The resulting average deflection at each cycle interval was then subjected to a non-linear regression analysis.

Results: Mean peak insertion torques for the DT and ST screws were 5.88Nm and 3.69Nm, respectively ($P<0.01$). The mean peak extraction torque for the DT screw was 4.30Nm, as compared to the mean peak ST screw extraction torque of 2.61Nm ($P = 0.02$).

The non-linear analyses of each screw type resulted in an exponential fit with r2 values and half-lives of 0.995 at 1375±74 cycles and 0.99 at 1235±93 cycles for the ST and DT screws, respectively. The fitted curves possessed a similar growth to approximately 1505 cycles. At this point, the ST curve increased at a greater rate than the DT curve, indicative of greater toggle for the ST screw.

Discussion: It has been proposed that the average individual will perform approximately 5,000 post-op gait (or toggle) cycles in the first two weeks.1 Using this data and the fact that a patient undergoing surgery would not completely fuse in the first three months, a difference of 50% in deflection would occur at 12,100 cycles, or 4-5 weeks post-operative.[1] The effects upon healing and fusion rate using a dual-threaded screw design at this point are unknown. However, assuming that a less toggling rod-screw construct would lead to an increased fusion rate, the fatigue data presented in this study suggest that the dual-threaded design could aid in a more stable construct.

Conclusion: While the static tests did not elucidate differences in pull-out strength between the two screw designs, the toggle fatigue testing revealed that beyond approximately 1500 cycles the DT screw displayed a reduction in toggle deflection rate and subsequently a decreased net deflection. Such performance may likely improve the likelihood of fusion due to the increased stability.

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New Methods for Quantifying Asymmetric Gait

Elizabeth Hsiao-Wecksler
Assistant Professor
Mechanical Science & Engineering, University of Illinois

K. Alex Shorter
Graduate Research Assistant
Mechanical Science & Engineering, University of Illinois

Louis A. DiBerardino
Graduate Research Assistant
Mechanical Science & Engineering, University of Illinois

Lower limb orthopedic problems frequently result in asymmetric gait patterns. Quantitative gait analysis, in combination with qualitative observational analysis, is a versatile clinical tool used to identify pathology or acute injury and assess recovery from injury or surgery [1]. Quantitative tools typically consist of univariate gait parameters that measure events at discrete and easily defined points in time (e.g., heel-strike, mid-stance, toe-off) [2]. Such measures, however, fail to capture the motion that occurs between these discrete temporal events. These methods also fail to assess how orthopedic problems at one joint can severely alter the behavior of other joints in both the ipsilateral and contralateral limbs. In this talk, we will present some recent advancements in techniques to quantitatively characterize asymmetric gait patterns using two methods from our group (Regions of Deviation Analysis [3], and Elliptical Fourier Analysis [4]). Regions of Deviation Analysis provides information about the magnitude of the asymmetry resulting from injury, the timing in the gait cycle where gait is perturbed, and information about how a joint-specific injury affects the coordinated motion of associated joints. Elliptical Fourier Analysis provides information about the complexity and variability of joint motions. These techniques provide useful supplements to qualitative observational gait analysis and improvement over current univariate measures.

Orthopedic Potential for Polymer-Proteoglycan Composites through Development of Porous UHMWPE Morphologies

Christian Schwartz
Department of Mechanical Engineering, Texas A&M University

Kevin G. Plumlee
Research Assistant
Department of Mechanical Engineering, Texas A&M University

Ultra high molecular weight polyethylene (UHMWPE) has long been an essential component in orthopaedic bearing applications due to its durability, biocompatibility and wear resistance. While novel materials including hydrogels and bio-derived polymers show great potential in orthopaedics, such materials require the development of innovative fabrication and fixation techniques [1-3]. The development of controlled porous UHMWPE morphologies offers the opportunity to advance the state of the art in orthopaedic implants, and also expands the future potential for UHMWPE-based composites with novel bio-derived materials. Interconnected porous structures were generated in UHMWPE by means of a solute-leaching process. Sodium chloride was chosen as the porogen due to its natural biocompatibility, easy removal, and high availability. By varying the concentration and particle size of the porogen, the final pore morphology can be tailored to fit a desired application. Computational simulations of porogen distribution and leaching were examined to provide initial insight into the process. Experimental samples were prepared by dry mechanical mixing of sized NaCl particles and UHMWPE powders followed by compression molding. Samples were then soaked in water to remove the embedded salt, leaving a porous UHMWPE structure. The amount of removed porogen and resulting void density results were found to match very well with the numerical simulations. Limited percolation was achievable at initial NaCl concentrations of 50 weight percent, while salt concentrations of 60 wt% and higher allowed for 95% of the initial salt to be removed. SEM imaging revealed well-controlled pore size and shape with a uniform distribution within the matrix. Dynamic Mechanical Analysis (DMA) results showed that storage and loss moduli depend greatly on porosity, and to a lesser extent individual pore size. These results confirm that porous UHMWPE morphologies can be created with repeatable results that can be tailored to chosen orthopaedic applications.

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Patient-Specific Finite Element Meshing from Medical Image Data

Janelle Totten
Sales/Aplication Engineer
Materialise

Medical imaging and simulation software tools have long been used for measurement and design verification purposes. With recent advancement in technologies like rapid prototyping, virtual surgery, computational fluid dynamics, and finite element analysis, these software tools used in conjunction have opened the doors for the next generation of medical device design. Using patient-specific anatomical data as a starting point improves the accuracy of the model and adds confidence in the simulation result. An overview will be given on some of these applications with results and advantages.

An introduction will be offered on the use of the Mimics software to create patient-specific finite element meshes from medical image data.

Characteristics of a Saddle Joint—an Alternative Geometry for Bearing Surfaces

Antonio Valdevit
BME, Stevens Institute of Technology, NYU HJD

J.P. Errico
MPU, Stryker Spine

Ray Zubok
MPU, Stryker Spine

William Salveson
Design, Datum Industrial Design

Introduction: The use of conforming surfaces such as a ball and socket is common in the orthopedic implant industry. The authors present a saddle joint configuration that may provide an alternative to the ball and socket geometry for use in smaller articulating geometries.

Materials and Methods: The saddle joint geometry was fabricated from Co-Cr-Mo. With slightly dissimilar radii in the X and Y directions, the saddle joint is capable of ±7.5 degrees of angulation while permitting ±3 degrees of axial rotation prior to separation. Six saddle joints were mounted on a polyethylene block with 4mm screws, subsequently mounted within a testing machine and subjected to ten million cycles of loading from -30N to -300N at a frequency of 60Hz. Data was collected at 15,000 cycles and at intervals of 250,000 cycles thereafter.

In order to evaluate the durability of the saddle configuration under repeated motion a custom joint simulator was designed and fabricated so as to permit both undulation (±7.5 degrees per side) and oscillation (±3 degrees per side). Undulation is accomplished through an offset base at a preset distance from a rotating cam while oscillation is performed through the motion of a secondary arm mounted off-axis to a second cam. The test information input included applied load (70N), frequency (1.5Hz), the number of cycles between intervals (1 million) and total test cycles. Six saddle configurations were subjected to 10 million.

Results: In order to elucidate an overall evaluation of the device deflection, and hence integrity, a non-linear regression of the mean deflection data was performed and resulted in an exponential curve with a time constant equal to 852,400 cycles. An overall decrease in deflection from (0.068±0.001)mm to (0.05564±0.0002)mm was computed. No significant changes in deflection were noted beyond 1.5 million cycles ($P>0.05$) while no statistically significant difference in stiffness was detected beyond 3 million cycles ($P>0.05$). With respect to the wear material, regression analyses for rates of generated for cobalt and chromium were computed as 0.000002cm3/million cycles and 0.000216cm3/million cycles respectively. While evidence of wear is seen throughout the 10 million cycles of simulated motion, no evidence of cavitation or pitting was evident.

Discussion: While wear markings were evident on the articulating surfaces of the prosthesis components, no component failed to perform to the designed range of motion. With respect to the wear debris, it has been reported that approximately 10mg of material is lost by 5 million cycles in simulator tests involving metal-on-metal Co-Cr hip components. Using the methods in this study lead to a mass loss of less than 8mg at 5 million cycles. The fatigue response of this design has shown that such a geometric configuration can sustain loads on the order of 70N.

Conclusions: These mechanical and material characteristics have demonstrated that a saddle design may be applicable in cases where large loads are rare and geometric constraints make application of the traditional ball and socket design difficult. Applications may include such joints as the elbow, wrist and cervical spine.

Stress Analysis of Ohio Total Ankle Replacement Models

Shawn Gargac*
Graduate Research Assistant
Department of Biomedical, Industrial, and Human Factors Engineering, Wright State University
gargac.2@wright.edu

Tarun Goswami
Department of Biomedical, Industrial, and Human Factors Engineering, Wright State University

Total ankle replacement (TAR) has recently emerged as a successful alternative to ankle arthrodesis (fusion). Unfortunately, the current implants have suffered from many complications including fractures, loosening, component subsidence, and poor wound healing. A set of new designs (The Ohio TAR)** have been developed that aim to offer a better alternative to existing implants. Three-dimensional finite element models were created of the designs using COSMOSWorks (SolidWorks Corp.). The implant components were modeled using ten node tetrahedral elements. Contact between the components was defined with a coefficient of friction of 0.04. A force of 4,448 N (five times body weight) was applied to the distal surface of the talar component. The proximal (bone-contacting) surfaces of the tibial component were constrained in all directions. Varying element sizes of 2.5, 1.75, and 1.25 mm were used. The optimization of individual components is currently being performed, and these results will be presented at this symposium.

**Patent Pending

In Vitro Mechanics of a Self-Adjusting Spinal Spacer

Michael Kvitnitsky
Mechanical Engineering, Stevens Institute of Technology

Antonio Valdevit
Biomedical Engineering, Stevens Institute of Technology

Ester Rodrigez
Biomedical Engineering, Stevens Institute of Technology

Introduction: While traditional anterior fusion devices are of fixed height, adjustable height devices have emerged. These devices are generally introduced into the disc spaced in a retracted mode and are then subsequently distracted to the appropriate height. A novel divergence from these expandable devices is the introduction of a self adjusting spacer. Such a device would expand to take up the intervertebral space yet provide sufficient mechanical stiffness so as to stabilize the segment in order to promote fusion. In this study a self adjusting height spacer was evaluated and compared to a fixed height spacer in an in vitro model.

Materials and Methods: Five calf specimens from L1 to S1 were prepared and mounted in a custom fixture that permitted flexion, extension and lateral bending and rotation without disruption of specimen alignment. Specimen loading was accomplished using a materials testing machine in displacement control at 1mm/s to a central deflection of 5mm resulting in an angular deflection of approximately 4o at the L3-L4 implantation site. Intervertebral disc deflections were continuously recorded for 6 cycles with the aid of radially deflecting transducers calibrated prior to use and mounted to metallic posts using an adhesive. The deflections were recorded from both the anterior and lateral aspects of the discs. The maximum deflection at each of the locations cited was extracted from the sixth loading cycle. Specimens were testing in the intact condition and again following surgical intervention that consisted of fixed height and adjusting height spinal spacer without supplemental screw fixation. Site specific deflection data in each loading mode was combined for both the anterior and lateral aspects. For the two surgical procedures, the resulting combined deflection was expressed as a percentage of the intact specimen deflection. Statistical comparisons were performed using repeated measures ANOVA and Turkey's post-hoc procedure for individual group comparisons.

Results: In flexion, the adjustable spacer displayed more motion at the surgical site as compared to the fixed height cage. While the motion was greater it was not statistically significant. In extension, the fixed height spacer displayed significantly more motion as compared to the adjusting spacer ($P<0.05$). In both lateral bending and torsion, the fixed height spacer displayed increased motion as compared to the adjustable cage but in both cased the increase was not statistically significant.

Discussion: This study indicated that a self adjusting spinal cage can provide a sufficient degree of stability in order to enhance bone bridging across the intervertebral space to achieve fusion. Such a device possesses the ability to not only sustain the axial compressive loads but adjust so as to maintain endplate contact in extension, where a fixed height device may display separation from the intervertebral endplate. This study represents a worst case scenario with respect to mechanical evaluation of these devices. Clinically such intervertebral spacers are employed with supplemental posterior fixation consisting of pedicle screws and rods. The adjusting cage displayed performance comparable to the intact specimen in all loading modes except flexion as compared to increased motion for the fixed height device in all loading modes.

Conclusions: A self adjust intervertebral spacer has been designed and evaluated in-vitro. The mechanical performance of the device is comparable to a fixed height device yet provides the clinician with continuous endplate contact and patient specific height when inserted.

Temporomandibular Joint Model Development

Shirish Ingawale
Graduate Student
Biomedical, Industrial and Human Factors Engineering, Wright State University

Tarun Goswami
Associate Professor
Biomedical, Industrial and Human Factors Engineering, Wright State University

About 30 million people in USA suffer from temporomandibular disorders (TMD). Although several non-surgical and surgical treatment options are available, reconstruction with either partial or total joint prosthesis is the only potential treatment option in certain TMD conditions. The outcome assessments of three Food and Drug Administration (FDA) approved temporomandibular joint (TMJ) implants have shown mixed success. Therefore, there is a need to develop anatomically more viable TMJ models for better understanding of TMJ structure and function, and to propose more efficient implant designs. Our research focuses on processing the computed tomography (CT) images of normal TMJ to develop appropriate three dimensional models. We have developed 3-D models from CT images of 16 subjects using Mimics® software (Materialise, Ann Arbor, MI, USA). Our future work, which constitutes research undergoing at Wright State University, will involve assigning implants to the TMJ models. The finite element analysis of the TMJ models, with and without implants, will be performed for better understanding of the joint movements, associated forces, and resultant stresses in normal and symptomatic TMJs.

SYMPOSIUM

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The 4th Symposium on Mechanics of Soft Materials and Tissues

ORGANIZERS:

Thao D. Nguyen, *Department of Mechanical Engineering, Johns Hopkins University*

H. Jerry Qi, *Department of Mechanical Engineering, University of Colorado*

Nonlinear Viscoelastic Relaxation and Recovery of Porcine Flexor Tendon

Sarah Duenwald
Research Assistant
Biomedical Engineering, University of Wisconsin, Madison

Ray Vanderby, Jr.
Professor
Biomedical Engineering and Orthopedic Surgery, University of Wisconsin, Madison

Roderic Lakes
Professor
Engineering Physics and Biomedical Engineering, University of Wisconsin, Madison

Soft biological tissues such as tendon are known to be viscoelastic[1,2]. Most research in this area focuses solely on relaxation[3] and creep[2,3] behavior after applied loading but neglect the recovery behavior after loads are removed. This study uses the porcine digital flexor tendons to study recovery following stress relaxation. It also studies stress relaxation at various levels of strain in order to check the ability of quasi-linear viscoelastic (QLV) to robustly model tendon recovery behavior.

Twenty porcine flexor tendons were carefully dissected. Ten were used to study recovery, and ten to study relaxation at various applied strains. Prior to testing, tendons were placed in PBS solution and mounted for testing. They were preloaded to 1N, preconditioned to 2% strain, and returned to preload for 1000 seconds prior to further testing. To study recovery, involved tendons being pulled to 2% strain, relaxing for 100 seconds, returned to preload for 1000 seconds, pulled to 6% strain for 100 seconds, then dropped to 2% strain to recover. To study relaxation at various strains, tendons were pulled to 1, 2, 3, 4, 5, and 6% strains relaxing for 100 seconds, with unloaded periods of 1000 seconds between each test.

Testing shows that recovery curves are fit well with a power law equation, but proceed at a much slower rate than relaxation. Initial recovery proceeds quickly, almost elastically, then slows dramatically, never reaching predicted levels within the time allotted for the experiment. Testing at various strain levels shows that stress relaxation proceeds more quickly at higher strains (e.g. 6%) than at lower strains (e.g. 2%). This nonlinearity cannot be modeled with QLV.

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Native and Engineered Knee Ligament Mechanics

Ellen Arruda
Department of Mechanical Engineering, University of Michigan

Jinjin Ma
Department of Mechanical Engineering, University of Michigan

The incidence of knee ligament rupture in the US has increased drastically in recent years, particularly among the pediatric population, leading to an increased urgency for engineered replacement tissue. This talk discusses the mechanical requirements for the medial collateral (MCL) and anterior cruciate (ACL) ligaments, two of the most commonly ruptured ligaments in the knee. We examine the functional gradient in the response of these ligaments and examine the ability of engineered ligament to remodel and grow in response to the mechanical environment in vivo as it functions as ligament replacement tissue. We also present a computational model of the poroviscoelastic response of ligament and comment on its efficacy as a tool for examining the physiological basis for functionally graded response in knee ligaments.

A Constitutive Model Considering the Orthotropy of the Elastic and Collagen Fiber Networks

Philip Kao
Graduate Student
Department of Mechanical Engineering, University of Colorado

Steven R. Lammers
Graduate Student
Department of Mechanical Engineering, University of Colorado

H. Jerry Qi
Department of Mechanical Engineering, University of Colorado

Robin Shandas
Department of Mechancial Engineering, University of Colorado

The artery wall is mainly comprised of smooth muscle cells, elastic lamina and collagen fibers. This model uses a hyper-elastic strain energy function comprised of an orthotropic Neo-Hookean-like network and an orthotropic fiber network to approximate the combined response of the artery wall. The Neo-Hookean-like network models the elastic network and ground matrix, and the fiber network models the collagen fiber bundles. The Neo-Hookean-like network consists of an isotropic Neo-Nookean component, with Neo-Hookean fiber reinforcements ([1]) in two, orthogonal directions, aligned with the circumferential and axial directions of the artery. The fiber network uses a fiber constitutive model developed by Yannas and Comninou [2] for collagen fiber bundles in tendons. This fiber model is a sinusoidal elastic beam with given bending rigidity and extensional stiffness. The fibers have an ellipsoidal distribution, and strain is calculated as such, as in Gasser, et al. [3], with major axes aligned with the axial and circumferential directions. Using data from elastic-network-only (digested) and fresh samples, in conjunction with histological information, model parameters are fit to the male Holstein calf animal model. Animals with hypoxia-induced pulmonary hypertension and normotensive animals are analyzed.

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Finite Element Modeling of Intraneural Ganglion Cysts of the Common Peroneal Nerve

Gregory Odegard
Assistant Professor
Department of Mechanical Engineering–Engineering Mechanics, Michigan Technological University

Shreehari Elangovan
Graduate Research Assistant
Department of Mechanical Engineering–Engineering Mechanics, Michigan Technological University

Duane Morrow
Biomechanics and Motion Analysis Lab, Mayo Clinic

Robert Spinner
Departments of Neurosurgery and Orthopedic Surgery, Mayo Clinic

Intraneural Ganglion Cysts (IGCs) are mucinous cysts which form within the epineurium of peripheral nerves, most commonly the Common Peroneal Nerve (CPN). They produce neurologic deficit, and their pathogenesis and treatment are subjects of intense debate for clinicians. Previous studies [1] support the theory that synovial fluid form the superior tibiofibular joint enters the articular branch of the CPN subsequent to joint capsule disruption through injury. The increased pressure caused by continuous influx of fluid compresses nerve fascicles, expands the nerve radially, and causes further propagation proximally into the CPN. To effectively treat IGCs and eliminate the common situation of postoperative recurrence, surgeons would benefit from an understanding of the underlying mechanics that influence cyst growth. The objective of this study is to introduce computational modeling as a tool for analysis of cyst development. In particular, this study will explore the phenomenon of proximal cyst propagation.

A three-dimensional finite element analysis (FEA) of the junction between the articular and the deep branches of the CPN has been constructed with a pressurized cyst propagating down the articular nerve branch. The dimensions of the model have been obtained from intra-operative and MRI images. The model is meshed with 10-node tetrahedral elements in ANSYS. The nerve fascicles and the epineurium are modeled as hyperelastic materials. Results of the FEA modeling indicate that the highest principal stresses occur at the tip of the cysts nearest the proximal section of the junction, which causes the cyst to propagate proximally, as observed clinically.

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Collagen Fiber Recruitment Structural Constitutive Models for Valvular Tissues

Michael Sacks
W.K. Whiteford Professor
Bioengineering, University of Pittsburgh

Advanced simulations of heart valve function requires more realistic and sophisticated structural constitutive models to predict the stress environment of cells for mechano-physiological questions and account for regional variations and layer properties. A structural model reflects the physiological structural kinematics of collagen fibers under deformation is thus presented here. Whole porcine hearts were obtained and the aortic valve leaflets (AVL), mitral valve anterior and posterior leaflets (MVAL and MVPL) were then prepared removed and square specimens were dissected from each valve leaflets. Each specimen was preconditioned then subjected to an equi-biaxial strain state in order to determine the effective fiber ensemble stress-strain response, which was then fitted to an appropriate recruitment function. In general, we observed that 1) heart valve tissues exhibit a long toe region due to small number of recruited fibers at lower strain level, 2) stress-strain curve becomes linear at high strain due to complete recruitment of the collagen fibers and 3) most fibers are recruited very quickly near upper bound strain limit. Most interestingly, the effective collagen fiber modulus for all three left side valve types was all ~68 kPa, with all fibers fully recruited by ~30% strain. Our purpose in the present study was to demonstrate that the constituent fibers of the left side valve leaflets can be simulated using a fiber recruitment model. Moreover, we demonstrated use of recruitment models can provide for more accurate simulations of valvular tissues at stress levels beyond those utilized in parameter determination.

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Identifying the Distribution of Elastic Properties in Thin Soft Tissues

Jia Lu
Associate Professor
Department of Mechanical and Industrial Engineering, Center for Computer Aided Design, The University of Iowa

Xuefeng Zhao
Research Assistant
Department of Mechanical and Industrial Engineering, Center for Computer Aided Design, The University of Iowa

Material identification for living tissues presents considerable challenge due to complications arising from nonlinearity, anisotropy, heterogeneity, and patient-specificity. More often than not, methods of characterizing the tissues need to be non-invasive. In our recent works [1, 2], we developed a pointwise identification method that can sharply characterize the heterogeneous properties of nonlinear membranes. The method builds on the static determinacy property of membrane equilibrium. We devised a method of stress analysis that can solve the stress distribution in a pressurized membrane without knowing the wall elastic properties in question. Based on independently acquired stress and strain data, the material property can be characterized pointwise by means of constitutive regression. In this presentation, we report numerical and experimental investigations on the effectiveness of the method as it applies to anisotropic, heterogeneous soft tissues. Virtual (numerical) experiments were conducted for a cerebral aneurysm model reconstructed from medical images. The inflation motion was simulated using finite element analysis assuming that the wall tissue follows a Fung-type constitutive model with location-dependent parameters. The subsequent application of the identification method rendered an accurate estimation of the assumed heterogeneous properties. We also conducted organ-level tests on chicken crops. A chicken crop was inflated to various pressures, and its deformed configurations were recorded through an Optical Motion Capture System, followed by the identification of the elastic parameters. The predictive capability of the identified model was verified by comparing the measured and finite element predicted shapes under selected pressures. The parameters were also compared to those from controlled specimen experiments on excised pieces.

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Shear Piezoelectricity in Individual 100 nm-Diameter Collagen Type I Fibrils

Majid Minary-Jolandan*
Graduate Research Assistant
Mechanical Science and Engineering, University of Illinois
mminary2@uiuc.edu

Min-Feng Yu
Assistant Professor
Mechanical Science and Engineering, University of Illinois

It is a long-held finding that a number of biological materials, such as bone, skin and connective tissues such tendon, show piezoelectric behavior similar to that of certain crystalline materials [1]. It has been postulated that the electrical charges produced under stress in such materials can stimulate cellular response and thus the growth and healing of these tissues [2]. More specifically, this piezoelectric effect in bone has been suggested as an explanation for the Wolff's law [3]. Till now, this behavior has been studied in bulk samples of these tissues where both piezoelectric and non-piezoelectric components are present, complicating the acquired piezoelectric response. However, considering the crystal structure of the different components in theses biological materials, only collagen fibrils may contribute to this effect, since the other components such as hydroxyapatite minerals in bone are non-piezoelectric materials. Collagen is the most abundant protein in mammals and it is a major constituent of all extracellular matrices with numerous developmental and physiological functions [4]. We studied piezoelectric effect at nanometer scale, in single collagen fibrils with ~100 nm-diameters and several tens of microns long, isolated from achilles tendons. The piezo force microscopy technique is applied in vertical and lateral modes to examine piezoelectric behavior of individual collagen fibrils in radial and axial direction. The results reveal that collagen fibrils behave predominantly as shear piezoelectric materials with axial polarization. The shear piezoelectric coefficient is on the order of ~1 pm/V and the polarization direction is maintained throughout the length of the fibril. Considering that the effective load transfer mechanism between tropocollagen molecules in a collagen fibril is shearing, such shear piezoelectric behavior may play a significant role in growth and healing in bone and connective tissues. Furthermore, the results confirm the nanoscale origin of piezoelectricity in bone and tendons.

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Torsional Buckling and Supercoiling of Fluctuating DNA

Prashant Purohit
Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

Several decades of experimental and theoretical research into the mechanics of dsDNA has lead to a theory that describes it as a fluctuating elastic rod with well characterized bending and twisting moduli. An interesting problem within this realm is that of plectoneme formation in DNA as it is simultaneously put under tensile and torsional stress. The mechanics of plectonemes is an interesting subject in its own right since DNA exists in the form of plectonemes within cells, and the torque required to unravel them plays a role in the regulation of genes [1]. In this presentation we will show how ideas from the Kirchhoff theory of filaments can be used to find semi-analytical solutions for the average shape of the fluctuating DNA with plectonemes under the assumption that there is no self-contact. Our method consists of combining a helical solution of the rod with a non-planar localizing solution in such a way that the force, moment, position and slope remain continuous everywhere along the rod [2]. An interesting testable result of our calculations is the prediction of a sudden change in extension at buckling which does not seem to have been emphasized in earlier theoretical models or experiments. Recent experiments have qualitatively confirmed our predictions [3].

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Determining Material Properties from an Oscillating Sphere in Viscoelastic Media

Kathleen Toohey*
Postdoc
Bioengineering, University of Illinois
ktoohey@uiuc.edu

Marko Orescanin
Graduate Student
Electrical and Computer Engineering, University of Illinois

Michael Insana
Professor
Bioengineering, University of Illinois

The material properties of biological systems affect and are affected by the presence of cells. Accurate, quantitative measurements of the viscoelastic properties of cell scaffolds provide insights into how cells modify their environment normally and with disease.

Tracking the motion of a sphere oscillating in a medium is a noninvasive method for measuring material properties. External forces to move the sphere can be applied in a variety of ways (acoustic radiation forcing or magnetic field forcing) and as different functions of time (impulse, step, or harmonic). Ultrasound and other imaging techniques are capable of recording the motion of the sphere as it responds to the applied force. In this work, we introduce a new viscoelastic system model (VE1) to predict the motion of a sphere under an applied force and compare it with an elastic material model [1] and a demonstrated viscoelastic material model [1] (VE2). VE1 and VE2 each use shear modulus and shear viscosity to characterize the system under step loading and sinusoidal oscillations.

An advantage of the VE1 model is that for the step forcing function the solution is analytical, whereas the solution for the VE2 model must be numerically evaluated. The VE1 model can therefore be used easily for curve fitting to experimental data to extract the viscoelastic material properties. Here, curve fitting to data was performed for the elastic and VE1 models. Parameters from the VE1 best fit were then substituted into the VE2 model for comparison.

An applied step in force is followed by the release of the force and the solutions to all three models are compared with experimental data from tests of two gelatin concentrations with an embedded steel sphere. Displacements from VE1 and VE2 show similar oscillations as the sphere relaxes back to its undisturbed position, while the displacement from the elastic model oscillates with larger amplitude. For 3%-concentration gelatin, with low stiffness and viscosity, the VE1 and VE2 models fit the displacement data very well, with mean squared errors (MSE) of 4E-14 and 1E-13. In 4%-concentration gelatin, where the stiffness and viscosity are higher and similar to soft tissues, the viscoelastic fits are also excellent. The elastic model does not fit the experimental data as well as the viscoelastic models, clearly showing the significant viscoelastic response of the material to this force stimulus bandwidth.

Single-frequency sinusoidal forcing of the sphere is used to test the validity of the different viscoelastic models. The viscoelastic response of the material to forced oscillations describes the mechano-environment of cells, which is important for understanding the development of natural and engineered soft tissues.

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Inhomogeneous Swelling of a Gel in Equilibrium with a Solvent and Mechanical Load

Wei Hong
School of Engineering and Applied Sciences, Harvard University

Zishun Liu
Institute of High Performance Computing

Zhigang Suo
School of Engineering and Applied Sciences, Harvard University

A network of polymers can imbibe a large quantity of a solvent and swell, resulting in a gel. The swelling process can be markedly influenced by a mechanical load and geometric constraint. When the network, solvent, and mechanical load equilibrate, the gel usually swells by a field of inhomogeneous and anisotropic deformation. We show that this field in the swollen gel is equivalent to that in a hyperelastic solid. We implement this theory in the finite-element package, ABAQUS, and analyze examples of swelling-induced deformation, contact, and bifurcation. Because commercial software like ABAQUS is widely available, this work may provide a powerful tool to study complex phenomena in gels.

Control of the Stress Relaxation Properties of Polymeric Hydrogels with Hybrid Crosslinkings

Xuanhe Zhao
School of Engineering and Applied Science, Harvard University

Nathaniel D. Huebsch
School of Engineering and Applied Science, Harvard University

David J. Mooney
Professor
School of Engineering and Applied Science, Harvard University

Zhigang Suo
Professor
School of Engineering and Applied Science, Harvard University

Hydrogels have been extensively studied as materials in various biomedical applications due to their high degree of biocompatibility. Especially in tissue engineering, hydrogels have been widely used as matrices to grow new tissues and organs, and as delivery vehicles of growth factors and cells. For reconstruction of tissues or organs, hydrogels are generally embedded in a mechanically dynamic environment, subject to forces from bones, muscles and blood vessels. In order to protect the encapsulated components (e.g. cells and growth factors), it is necessary to maintain the structural integrity of hydrogels. In addition, controlling the mechanical properties of the hydrogels is an important way in regulating the adhesion and gene expression of the cells.

Previous studies have demonstrated that various mechanical properties of hydrogels including rigidity, fracture toughness, swelling ratios, and large strain hysteresis can be independent controlled. Here, we focus on another mechanical property critical to hydrogels' application in tissue engineering, i.e. stress relaxation.

We use alginate gel as an example hydrogel. Alginate gel can form via either ionic or covalent crosslinkings of polymer chains. We show that the crosslink types strongly affect the stress relaxation property of hydrogels. The stress relaxation in covalently crosslinked hydrogel is mainly due to the migration of water molecules. The reversible crosslinking/decrosslinking of polymer chains account for the stress relaxation of ionically crosslinked hydrogel. We form a hydrogel in a hybrid way with both ionic and covalent crosslinkings. By varying the ratio of ionical and covalent crosslinks in a hydrogel, one can independently tune its stress-relaxation behavior while maintaining its rigidity and swelling ratio unchanged. In addition, the hybrid hydrogel has a fracture toughness much higher than the corresponding hydrogel with pure covalently crosslinks.

Modeling the Coupled Diffusion and Swelling Deformation of Hydrogels

Kristofer Westbrook
Graduate Student
Mechancial Engineering, University of Colorado

H. Jerry Qi
Assistant Professor
Mechanical Engineering, University of Colorado

Environmentally responsive (ER) hydrogels are hydrogels that respond to environmental stimuli, such as temperature, pH, or an electric field, by dramatically changing their volume and hence holding or releasing a large amount of water. In many applications of ER hydrogels, it is very important that the volume change of hydrogels as a function of environmental stimuli and time can be precisely controlled. Diffusion in such polymers is a complicated rate controlling process between the mechanical relaxation effects associated with the viscoelastic behavior of polymers and the relative diffusion time scale associated with the mutual diffusion process. In many cases, diffusion in polymers does not follow classical theory and the various types of anomalies are often referenced as non-Fickian or anomalous diffusion behavior. Proposed models that capture these swelling anomalies are able to capture the swelling front separating the swollen and collapsed phases in the material [1,2]. More recently [3], the swelling behavior of ER hydrogels is modeled by considering an evolving interface separating the two phases which can be correlated to a similar anomalous behavior called Case II diffusion. We propose a 2D model coupling the diffusion and swelling deformation of polymer materials which takes into account the shear effects associated with the interface. The requirements for the existence of a sharp interface and the evolution of this interface through the material are considered. The results of our model and other models are then compared.

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Dynamic Compressive Response of Soft Biological Tissues

Weinong Chen
Professor
Aeronautics, Astronautics and Materials Engineering, Purdue University

Dynamic response of soft biological tissues under impact loading is desired to be quantified for an understanding of high-rate deformation, damage, and injury mechanisms in the tissues. However, characterization of soft tissue response to high-rate loading faces significant experimental challenges. If testing conditions are not properly controlled, inertia effects may over-shadow the mechanical response of tissues. In this presentation, we summarize the technical challenges in dynamic compressive characterization of soft tissues by using a split Hopkinson pressure bar (SHPB). To conduct valid dynamic experiments, besides employing pulse shaping techniques and highly sensitive transducers, annular thin specimens are needed to minimize the radial inertia effects. Using this method, we obtained the compressive behavior of a bovine brain white matter and a porcine muscle along and perpendicular to the fiber direction from quasi-static to dynamic strain rates. The experimental techniques and results will be presented and discussed.

In Vitro Dynamic Response of Porcine Brain Tissue in Uniaxial Compression and Indentation

Thibault Prevost
DMSE, Massachusetts
Institute of Technology

Simona Socrate
Mechanical Engineering, Massachusetts Institute of Technology

Subra Suresh
DMSE, Massachusetts Institute of Technology

In this work, a large strain, non-linear, poro-viscoelastic model is used to simulate the dynamic response of porcine brain tissue measured in vitro under different modes of deformation (compression and indentation). Mixed gray and white matter specimens were excised from the cortical region of porcine brains and tested within 12 hours post mortem. The specimens were subjected to cyclic(load-unload) segments at constant strain rate to 50% nominal strain at frequencies between .01Hz and 10Hz in uniaxial unconfined compression. Stress relaxation tests were also performed to characterize the material behavior at longer time scales. Local axial and lateral strains throughout each deformation history were captured using a video extensometer. Based on lateral and axial stretch measurements, the volumetric response of the material in uniaxial compression was obtained. Indentation testing using a 12.5mm diameter spherical indenter was performed to a depth of 7mm following a loading protocol similar to that described for the uniaxial compression tests. A surface-tracking secondary sensor was used to augment the force-displacement indentation data with information relating to the volumetric compliance of the material [1]. The objective of performing indentation tests on the in vitro specimens was to identify a suitable loading protocol for an upcoming in vivo indentation study on porcine brain tissue. The tissue response exhibited substantial nonlinearity, hysteresis, conditioning and rate dependence. In order to capture the essential features of the cortical tissue response, a three-dimensional poro-viscoelastic model was developed. The model was implemented in a finite element framework and model parameters were optimized to fit the load-unload as well as the stress relaxation behavior of the tissue in unconfined compression. The adequacy of the proposed constitutive formulation was assessed by comparing model predictions and experimental response of the tissue to indentation.

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Explosive Blast Loading Experiments of Model Systems: Characterization and Mitigation

Steven Son*
Professor
Mechanical Engineering, Purdue University
sson@purdue.edu

Matthew D. Alley
Research Assistant
Mechanical Engineering, Purdue University

Recent studies have shown that wartime internal, non-penetrating (closed) brain injuries have increased roughly 45% since the Vietnam War. The modern improvements to body armor have decreased the number of blast fatalities and therefore focused attention on closed brain injuries sustained by blast survivors. The consequences of these traumatic brain injuries (TBI) range from mild headaches and swelling, to concussion and brain function deficits, to death. This study aims to investigate and characterize the interaction of explosive blast waves through various model medium including anatomical systems. We have developed physical models and a systematic approach for testing TBI mechanisms and occurrences, which could also lead to possible mitigation techniques for blast injuries. The models involve a series of increasingly complex head structures. Initially, a polycarbonate sphere filled with instrumented ballistics gel roughly approximating the size and volume of a human skull/brain is being used. After characterizing the blast from this model, a stereo lithography skull structure will be utilized with a more accurate brain simulant. Surrounding tissue simulants and muscular/vascular/skeletal features will potentially be included to create an anthropomorphic model. Small explosive charges are directed at the models to produce a realistic blast wave in a laboratory setting. The models are instrumented with pressure transducers, accelerometers, and strain gages to study the response of the model to the explosive stimuli. In addition, the use of high speed shadowgraphy provides visualization of the blast wave interaction with the head model. These results suggest the reflection and coalescing of shock waves inside the head may be the cause of some TBI.

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Mechanical Response of Neuronal Cells for Understanding Mechanisms of Traumatic Brain Injury

Kristin Bernick
Department of Biological Engineering, Massachusetts Institute of Technology

Thibault Prevost
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Simona Socrate
Department of Mechanical Engineering, Massachusetts Institute of Technology

Subra Suresh
Department of Materials Science and Engineering, Massachusetts Institute of Technology

Blast Traumatic Brain Injury (bTBI) is becoming increasingly prevalent in soldiers returning from combat. Currently, there is limited information on the effect of exposure to blast waves on the human head. Through this project we hope to understand the role mechanical response of neuronal cells and tissues plays in injury and disease states (specifically bTBI). This project combines clinical, experimental, and modeling studies with the goal of determining the cell and tissue-level injury mechanisms. One necessary element to achieve this goal is measurement of in vitro and in vivo mechanical properties of brain tissue and cells. Here, the experimental work at the cellular level is described.

In this study, we investigated the mechanical properties of healthy neurons using an atomic force microscope. Dissociated cortical neurons from neonatal rats were allowed to mature in culture, and subsequently, the cell body was indented using a 45um polystyrene microsphere attached to an AFM probe. The cells were subjected to a sequence of load-unload segments at three consecutive displacement rates followed by one stress relaxation test. The neuron response showed nonlinearity, hysteresis, and rate dependence. Upcoming studies will compare the mechanical response of neurons to that of glial cells (both astrocytes and oligodendrocytes). In addition, the results will be integrated in a finite element model of a single neuron and used for multi-scale modeling.

Constitutive Modeling of Rate-Dependent Stress-Strain Behavior of Human Liver Tissue in Blunt Impact Loading

Rebecca Dupaix
Assistant Professor
Mechanical Engineering, The Ohio State University

Jessica L. Sparks
Assistant Professor
Biomedical Engineering, Wake Forest University School of Medicine

The liver is one of the most frequently injured abdominal organs in motor vehicle crashes, and blunt liver injury is associated with mortality rates as high as 30% in cases requiring operative intervention. An understanding of the mechanical behavior of the liver under high strain rate loading conditions could aid in the development of vehicle safety measures to reduce the occurrence of blunt liver injury. The purpose of this study was to develop a constitutive model of the stress-strain behavior of human liver tissue in blunt impact loading.

Liver specimens from 13 unembalmed cadavers were tested within 36 hours of death. Specimens were perfused with heated (37 °C) normal saline solution at physiological pressures. A drop tower was used to apply blunt impact at varying velocities ranging from 1 to 6 m/s. Forces were recorded by a load cell that was mechanically isolated and mounted flush with the flat surface of the impact plate. Force from the isolated load cell was divided by the load cell cross-sectional area to calculate the stress applied to the liver. Strain was calculated from the displacement of the liver at its point of maximum thickness.

A constitutive model previously developed for finite strain behavior of amorphous polymers was adapted to successfully model the observed liver behavior [1]. The elements of the model include a nonlinear spring in parallel with a linear spring and nonlinear dash-pot. The model captures three features of liver stress-strain behavior in impact loading: (1) a relatively stiff initial modulus, (2) a rate-dependent yield or rollover to viscous "flow" behavior, and (3) strain hardening at large strains.

The model developed in this work capitalizes on similarities between the mechanical behavior of amorphous polymers and soft biological tissue such as the liver. This study represents a novel application of polymer mechanics concepts to understand the rate dependent large strain behavior of human liver tissue under high strain rate loading. Applications of this research include finite element simulations of injury-producing abdominal impact events. In addition, the techniques developed in this work could be applied to a variety of soft biological tissues with fine collagenous frameworks similar to that of the liver.

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The Strain Rate-Dependent Response of Bovine Liver Tissue

Kumar Vemaganti
Associate Professor
Mechanical Engineering, University of Cincinnati

Esra Roan
Research Assistant Professor
Biomedical Engineering, Mechanical Engineering, University of Memphis

Like most soft cellular tissues, the liver exhibits a time-dependent hyperviscoelastic mechanical behavior. To accurately capture this complex response of liver tissue, its constitutive model must account for both the viscous and nonlinear contributions. Traditional approaches, like the quasi-linear viscoelastic (QLV) approach [1] or the convolution integral approach [2], are suitable for capturing long-term memory effects, but are less successful in describing short-term effects. In such cases, a "fast" formulation that splits the strain energy into hyperelastic and viscoelastic contributions may be a viable alternative [3].

In this work, bovine liver tissue is tested in uniaxial compression at various strain rates. A no-slip edge condition is used in these experiments so that friction is not a consideration in our tests on soft tissue, and a correction factor approach [4] is used to account for the resulting non-uniform states of stress and strain. Results show that the fast split formulation is the better alternative and provides a good description of the viscohyperelastic response over two orders of magnitude of strain rates.

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Ionic Polymer-Metal Composites as Soft Actuators and Sensors

Sia Nemat-Nasser
Distinguished Professor
Center of Excellence for Advanced Materials/MAE, University of California, San Diego

Ionomeric polymer-metal composites (IPMCs) as bending actuators and sensors are sometimes referred to as "soft actuators-sensors" or "artificial muscles." When an IPMC in the solvated (i.e., hydrated) state is stimulated with a suddenly applied small step-potential, the composite undergoes bending deformation. The magnitude and speed of the deflection depend on the many factors, including the structure of the electrodes, the nature and the amount of the solvent uptake, and other conditions (e.g., the time-variation of the imposed voltage). When an IPMC membrane is suddenly bent, a small voltage of the order of millivolts is produced across its faces. Hence, IPMCs of this kind can serve as soft actuators and sensors.

With water as the solvent, the applied electric potential must be limited to less than 1.3V at room temperature, to avoid electrolysis. Moreover, water evaporation in open air presents additional problems. These and related factors limit the application of IPMCs with water as the solvent. Both Nafion- and Flemion-based IPMCs may be solvated with ethylene glycol, glycerol, and crown ethers. IPMCs with these solvents have greater solvent uptake, and can be subjected to relatively high voltages without electrolysis. They can be actuated in open air for rather long time periods, and at low temperatures. They may be good actuators when high-speed actuation is not necessary. Remarkably, solvents are found to have profound effects on the nature of the IPMCs' actuation. The lecture gives an overview of the recent experimental and theoretical results in this fascinating research area.

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A Thermoviscoelastic Model for Amorphous Shape Memory Polymers: Incorporating Structural and Stress Relaxation

Thao Nguyen
Assistant Professor
Mechanical Engineering, Johns Hopkins University

Thermally activated shape memory polymers (SMP) are soft active materials that deform in respond to a specific temperature event. The permanent shape of an SMP device is manufactured using conventional polymer processing techniques, and the temporary shape can be programmed by a thermocycle [1].

The primary mechanisms of the shape memory effect and its time dependence are structural and stress relaxation. Structural relaxation is the time-dependent process in which the macromolecular structure and structure-dependent properties (e.g., the viscosity) evolve to equilibrium in response to a temperature and/or pressure change. Similarly, stress relaxation is the time-dependent process in which the stress response evolves to equilibrium in response to a change in deformation. To examine the importance of the structural and stress relaxation mechanisms, a constitutive model has been developed that incorporates structural relaxation in the glass transition region, viscoelasticity in the rubbery and transition regions, and viscoplasticity in the glassy region [2]. This work represents a new approach to modeling the thermomechanical behavior of amorphous SMPs that is fundamentally different than current phase transition approaches [3].

The model was implemented in a finite element program and applied to simulate a series of thermomechanical experiments and constrained and unconstrained recovery experiments. Results showed excellent agreement with experiments for the strain-temperature response and the isothermal uniaxial stress-strain response for different temperatures and strain rate. For unconstrained recovery, the model achieved full strain recovery. The onset of strain recovery predicted by the model agreed well with experiments. However, the recovery time was faster than observed in experiments. For the constrained recovery experiments, the model predicted many features of the hysteresis in the stress-temperature response, but some discrepancies remain. Currently, we are investigating the causes of the discrepancies between experiments and simulations.

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Mechanical Instabilities in Liquid Crystal Elastomers

Robin Selinger
Department of Chemical Physics, Liquid Crystal Institute, Kent State University

Badel Mbanga
Research Assistant
Department of Chemical Physics, Liquid Crystal Institute, Kent State University

Jonathan V. Selinger
Department of Chemical Physics, Liquid Crystal Institute, Kent State University

Liquid crystal elastomers (LCE) are cross-linked polymer networks covalently bonded with liquid crystal mesogens. They combine the high extensibility of rubbers with the orientational order of liquid crystalline materials to produce highly nonlinear elastic effects. In the nematic phase, due to strong coupling between mechanical strain and orientational order, these materials display strain-induced instabilities associated with formation and evolution of orientational domains. When an LCE crosslinked in the nematic phase is stretched perpendicular the director, striped orientational domains are observed with alternating director orientations[Kundler,Macromol. Rapid. Commun. 16, 1997].

We model this phenomenon using a novel finite element elastodynamics simulation method. We investigate the dependence of the material response on both intrinsic parameters such as elastic constants and other parameters emanating from purely geometrical considerations such as the angle between the applied strain and the nematic director orientation. We show that the formation of striped domains is possible only for strains applied above a certain threshold angle from the nematic director. Moreover, we demonstrate that the stripe instability that results during deformation of these materials is the underlying cause of their soft elastic response.

Our simulations yield both qualitative and quantitative agreement with experimental observations. This model allows us to explore the fundamental physics governing dynamic mechanical response of nematic elastomers and also provides a potentially useful computational tool for engineering device applications.

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An Advanced Thermomechanical Constitutive Model for Ultra-high Molecular Weight Polyethylene

Jorgen Bergstrom
Managing Engineer
Veryst Engineering, LLC

Jeffrey E. Bischoff
Senior Engineer
Zimmer

Ultra-high molecular weight polyethylene (UHMWPE) is a material that is extensively used in biomedical devices due to its good mechanical properties, including high impact and wear resistance. In these applications the UHMWPE is often deformed beyond the limit where linear viscoelasticity is accurate, and traditional metal plasticity models are not suitable since the applied loads are not monotonic. To overcome these limitations we have developed an advanced thermomechanical constitutive model for UHWMPE. In this new model the micostructure of the material is represented using three distinct structural domains that capture the experimentally observed non-linear, time- and temperature-dependent response at both small and large strains. The theory for the model is presented, and the model calibration and validation exemplified by direct comparison with experimental data.

Constitutive Modeling of Poly(methyl methacrylate) (PMMA) at Large Strains near the Glass Transition

Kamakshi Singh
Graduate Student
Department of Mechanical Engineering, The Ohio State University

Rebecca B. Dupaix
Department of Mechanical Engineering, The Ohio State University

Poly(methyl methacrylate) (PMMA) has a wide number of applications ranging from embossing to thermoforming. Like all other polymers it shows a substantial change in physical behavior near the glass transition temperature (Tg). PMMA can be deformed above Tg without the application of a large force and then can be cooled just below Tg to sustain the deformation. Hence, developing a model that accurately predicts the behavior of PMMA around Tg has wide industrial applications. Flow behavior of PMMA is highly sensitive to changes in temperatures and strain rates around Tg which makes the problem on hand more difficult. A limited number of material models have been developed to try to capture both the temperature and the strain rate dependence. In this work, we compare three existing models with a range of experimental data.

Uniaxial and plane strain experiments were conducted on uncross-linked PMMA at various temperatures ranging from 82 to 132 °C (Tg ~ 102 °C) and strain rates from 0.2/min to 4.0/min to a strain level of 140%. The data collected was compared with three existing material models—(i) Model by Dupaix-Boyce[1], (ii) Model by Doi-Edwards[2], and (iii) Model by Dooling-Buckley[3]. The Dupaix-Boyce model has been shown to work well at lower temperatures (below and around Tg), the Doi-Edwards model has been shown to work well at higher temperatures (well above Tg) and the Dooling-Buckley model has been shown to capture temperature dependence above Tg, but not rate dependence. Our work investigates the ability of all three models to capture the flow of the material behavior over a wide range of strain rates and temperature of significance in industrial applications.

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On the Specific Characteristics of Soft Polymers in Nanoindentation Tests

Susan Enders
Engineering Mechanics, University of Nebraska, Lincoln

Julia Deuschle
Thin Films and Biological Systems, Max-Planck-Institute for Metals Research

Matthias Deuschle
Dipl.-Ing.
Institute of Statics and Dynamics of Aerospace Structures, University of Stuttgart

Johann Michler
Materials Science & Technology, EMPA Thun

Gerhard Buerki
Materials Science & Technology, EMPA Thun

Emerson de Souza
Thin Films and Biological Systems, Max-Planck-Institute for Metals Research

The wide need of mechanical characterization of soft polymers and biomaterials by using techniques like nanoindentation, which were originally designed to test hard and stiff materials , e.g. metals and ceramics calls for a critical investigation of the behavior of soft elastomers under high local loading. In our research we focused on the two crucial points in indentation testing—1) contact determination and 2) size of the true contact area during the experiment. In this investigation the contact evolution and the deformation behavior of Polydimethylsiloxane (PDMS) was studied during indentation in-situ inside an SEM and by observation in a light-microscope. Since detailed information on the true contact area and the amount of sink-in can be acquired from finite element analysis, simulations on the indentation process have been performed in order to complement the in-situ testing. Through the combination of these techniques several individual error sources in the conventional contact area determination have been identified and quantified for two different Polydimethylsiloxane elastomers. We then applied the now improved dynamic nanoindentation tests for the determination of storage modulus, loss modulus and hardness of PDMS samples of 8 different crosslinking densities. Furthermore, the influence of the curing time was investigated for 3 different crosslinking stages. The results of our investigation revealed that the elastic moduli of our samples cover a range of 2 orders of magnitude, and for one and the same PDMS the modulus may increase by a factor of 10 as a function of curing time. Complementary tensile tests were performed to validate the nanoindentation results and to determine the Poisson's ratios of 6 different PDMS samples. In contradiction to the general assumption, the Poisson's ratios obtained deviate from 0.5, thus indicating a viscoelastic rather than ideal rubbery behavior.

An Elastic Micropolar Mixture Theory for Predicting Elastic Properties of Cellular Materials

Gregory Odegard*
Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University
gmodegar@mtu.edu

Shreehari Elangovan
PhD Candidate
Mechanical Engineering and Engineering Mechanics, Michigan Technological University

Burhanettin S. Altan
Proprietor
Tiger Strategy, LLC

Cellular materials have good specific stiffness and specific strength and hence are excellent candidates for various light weight applications in structural engineering. However, the microstructural complexity, caused by random interconnection of material struts, poses significant problems for accurately modeling their mechanical behavior. Current modeling approaches of cellular materials include FEA and analytical methods. While FEA has the ability to accurately predict mechanical behavior for a wide range of cellular microstructures [1], the model building and solution procedures can be time-consuming and expensive. Analytical approaches [2] tend to be more efficient that FEA but they often cannot directly incorporate the non-periodic microstructure that are found in a majority of cellular materials without resorting to the use of empirical data. Therefore, there is a need to establish an analytical approach that is efficient and accurate, and yet capable of accounting for the random cellular microstructure which is the objective of this study. In this vein, two regular triangular lattices are superimposed to create a conceptual random lattice that is representative of a random two dimensional cellular material. The equivalent continuum representing the conceptual lattice is arrived in two steps: first, the equivalent micropolar continuum of each regular triangular lattice is obtained, second, the two micropolar continua are superimposed using the micropolar mixture theory. The developed model is used to predict properties of balsa wood, a candidate two dimensional cellular material, and good correlation in the results is obtained.

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Initial Yield Behavior of Stretching and Bending Dominated Metallic Cellular Solids

Maen Alkhader
Department of Mechanical, Material and Aerospace Engineering, Illinois Institute of Technology

Murat Vural
Department of Mechanical, Material and Aerospace Engineering, Illinois Institute of Technology

The 2D initial yield behavior of open cell cellular strut-lattice materials is investigated under biaxial loading using finite element simulations. The sensitivity of the initial yield surface to the dominant deformation mode, either stretching or bending, is explored in this work. Low connectivity and high connectivity specimens which deform by local bending and strut stretching, respectively were utilized. The effect of manufacturing induced imperfections on the initial yield surface is examined for both stretching dominated and bending dominated specimens. A quantitative measure to describe the dominant deformation mechanism under multiple loading is proposed. This measure is derived by partitioning the elastic energy of each element into bending energy and stretching energy, and then finding the elemental level distribution of the ratio between stretching energy to total energy. The distribution points directly to the dominant mode of deformation. Phenomenological yield functions are developed to characterize the initial yield behavior of stretching and bending dominated strut-lattice materials under a full range of in-plane biaxial conditions. The phenomenological yield functions have a physical base as they are derived from the total elastic energy density. The phenomenological yield functions are capable of describing the initial yield surface of cellular solids with small and moderate plastic anisotropy. Moreover, the yield functions are convex and smooth.

Dynamics of Biomechanical Processes

SYMPOSIUM
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ORGANIZERS:

Elizabeth Hsiao-Wecksler, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Harry Dankowicz, *Department of Mechanical Science and Engineering, University of Illinois ata Urbana-Champaign*

Stability and Goal Equivalence in Inter-stride Fluctuations of Treadmill Walking

Joseph P. Cusumano
Professor
Penn State University

Joby John
Graduate Research Associate
Penn State University

Jonathan B. Dingwell
Associate Professor
University of Texas

Fluctuations in the repeated performance of human movements have been the focus of much study because they are widely believed to provide important information about the function and health of the neuromotor system [1, 2]. The work described here uses the concepts of goal equivalence and goal equivalent manifolds (GEMs) [3, 4] to gain new insights into the nature and structure of neuromotor control used during human treadmill walking. We present the results of an experimental study of the inter-stride dynamics of 17 healthy subjects. The GEM consists of the set of all relevant body states required for perfect task execution, which in the given walking task was hypothesized to be defined by the goal of steady walking at constant speed. Given this task hypothesis, or goal function, a hierarchical control structure is then posited to drive the body states onto the resulting GEM. Properly normalized stride variability data strongly confirmed the use of the hypothesized goal function by all subjects. Furthermore, the associated linear GEM in the stride-length and stride-time plane allowed for a particularly useful decomposition of the dynamics. Fluctuations in the stride dynamics were studied using detrended fluctuation analysis (DFA) [4-5]. The fluctuations along the GEM exhibited statistically persistent correlations, while fluctuations perpendicular to the GEM exhibited anti-persistent correlations. That is, perturbations normal to the GEM, that cause deviations from the mean walking speed, tend to be followed by perturbations in the opposite direction, thus suggesting control effort; while perturbations tangent to the GEM, that do not affect the mean walking speed, tend to go uncorrected. The correlation results are supported by estimation of the stability multipliers for normal and tangential perturbations: normal multipliers are found to be negative with magnitude much smaller than 1, indicating strongly stable control, while the tangential multipliers are positive and slightly smaller than 1, indicating weak stability and indifferent control. These results taken together represent the first ever demonstration of goal equivalent control in a human movement system.

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Variability, Covariation, and Sensorimotor Noise in Motor Learning and Retention

Dagmar Sternad
Department of Integrative Biosciences and Kinesiology, Pennsylvania State University

Reduction of random fluctuations or "motor noise" across practice is considered a major characteristic of motor learning evidenced in many demonstrations where improved accuracy correlates with decreases in variability over repeated movement executions. Variability is specifically informative when a task is redundant, i.e., the same result can be obtained by many different strategies. In recent experimental and theoretical work we developed a new method of decomposing variability in performance to allow further insights into determinants of change in behavior. Our approach permitted answers to three specific questions: Is it only random fluctuations that diminish with practice? Can variability be decreased in selected variables? How can variability be manipulated by interventions such as in rehabilitation practices?

The basis for our studies is a decomposition of variability into three conceptually and quantitatively distinct factors: (1) Discovery of error-tolerant strategies (Tolerance); (2) exploitation of covariation between essential variables (Covariation); and (3) reduction of dispersion or "noise" (Noise). The so-called TCN-method quantifies the contributions of each of these components in task performance.

In all experiments a throwing task served as our model system. Using a virtual set-up subjects threw a pendular projectile in a simulated concentric force field to hit a target. The movement was experimentally constrained such that only two variables, angle and velocity of ball release, fully determined the projectiles trajectory and accuracy of the throw. The set of successful solutions defines a nonlinear solution manifold. Importantly, different locations of the manifold are differentially sensitive to error.

Experiment 1 examined performance changes with practice and showed that the largest contribution to learning was due to Tolerance, followed by Covariation, with reduction of Noise contributing the least. These results highlight that skill improvement consists largely of subjects' increasing sensitivity to subtle aspects of redundancy in execution, rather than simply reducing noise. Experiment 2 contrasted the hypotheses that variability is aligned with the solution manifold by covariation or that "signal-dependent noise" in minimized. In a task where successful strategies were redundant in the velocity dimension, results showed that executions exploited the redundancy of the task and rather than minimizing velocity, i.e., "signal strength". Experiment 3 examined how highly skilled performance can still be influenced by adding error-dependent noise. During practice sessions with added noise subjects could reduce their variability to maintain accuracy. Importantly, subjects maintained their low variability even after this noise was removed. The results have implications for training and rehabilitation.

Generalization of Dynamic Learning for Posture and Movement

Alaa Ahmed*
Research Associate
Engineering, University of Cambridge
aaa52@cam.ac.uk

Daniel Wolpert
Professor
Engineering, University of Cambridge

Skillful movement depends upon our ability to predict the consequences that our actions have on our bodies and environment. It is widely accepted that this predictive control relies on a central representation (internal model) of the internal and external dynamics. However, it is not known whether learning novel dynamics of the arm in a seated position will generalize to the same movement performed while standing. In addition, will the postural system be able to generalize to standing and predict and compensate for the destabilizing consequences of these dynamics on posture?

Initially, seated subjects made reaching movements to targets in the horizontal plane while grasping the handle of a robotic, force-generating, manipulandum. Their reaching movements were perturbed with a force proportional to their movement velocity, but perpendicular in direction. Following the seated trials, subjects stood on a force plate and performed another set of reaching movements in the presence of the force perturbations. Handle position, robot-generated forces, and forceplate forces were recorded at 500 Hz. To assess learning of the dynamics in both the seated and standing conditions, we examined movement error on each trial. Quality of learning was assessed with random catch trials, where hand movement was restricted to a path along the target vector, using a force channel. Feedforward control of posture in the standing position was measured as the position and velocity of the center of pressure at the onset of hand movement. Movement of the center of pressure in the direction of the impending perturbing force indicates anticipatory control.

All participants learned to make relatively accurate reaching movements to the target while seated, and significantly reduced their movement error. Upon switching to a standing posture, hand error remained reduced. Similarly, by the end of the sitting phase, participants generated significant anticipatory forces on catch trials and this performance was maintained upon changing to a standing posture. However, on standing subjects did not initially compensate for the postural perturbation in an anticipatory manner and generated similar postural responses as found when reaching in the absence of a force field. Over the course of several trials, anticipatory postural responses developed. These findings indicate that learned dynamics of the arm generalizes from sitting to standing but that the postural system does not generalize anticipatory mechanisms between body postures.

Energy-Efficient Speed Regulation of Bipedal Robot Walking via Biomimetic Control Design

Jonathan K. Holm
Research Assistant
Coordinated Science Laboratory, University of Illinois

Mark W. Spong
Professor
Coordinated Science Laboratory, University of Illinois

Recent results in passive-dynamic locomotion have led to the development of bipedal robots with remarkable energy efficiency, in some cases with energy efficiency as high as that of human walking [1]. However, passive-dynamic locomotion affords no more than one period-1 walking cycle for any given slope, therefore providing efficient walking for a single, fixed speed. Several authors [2,3] have introduced controls that allow a range of walking speeds by time-scaling the fundamental passive-dynamic walking cycle. Such controls suffer from large energy requirements and may be implemented only on fully actuated robots.

A new control is introduced here that achieves speed regulation for bipedal walking with substantially lower energy requirements than previously reported speed-regulating controls. This control also requires fewer actuators than previous approaches. Development of the control centers around duplicating two key features of human biomechanics: monotonic change in step length as speed is varied [5] and supply of mechanical energy for walking primarily at the ankle joint [4]. With these objectives in mind, the biomimetic control is designed under an energy shaping framework subject to underactuation constraints. In particular, we show how the natural kinetic energy of a bipedal robot may be modified by feedback control using actuation at the ankle alone to accomplish energy-efficient speed regulation.

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Biomechanics, Energetics, and Neural Control of Walking with Robotic Lower Limb Exoskeletons

Daniel Ferris*
Associate Professor
Movement Science, University of Michigan
ferrisdp@umich.edu

Advances in mechatronics and computer technology have enabled engineers around the world to develop robotic exoskeletons for assisting human movement. Some of the most advanced exoskeletons that have been built include the ExoHiker, HAL, and the XOS Exoskeleton [1]. Yet, in spite of these and other amazing robotic accomplishments, we still have relatively little understanding of how humans alter their biomechanics, energetics, and neural control to mechanical gait assistance [2]. In the University of Michigan Human Neuromechanics Laboratory, we build simple one joint robotic exoskeletons controlled by the user's own electromyography signals (i.e. proportional myoelectric control). Our goal is not to produce products for commercialization but to study the human physiological response to mechanical assistance. Our experiments on human walking with robotic exoskeletons have allowed us to reveal new insights into principles of locomotor adaptation [3], relationships between biomechanics and energetics [4], and human adaptation to different control approaches [5]. Our ongoing studies examine the mechanics of gait perturbations and the potential therapeutic effects of exoskeletons with proportional myoelectric control in gait rehabilitation after spinal cord injury. Results from these types of carefully controlled investigations can greatly expand our basic knowledge of human physiology and provide critical insight into the design of robotic devices for assisting and rehabilitating human gait.

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Skeletal Muscle Energetics and Function during Human Locomotion

Paul DeVita*
Professor
Exercise and Sport Science, East Carolina University
devitap@ecu.edu

Patrick Rider
Exercise and Sport Science, East Carolina University

Stan Solnik
Exercise and Sport Science, East Carolina University

Ben Long
Exercise and Sport Science, East Carolina University

Kevin Via
Exercise and Sport Science, East Carolina University

Tibor Hortobagyi
Exercise and Sport Science, East Carolina University

Although muscles produce both positive and negative work in all gaits, inclined and declined gaits are biased towards energy generation and dissipation respectively and level gaits balance energy generation and dissipation. We showed however that net positive muscle work in ascending stair and ramp walking was larger than net negative muscle work in descending stair and ramp walking and that net muscle work was positive in level walking [1]. Thus, we present a new paradigm of muscle function: muscle work is biased towards energy generation over dissipation in locomotion. Our working hypotheses are: skeletal muscles generate more mechanical energy in gaits that raise the center of mass compared to the mechanical energy they dissipate in gaits that lower the center of mass despite equivalent changes in total energy and skeletal muscles generate a net positive amount of mechanical energy in level gaits despite the maintenance of a constant amount of total energy. We explored these hypotheses through inverse dynamic analyses of human walking and running on 10° sloped and level surfaces using three dimensional ground reaction forces and kinematics. Our first experiment showed that lower extremity muscle work was 28% greater in incline vs. decline running (1.32 vs. –1.03 J/kgm, $p < 0.001$) at 1.5 m/s despite equivalent changes in total body energy (|1.48| J/kgm). The next experiment showed the positive bias in muscle function in non-level running was directly related to running speed (i.e. a significant interaction for muscle work existed between gait direction and speed, $p<0.05$). Muscle work was identical in incline running at 2.8, 3.5, and 4.4 m/s (0.70 J/kgm) but decreased –0.58, –0.51, to –0.44 J/kgm with speed in decline running. Thus, positive vs. negative muscle work was 21%, 40% and 64% larger in incline vs decline running as speed increased. Lastly, despite no change in total energy, net muscle work was positive in both level walking and level running (both 0.17 J/kg). These data lend support to the idea that muscle work is biased towards energy generation over dissipation in locomotion through a variety of gaits tasks.

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Feasibility of Dynamic Entrainment with Ankle Mechanical Perturbation to Treat Human Locomotor Deficits

Jooeun Ahn
Research Assistant
Department of Mechanical Engineering, Massachusetts Institute of Technology

Neville Hogan
Departments of Mechanical Engineering, Brain and Cognitive Sciences, Massachusetts Institute of Technology

Despite advances in cellular and molecular therapies, sensory-motor training is required to assist recovery after neurological injury (e.g., stroke, spinal cord injury). Human-interactive robots can deliver sensory-motor treatment safely and numerous studies have shown their effectiveness for upper-limb therapy. To treat the lower extremity, we introduced Anklebot [1] a machine that can simultaneously apply forces at the ankle in plantar/dorsi-flexion and inversion/eversion. It may be used seated or standing, walking on a treadmill or moving overground. Here we describe initial attempts to explore how it might be used for balance and locomotion therapy.

Much of the coordination required to walk may emerge from the natural nonlinear dynamics of the lower limbs [2]. As Anklebot was carefully designed to allow the expression of natural dynamics, we tested whether it might be applied to assist dynamic walking, possibly recruiting and entraining residual pattern generators in the lumbar cord. Analysis indicated that, with suitable control, Anklebot can offset the essential energy loss due to foot-ground collision and stabilize sagittal-plane limb motion patterns. It may simultaneously assist lateral (frontal-plane) balance. Difficult to train on a treadmill, this is an essential component of normal locomotion, especially important during turns.

In a pilot experiment, we perturbed the gait of unimpaired human subjects by applying torque to the ankle at various frequencies. With a properly designed perturbation, 8 subjects out of 10 exhibited entrained gaits: their gait frequencies were adapted to the frequency of mechanical perturbation, and they synchronized their ankle actuation with the torque supplied by the robot. Entraining human gait with periodic torque from a robot may provide an approach to walking therapy that is uniquely supportive of normal biological function. Based on a patient's performance, a robot may entrain the patient's walking frequency and gradually "drag" it towards a normal walking frequency. By controlling the robotic torque frequency and amplitude, assistance can be adjusted continuously to promote patient participation, an essential element of successful upper-extremity neuro-restoration. Moreover, this approach may be able to promote recovery without significant involvement of supraspinal input, especially important for rehabilitation after spinal cord injury.

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Elliptical Fourier Analysis of Joint Angle Phase Portraits: Application to Simulated Injury

Louis DiBerardino III
Department of Mechanical Science and Engineering, University of Illinois

Jesse Spencer-Smith
Department of Psychology, University of Illinois

John Polk
Department of Anthropology, University of Illinois

Karl Rosengren
Departments of Psychology and Kinesiology, University of Illinois

Elizabeth Hsiao-Wecksler
Department of Mechanical Science and Engineering, University of Illinois
ethw@illinois.edu

Human gait can be described as a complex dynamical system. Clinicians and researchers characterizing gait have typically examined a limited number of variables at a time, and mainly described gait using univariate and qualitative methods. Phase portraits of a leg segment's angular displacement versus velocity are commonly used to illustrate the complexity of a population's gait, or the differences in complexity and variability between populations. Past studies have mainly focused on simplistic measures of the phase portraits and qualitative descriptions of their behavior [1]. In our previous work, we have applied a method [2] for describing closed contours with elliptical Fourier series to aid in quantifying the changes in gait complexity and variability throughout gait development [3]. We have also investigated differences between healthy children and those diagnosed with developmental coordination disorder [4]. We now apply this quantitative analysis of phase portraits to a population with simulated injury. We recorded kinematic data for 20 healthy adults walking on a treadmill for 21 consecutive gait cycles with and without a knee brace to prevent flexion and create an exaggerated effect of injury. We found a drastic decrease in complexity and variability of the foot, shank and thigh segments on the braced leg. These changes were expected since the brace limited the allowable motion of that leg; however, our approach enables greater quantification of the variation from normal. Using this approach we were not able to detect changes in complexity of the contralateral limb during bracing, which would display a compensation for the decreased range of motion of the braced knee. Only a slight trend was observed. The overall result of the study is encouraging in that our methods displayed the expected differences between the braced and non-braced leg very well, however it seems that this method lacks the sensitivity to detect changes in the movement pattern of the contralateral limb.

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A Linear Controller in Combination with a Model of the Ankle Torque Generation Process for Control System of Human Standing Balance

Kei Masani
Scientist
Lyndhurst Centre, Toronto Rehabilitation Institute

Albert H. Vette
PhD Candidate
Institute of Biomaterials and Biomedical Engineering, University of Toronto

Milos R. Popovic
Associate Professor
Institute of Biomaterials and Biomedical Engineering, University of Toronto

In the clinical field, postural sway during quiet standing has been used to assess the balance ability of various populations. The physiological control system of balancing the body in the upright posture has been intensively studied and debated. A feed-forward control mechanism has been proposed to regulate the neural torque that can compensate for the neural transmission delay [1]. On the contrary, also a simple linear feedback model has been suggested to represent the neural control system [2]. In this context, it has been shown by our team that a neural feedback system regulated by a proportional and derivative (PD) controller with a high derivative gain can stabilize the postural control system despite the neural transmission delay [3]. Additionally, we recently demonstrated that the ankle torque generation process is a source of a large delay in the control system, and that a neural controller with a high derivative gain can stabilize the body despite this large delay as long as half of the required torque is provided by mechanical stiffness around the ankle joint [4]. The identified postural control model successfully accounts for the fluctuation of the resultant ankle torque during quiet standing [5]. Further, our postural control model has the potential to characterize the differences in the control schemes of the elderly and the young. For example, the lower stability in the elderly is primarily caused by a smaller stiffness and, as a consequence, the elderly highly depend on the neural derivative gain to compensate for a long feedback time delay.

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Modeling and Analysis of Posturographic Data Using Markov Chains

Pilwon Hur
PhD Candidate
Department of Mechanical Science and Engineering, University of Illinois

K. Alex Shorter
PhD Candidate
Department of Mechanical Science and Engineering, University of Illinois

Elizabeth T. Hsiao-Wecksler*
Department of Mechanical Science and Engineering, University of Illinois
ethw@illinois.edu

Posturographic data collected during quiet stance using force plates is widely used to assess postural stability [1]. Center of pressure (COP), the location of the resultant reaction force underneath the subject's feet, is a commonly used experimental variable for several types of analyses. Traditionally, COP data has been analyzed using measures that describe the shape or speed of the trajectory [1]. However, these parameters do not provide insight into the physiological system as a whole, and have been shown to have questionable reliability [2]. Collins and DeLuca addressed this problem by modeling the COP trajectory as a one or two dimensional random walk, and created Stabilogram Diffusion Analysis (SDA, a stochastic analysis) to characterize short term (open loop) and long term (closed loop) postural control strategies [3]. While SDA characterizes underlying behavior in the data set, the characterization of the long term behavior can be improved. The goal of this work was to utilize a Markov chain model of the COP data to provide new insight into the long term behavior of quiet standing data.

In this study, we consider the COP as the output that results from the stabilizing mechanism of the human postural control system. This dynamical system is a stochastic process and does not have closed form equations [3]. As a result, a Markov chain with a finite state space was used to describe the system's dynamic evolution. States were defined as set distances away from a center point (i.e., the average value of the COP for the entire trial). The transition probability from one state to another was described with a probability transition matrix (P) [4]. In our case, P was defined as the probability that the current state (a given distance from the mean COP value to the current COP value) will evolve to another state. The invariant density of the Markov chain was found using the probability transition matrix, P. Invariant density is the distribution where the Markov chain converges regardless of the system's initial conditions and describes the asymptotic behavior of the system [4]. Invariant density describes the probability of finding the COP at any given distance away from the center. The peak value of the invariant density can be interpreted physically as the distance within which the COP is most likely to be found. Spectral decomposition was used to compute the approximate time for the COP to reach its invariant density.

Using the derived invariant density, four parameters that describe the long term behavior of the system were defined: peak probability (Ppeak), distance from center to peak probability (Dpeak), distance to 95% cumulative probability (D95), and time to reach Invariant Density (Tinv). Quiet stance trials were conducted with three different age groups: young adult (YA), middle-aged adult (MA), and old adult (OA). The results showed Ppeak decreased as age increased, while Dpeak, D95, and Tinv increased as age increased. YA and MA age groups were statistically different from OA at two parameters ($p<0.05$): Ppeak ($p=0.001$) and D95 ($p<0.001$). Additionally, a nearly significant difference was present in Tinv ($p=0.07$). Therefore, invariant density analysis (IDA) can be used as a tool to characterize posturographic data.

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Inter-trial Dynamics in a Shuffleboard Task: Theory and Experiment

Joby John
Graduate Research Assistant
Penn State University

Joseph P. Cusumano
Penn State University

Variability is apparent in all human movement, and is observable in repeated performance of goal-oriented tasks [1]. The effect of this variability on performance can be understood by studying the inter-trial dynamics involved and by analyzing the data from repeated trials in light of the concepts of goal function and goal equivalent manifold (GEM) [2, 3]. We present a modeling paradigm for inter-trial task dynamics that allows one to understand how performance, as measured by goal level variability, is generated. The modeling approach involves a precise definition of the task using a goal function, an in-trial controller or action template, and an inter-trial controller that uses goal-level error feedback to closes the perception-action loop [4, 5]. We describe the modeling methodology in general terms, and discuss the development of a virtual physics shuffleboard experiment for testing theoretical predictions from the models. The GEM for the shuffleboard task is completely determined by the release position and velocity of the puck, as these variables completely determine whether the subject attains the goal or not in any given trial. The subject performs the task using a custom-made manipulandum that moves a virtual puck in the virtual 3D environment. Visual feedback of the current trial's goal-level error is used to correct the subsequent trial in an attempt to converge on the GEM and hence attain the goal. The subject controls only end-effector used to launch the puck for each trial: other components of the perception-action loop, such as the physics, shuffleboard court geometry, and the representation of the goal-level error, are handled by the virtual environment. We illustrate how the dynamical task models drive the analysis of data from the experiments. Specifically, we discuss the decomposition of body variability into goal-relevant and goal-irrelevant components, and use the data to obtain a body-goal variability map [2] that shows how goal-level error is related to body-level variability. We conclude by discussing how the modeling methodology and the data analysis methods presented here can be used to model a whole class of discrete tasks by replacing components of the perception-action loop accordingly. In addition, the "human in the loop" computer interface used for our experiment provides a rich ground for easy implementation of various alternative experimental protocols.

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Analysis and Classification Methods for Healthy and Cruciate-Deficient Dogs

Louis DiBerardino III
Mechanical Science and Engineering, University of Illinois

Sungjin Hong
Psychology, University of Illinois

Chantal Ragetly
Veterinary Clinical Medicine, University of Illinois

Jason Thomas
Mechanical Science and Engineering, University of Illinois

Elizabeth Hsiao-Wecksler*
Mechanical Science & Engineering, University of Illinois
ethw@illinois.edu

Testing and analysis of canine gait dynamics has been quite limited. Also, due to the inherent problems of recording forces with quadrupeds, many studies focus only on kinematics or ground reaction forces alone [1,2]. Here, we try to apply similar techniques used in distinguishing injured and healthy human gait to populations of injured and healthy dogs. Previously obtained motion data [3] for 12 healthy adult Labrador Retrievers and 10 with unilateral cranial cruciate ligament injury trotting over ground with a single force plate were analyzed. The goal of this work is to temporally determine how these groups differ using normally studied gait variables such as joint angular position or moment, and also create a classification function that has the ability to correctly diagnose future dogs based on their gait dynamics. In order to determine the significantly different time regions, we modify the technique developed by Shorter, et al. [4] by applying a two-sample t-test between the groups for each time point. The regions where the null hypothesis of equal group means is rejected for each variable agree quite well with the "regions of deviation" as defined by Shorter, et. al., while providing results based on an improved statistical foundation. Each of the significant time points is then considered a separate variable for the purpose of creating a discriminant function between the groups. Only the first nine principal components were used since the number of observations (subjects) in each group must be greater than the number of variables (time points) used to discriminate the two groups. The classification accuracy of the function was evaluated by a holdout method, which derives a discriminant function from data for all but one subject to classify it with. Preliminary results are encouraging, with only three misclassifications out of 22. It seems to be quite possible, with the addition of other gait parameters or EMG of muscle activity, to almost perfectly diagnose or track recovery of an injured dog using these techniques on experimental gait dynamics.

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Bifurcations Drawn by the Cell Mapping Method for Gait Asymmetries Based on Passive Dynamic Walking

Jae-Sung Moon
PhD Student
Coordinated Science Laboratory, University of Illinois

Mark W. Spong
Coordinated Science Laboratory, University of Illinois

Bifurcations caused by asymmetries of a compass gait biped are exploited within the context of passive dynamic walking pioneered by McGeer [1]. The assumptions and development of the 2D model follow the methods of Gosami et. al. [2] and two different dynamics for left and right legs are derived to examine the asymmetries. Based on the idea of cell mapping proposed by Hsu [3], we introduce a generalized algorithm to plot bifurcation diagrams showing period doubling as parameters are varied. One of the parameters is the ratio of leg masses which represents the asymmetries and the other is the slope angle which exhibits a variety of bifurcations. It is found that the bifurcations can be grouped into six stages some of which have not been reported yet and we discuss the features of them in detail. The rate of convergence of the period doubling sequences is in good agreement with the Feigenbaum delta constant [4].

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Choosing the Right Postural Perturbation for Studies at the Threshold of Balance Recovery: Nature and Direction

Cecile Smeesters*
Associate Professor
Department of Mechanical Engineering, Université de Sherbrooke
Cecile.Smeesters@USherbrooke.ca

Kodjo Enyonam Moglo
Postdoctoral Student
Department of Mechanical Engineering, Université de Sherbrooke

Alessandro Telonio
Doctoral Student
Department of Mechanical Engineering, Université de Sherbrooke

Comparisons between experiments at the threshold of balance recovery, where avoiding a fall is not always possible, are complicated by A) differences in the nature of the postural perturbations and the presence (trip, slip or pull) or absence (lean, pull or translation) of initial velocity [1] as well as B) differences in loss of balance direction (forward, sideways or backward) [2-4]. In our first study we determined A1) the maximum forward lean angle (MLA) that 10 younger and 10 older healthy adults could be suddenly released from and still recover balance using a single step for 3 pull forces and A2) the maximum forward pull force (MPF) that they could suddenly sustain and still recover balance using a single step for 3 walking velocities [1]. Results showed that different postural perturbations are clearly not the same (increasing pull force decreased MLA and increasing walking velocity decreased MPF). They are however similar (stepping kinematics at MLA and MPF trials were nearly identical). They can thus be compared (lean angle positions and velocities at the end of reaction time for MLA and MPF trials formed a disturbance threshold line (DTL) separating falls from recoveries). Moreover, we found a 39% decrease of DTL with age. In our second study, the MLA that 16 younger and 16 older healthy adults could be suddenly released from and still recover balance using a single step was determined for B1) forward B2) sideways and B3) backward leans [2]. Results showed that lean direction significantly affected MLA (forward MLA > backward MLA > sideways MLA). Age also significantly affected MLA (29% forward, 24% backward and 36% sideways age-related reduction). Moreover, age and lean direction significantly affected stepping kinematics at MLA trials. Finally, while balance (11-17%) and reaction time (1-4%) also contributed, muscular power (65-72%) was the best predictors of the ability to recover balance to avoid a fall [3]. In fact, step velocity (65-83%) was the best performance measure to predict MLA [4]. We have thus demonstrated that all postural perturbations at the threshold of balance recovery, whether with or without initial velocities, appear to be equally valid to study falls. However, different loss of balance directions cannot be compared.

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Discriminating a Successful from a Failed Balance Recovery: Instruction and Harness Failures

Cécile Smeesters*
Department of Mechanical Engineering, Université de Sherbrooke
Cecile.Smeesters@USherbrooke.ca

Marc-André Cyr
Master's Student
Department of Mechanical Engineering, Université de Sherbrooke

In experiments at the threshold of balance recovery, where avoiding a fall is not always possible, an unsuccessful balance recovery is defined in two ways: the participant does not respect the instructions regarding how to recover balance (instruction failure) or the safety harness system assists the participant in balance recovery (harness failure) [1]. Our first objective was to determine the effect of instructions limiting the number of steps on the threshold of balance recovery [2-3]. Our second objective was to propose a method to determine the maximum allowable force on a safety harness cable to discriminate a successful from a failed balance recovery [4]. To do so, we determined the maximum forward lean angles that 28 younger adults could be suddenly released from and still recover balance using: i) only a single step, ii) no more than two steps and iii) no limit on the number of steps. For 12 of the participants, the coefficients of an asymptotic regression, between the maximum vertical force on the safety harness cable and the initial lean angle at each trial, were also evaluated by a least squares method. Results showed that a maximum allowable vertical force of five force constants (23.0% body weight on our safety harness system) insured that the initial lean angle reached 99% of its steady state value with respect to its initial value [4]. It thus discriminated well a successful (below the threshold) from a failed (above the threshold) balance recovery. Results also showed that instructions limiting the number of steps significantly affected the maximum lean angle but only by a maximum of 1deg [2-3]. Furthermore, at the maximum lean angles, they significantly affected reaction time, first weight transfer time, first stride time, first stride velocity, first stride length and second stride velocity but only by 8% on average. However, they did not affect muscular latencies, first stride height, first stride width, other second step kinematics or first step peak normalized joint torques. Since the maximum lean angles were similar and first step kinematics and kinetics were nearly identical, we have thus demonstrated that instructions limiting or not limiting the number of steps appear to be equally valid to study falls in younger adults.

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Relative Effects of Weight Loss and Strength Gain on Balance Recovery from a Forward Fall

Sara Matrangola*
Research Assistant
School of Biomedical Engineering and Sciences, Virginia Polytechnic Institute and State University
smatrang@vt.edu

Michael Madigan
Department of Engineering Science and Mechanics, Virginia Polytechnic Institute and State University

Obesity is a growing epidemic in the United States. Between 1999 and 2004, the prevalence of obesity increased from 27.5% to 31.1% in US adult men[1]. Obesity is associated with an increased risk of falls and subsequent injury [2]. Previous studies have shown weight loss [2] and strength training [3] to be beneficial to balance, but knowing which is more beneficial will allow researchers to design interventions to maximize the benefits in terms of balance and reducing risk of falls. Therefore, the purpose of the first study was to evaluate the effects of weight loss and strength training on balance recovery using a combination of laboratory experiments and mathematical modeling. Nine male subjects with BMI 30.1 to 36.9kg/m2 were released from a forward lean and attempted to recover balance using an ankle strategy. Lean angle was increased until subjects required a step or hip flexion to recover balance. The maximum lean angle, max, was used as the measure of balance recovery capability.

Experimental data was used as inputs to an inverted pendulum model of balance recovery. The 2-D model included a slender rod rotating about a hinge joint to model the body rotating about the ankle joints. A torque actuator about the ankle was used to represent the effect of the ankle muscles. Multiple simulations were used to determine the effects of strength (maximum ankle torque and ankle torque generation rate) and weight loss on max. Changes in weight and strength were linearly related to changes in max. A 6.6 ± 0.4% decrease in weight or 6.9 ± 0.9% increase in strength would be required to improve max by 1 degree. Based on these results, balance recovery using an ankle strategy can improve with both reductions in weight and increases in strength. In addition, weight loss may be a more effective intervention than strength gain at improving balance recovery capability.

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The Effects of Horizontal Support Surface and Visual Field Oscillations on the Orbital Stability of Human Walking

Jonathan B. Dingwell
Associate Professor
Kinesiology, University of Texas at Austin

Patricia M. McAndrew
Graduate Assistant
Biomedical Engineering, University of Texas at Austin

Jason M. Wilken
Director, Military Performance Lab, Center for the Intrepid, Brooke Army Medical Center

In robotics, walking is commonly assumed to exhibit limit cycle dynamics, where local stability is quantified using maximum Floquet multipliers (FM) [1]. In humans, Polio patients exhibited larger maximum FM (i.e., less stable) than healthy controls [2] and healthy elderly were similarly less stable than young subjects [3] during unperturbed walking. However, maximum FM did not increase when perturbations of increasing amplitude were applied to a passive dynamic model of walking [4]. Changes in FM have not been assessed in humans during perturbed walking. Therefore, this study determined how horizontal perturbations of the walking surface and visual field affected gait stability. Twelve young healthy subjects walked in a well-controlled virtual reality environment under 5 conditions: no perturbations (NOP), anterior-posterior platform (APP) or visual (APV) translations, or mediolateral platform (MLP) or visual (MLV) translations. Oscillations were applied as a continuous pseudo-random sum of sines. Kinematic data for the motions of a single marker placed on the 7th cervical (C7) vertebra were recorded and analyzed. Power spectral analyses of the C7 marker movements exhibited significantly greater spectral power at all perturbation frequencies for all conditions. Subjects also exhibited significantly increased kinematic variability during perturbed walking. Thus, the applied perturbations significantly altered each subjects' kinematics. To quantify orbital stability, maximum Floquet multipliers (FM) were computed for each time series. State-spaces were generated using 3-dimensional velocities and accelerations of the C7 marker. In spite of the significant kinematic deviations observed, subjects remained orbitally stable (maximum FM < 1) for all experimental conditions. Maximum FM magnitudes did NOT increase significantly for any perturbation condition, confirming previous modeling predictions [4]. These results indicate that inducing greater variability does not necessarily induce greater instability. What these FMs do not reflect, however, is how people achieved stability. While these FM appear to represent overall gait "stability", they may not in fact be sensitive enough to predict risk of falling.

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Local and Orbital Dynamic Stability of Walking in Healthy Young and Older Adults

Jonathan Dingwell
Associate Professor
Kinesiology, University of Texas at Austin

Hyun Gu Kang
Postdoctoral Fellow
Institute for Aging Research, Hebrew SeniorLife

Falls pose a tremendous risk to those over 65 and most falls occur during walking. Walking slower is common in the elderly [1], is related to fear of falls [2] and may help improve stability. In young adults, walking slower leads to improved local dynamic stability, despite also leading to greater variability [3]. However, very healthy active elderly who walk at the same preferred speeds as young adults still exhibit increased variability, which also increases at slower speeds [4]. This study was conducted to try to resolve this seeming paradox. Eighteen healthy older adults (72±6 yrs) and 17 height- and weight-matched young adults (23±3 yrs) walked on a treadmill at each of 5 speeds [4]. Motions of the trunk segment were recorded and used to quantify dynamic stability using local divergence exponents and maximum Floquet multipliers (FM) [5]. Isometric leg strengths and passive ranges of motion (ROM) were also measured to account for age-related differences. These healthy older subjects walked with the same preferred walking speeds as the younger subjects ($p = 0.860$) [4]. However, they also still exhibited greater local divergence exponents ($p<0.0001$) and higher maximum FM ($p<0.007$) than young adults at each walking speed. These older adults remained more unstable ($p<0.04$) even after adjusting for their decreased strength and flexibility. In both groups, local divergence exponents decreased at slower speeds and increased at faster speeds ($p<0.0001$), similar to [3]. Maximum FM showed similar changes with speed ($p<0.02$). These older adults were healthy enough to walk at normal speeds. However, they were still more locally unstable than the young adults, independent of walking speed. This greater instability was not explained by loss of strength or flexibility. Other age-related physiological changes, like increased neuromotor noise, may also be important determinants of walking stability.

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The Role of Proprioception in Modeling Dynamic Neuromotor Control of Joint Motion

Sara E. Wilson
Department of Mechanical Engineering, University of Kansas

Feedback control of joint motion requires the ability to sense joint motion. Proprioceptive (sensory) elements, such as the muscle spindle organs, play an important sensory role that should not be neglected when modeling dynamic control of joint motion. It has been suggested that such elements can have a nonlinear, proportional-derivative response which can include a sensory threshold [1]. Proprioception can be affected by age, disease, and occupational exposures. It is important to be able to model these changes in the nonlinear sensory response in order to understand the effects of age, disease and occupational exposures on dynamic motion. For example, we have observed that with occupational whole body vibration exposure, the ability to sense lumbar posture decreases [2]. This can be modeled as an increase in the sensory threshold. Using a simple, inverted pendulum model of the trunk with a single, time-delayed, thresholded, proportional response, an increase in the sensory threshold has a number of effects on the dynamic response to a perturbation including a delayed muscular response and increased trunk deflection. Experimentally, such effects have been confirmed to occur in sudden trunk loading experiments performed before and after vibration exposure [2-4]. This model can be further developed to include the proportional-derivative behavior of the muscle spindle organs. While this model is simple, it demonstrates the potential benefit of improving modeling of the sensory system in dynamic models of neuromotor joint control. Improved understanding of the feedback mechanisms that exist is necessary to better develop such models.

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Algorithms and Computer-Aided Tools for Predicting Progression of Three-Dimensional Spinal Deformity in Patients with Idiopathic Adolescent Scoliosis

Harry Dankowicz
Associate Professor
Mechanical Science and Engineering, University of Illinois

Jeffrey Shilt, MD
St. Alphonsus Regional Medical Center

Scoliosis affects about 2 % of the population and is most commonly seen in children 10 years or older. The current clinical paradigm for quantifying the degree and nature of the spinal deformity, assessing the need for external bracing or surgical correction, and designing the surgical corrective instrumentation is poorly resolved and highly personnel intensive. In a non-negligible number of cases, corrective surgery is unable to satisfactorily address the primary deformity or prevent the occurrence of postoperative, secondary deformities away from the region of fixation.

Management of adolescent scoliosis and prospective treatment analysis relies on the ability of the physician to predict the progression of severity of spinal deformation. A number of clinical measures, including gender, skeletal maturity, bone density, and brace treatment have been shown to provide information about the likelihood of progression and ultimate need for surgical intervention. This talk reports on an ongoing effort to develop a predictive computer-aided algorithm with which the progression of the three-dimensional deformity in patients with scoliosis can be monitored over time. Past work has resulted in the WINDOWS-based software application SPINECAD and a set of image-processing algorithms for reconstructing a three-dimensional representation of the vertebral column given reasonable-quality anterior-posterior and lateral radiographs; for quantifying the three-dimensional properties of the vertebral column; and for characterizing the deformity according to the Lenke classification scheme for scoliotic spines. In the current effort, an initial three-dimensional reconstruction of the spine is combined with the limited data provided by subsequent anterior-posterior radiographs, and with mathematical models of the rate of spinal growth and local rates of change of curve shape, to generate an estimated three-dimensional reconstruction of the spine without the need for additional lateral images, CT, or MRI scans.

A State Space Perspective of Dynamic Torso Stability

Martin L. Tanaka*
Instructor
Department of Orthopedic Surgery, Wake Forest University
mtanaka@wfubmc.edu

Shane D. Ross
Department of Engineering Science and Mechanics, Virginia Polytechnic Institute and State University

Low back pain is often associated with torso instability that may result in potentially injurious motion. Yet little information is available on the dynamic stability of the spine and core musculature. In previous experimental studies stability diffusion analysis [1] and the time series averaged finite time Lyapunov exponent (FTLE) [2] were calculated to determine the local dynamic stability of the system. However, additional information can be extracted from the time series data. Rather than averaging the Lyapunov exponents over state space to obtain a single scalar value (traditional method), one can generate a FTLE field. This field quantifies the expansion rate at different locations in state space and may be used to locate separatrices demarking the boundary between stable and unstable trajectories.

In order to improve the fundamental understanding of this medical condition, mathematical models were developed based on seated torso stability experiments. Lagrangian coherent structures (LCS), ridges in the state space distribution of the FTLE field, were used to locate basins of stability [3]. We demonstrate how LCS can be found from time series data without knowledge of the complete vector field as required by previous approaches [4]. As a result, this approach was shown to be well suited for biomechanics experiments where often only time series data is available. Furthermore, since LCS are robust to noise [5] this approach is even more attractive for use with experimental data analysis where noise sensitivity is an important issue. We also illustrate how morphing was used to identify stable PD control gain parameters for the forward dynamic simulation that could not otherwise be determined. Finally, we present the basins of stability for the models and locations of the equilibrium manifolds.

The basin of stability in state space provides a richer understanding of the system dynamics than a single scalar value (previous methods). The boundary, or recovery envelope, could be used in conjunction with sway data to define new measures of individual fall risk, e.g., the average distance of an individuals state from the boundary. In general, we believe the method demonstrated in this study provides a fruitful approach for extracting additional information from noisy experimental data, namely boundaries between qualitatively different kinds of motion.

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Nonlinear Localization and Targeted Energy Transfer Phenomena in Dynamical Systems

SYMPOSIUM N

ORGANIZER:

Alexander Vakakis, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Synchronous and Localized Dynamics in Systems of Torsional Vibration Absorbers

Steven Shaw*
Professor
Mechanical Engineering, Michigan State University
shawsw@msu.edu

Alan Haddow
Associate Professor
Mechanical Engineering, Michigan State University

Centrifugally driven pendulum absorbers are a proven means of reducing torsional vibrations in rotating machinery. These absorbers are naturally order-tuned, that is, their natural frequency is proportional to the mean rotor speed, making them effective for counteracting vibrations that arise from engine-order excitation [1]. The absorbers consist essentially of masses that passively move along prescribed paths relative to the rotor, typically using a bifilar (two point) suspension. Most absorber configurations employ a set of identical absorber masses arranged around and/or along the rotor in order to satisfy balancing and packaging constraints. In such cases the desired system response is synchronous, wherein all absorbers move with the same amplitude and phase. However, a set of identical absorbers possesses an inherent symmetry that leads to rich dynamics, including bifurcations of the synchronous response that result in a variety of non-synchronous responses. Common among these are localized responses in which one absorber experiences a response whose amplitude is much larger than the others [2]. These responses are detrimental to absorber function, since they result in a smaller operating range [3]. In this talk we survey these analytical results and describe controlled experiments which demonstrate a wide range of possible system responses, including localized motions. In addition, we show how one can avoid such responses by proper absorber path selection and describe ongoing development of these absorbers for fuel-efficient automotive engines.

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Exploration of Nonlinear Shunting Strategies as Effective Vibration Absorbers

Régis Viguié
Aerospace Engineer, PhD Student
Department of Aerospace and Mechanical Engineering (S3L), University of Liège

Gaëtan Kerschen
Department of Aerospace and Mechanical Engineering (S3L), University of Liège

Massimo Ruzzene
School of Aerospace Engineering, Georgia Institute of Technology

The tuned mass damper (TMD) is a simple and efficient device, but it is only effective when it is precisely tuned to the frequency of a particular vibration mode. In order to overcome this limitation, the nonlinear energy pumping phenomenon from a main mechanical structure to a local, passive nonlinear energy sink (NES) is investigated. Unlike the TMD, an NES has no preferential resonant frequency, which makes it a good candidate for vibration mitigation of MDOF linear and nonlinear vibrating structures. However, in addition to the rattle space requirements, the mechanical implementation of the nonlinear absorber poses serious challenges. This is why piezoelectric shunting is considered in this study. Specifically, the objective of the paper is to develop a suitable association of piezoelectric patches and nonlinear shunted electrical circuits, such that the effects of the NES would be electrically reproduced.

Numerical Evidence for Targeted Energy Transfer in Pure Plastic Oscillators and Damage Oscillators

Franziska Schmidt*
DR/DGCB/LGM, Ecole Nationale des Travaux Publics de l'Etat Franziska
SCHMIDT@entpe.fr

Claude-Henri Lamarque
Professor
DR/DGCB/LGM, Ecole Nationale des Travaux Publics de l'Etat

The phenomenon of targeted energy transfer is widely and deeply studied ([3, 4]) because it makes it possible to take off some energy from one specific structure we want to preserve and transfer it to another one. Generally, this last one, auxiliary structure is taken to be an essentially nonlinear (cubic) oscillator and this transfer is done by linear coupling between this last structure and the main one. Many other cases are studied in the literature, but the structure is generally supposed to be either linear elastic or at least smooth. So nor residual distortion, neither uncertainty in modelling is taken into account.

We use the system studied generally to show the phenomenon of energy pumping, but allowing the linear structure to undergo plastic deformation and residual damage (even initial). To do this, we introduce two different behaviors: one pure plastic behavior (see [1]) and one plastic behavior with damage (see[2]). We thus obtain a system of ordinary differential equations, some of them treating the memory variables. Then, we perform numerical simulations to investigate the behaviors of the free and forced dynamical systems leading to energy transfer when the behavior is elastic. The numerical results we obtain are coherent with some others we already had by studying the pure plastic system in introducing Saint-Venant elements. Thus we observe that differents consequences may appear: indeed energy transfer may happen or not, and if it occurs, it may be altered or not, due to the dissipation.

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On Energy Transfer: Theoretical Aspects, Numerical Results, and an Active Control Approach

José Manoel Balthazar*
Demac, UNESP Rio Claro
jmbaltha@rc.unesp.br

In this work, numerical investigations are carried out on a linear structure, weakly coupled to a small nonlinear attachment. The essential nonlinearity of the attachment enables it to resonate with any of the linearized modes of the structure leading to nonlinear energy pumping. The underlying dynamics governing this phenomenon is a 1: 1 resonance capture on a resonant manifold of the combined system. Properly designed nonlinear attachments with essential nonlinearities can act, in essence, as nonlinear energy sinks (NESs); that is, they passively absorb energies generated by transient disturbances in the main system to which they are weakly attached. In contrast to the classical linear vibration absorber whose effectiveness is restricted to narrowband frequency ranges, (NESs) effectively absorb energies of broadband transient disturbances.The term energy pumping is used here to refer to the irreversible transfer of vibration energy from its point of generation into a predetermined spatial area (the nonlinear energy sink) in which the vibration localizes and dissipates. It is to be emphasized that this transition of energy is controlled (i.e. it occurs over a wide range of initial conditions of the excitation), and it is one-way (i.e. energy does not flow out of the localizing area). There is an obvious advantage of such features in the context of vibration isolation: it promotes a very robust behavior of the isolator under a variety of excitations and without relying upon "special" procedures for eliminating the unwanted motions. Here, NESs) are considered with smooth and essential (nonlinearizable) nonlinearities that enabled resonance interactions of the NESs with modes of the (linear) main system possessing arbitrary eigenfrequencies. This may lead to resonance capture cascades, where, with decreasing overall energy due to damping, a (NES) interacts consequently with a series of linear modes (typically from high to low frequency), extracting a certain amount of energy from each before interacting with the next.

Identification of the Slow-Flow Dynamics of Transonic Aeroelastic Response from Time-Series Data

Young S. Lee
Postdoctoral Researcher
Aerospace Engineering, University of Illinois

Alexander F. Vakakis
Professor
Division of Mechanics, National Technical University of Athens

D. Michael McFarland
Research Associate Professor
Aerospace Engineering, University of Illinois

Gaetan Kerschen
Assistant Professor
Aerospace and Mechanical Engineering Department (LTAS), University of Liege

Lawrence A. Bergman
Professor
Aerospace Engineering, University of Illinois

Recent advances in the nonparametric identification of strongly nonlinear dynamic systems hold promise for generating low-order models capable of reproducing complex responses, including transient internal resonances, frequency shifts, and energy transfer between substructures [1, 2]. The techniques employed here build on the empirical mode decomposition and exploit the established relationship between the intrinsic mode functions extracted by the EMD and the slow-flow dynamics of the unknown system. In this paper, this slow-flow system identification (SFID) technique is applied to time-series data generated through the high-fidelity numerical simulation of the response of a flexible airfoil in transonic slow. Specifically, modal displacements and slopes obtained from linear finite element analysis of a jet-transport wing have been used along with the transonic small disturbance equations, as solved in discretized form by NASAs CAPTSDv program, to compute realistic aeroelastic responses under various flow conditions. SFID analysis of the resulting time histories has produced models exhibiting good quantitative agreement with the full simulation, capable of reproducing phenomena such as the transient heave response during the onset of pitch-dominated limit cycle oscillation. The results of this use of SFID are reviewed and their use in structural design alterations are investigated.

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On the Optimal Design of Goupillaud Type Layered Elastic Media

George A. Gazonas
Research Physicist
Weapons and Materials Research Directorate, U.S. Army Research Laboratory

Ani Velo
Department of Mathematics and Computer Science, University of San Diego

We study an optimal design problem involving wave propagation in a multilayered elastic medium subjected to a transient stress loading on one boundary. Optimal designs are those designs which minimize the stress wave amplitude for all time, in all layers. Exact solutions to optimal design problems of this nature (hyperbolic systems) are virtually nonexistent in the literature, but can be used for benchmarking or validating optimization codes which link formal nonlinear parameter estimation (optimization) routines with explicit finite element numerical codes [1]. Our previous work has presented exact analytical optimal designs for the two-layer case [1], and the extension to the three- and four-layer cases [2], but the solution to the five-layer case and natural extension to n-layers has remained elusive until now. To accomplish this, we use the method-of-characteristics to derive a system of linear recurrence relations for the stress amplitude in each layer of a multilayered elastic strip; these recurrence relations can be solved explicitly using the Mathematica software package for a system of up to three-layers. For systems of more than three layers, the algebraic complexity increases dramatically, but the recurrence relations can be simplified using z-transforms, and written in global matrix form [3]. The characteristic polynomial for the resulting system is palindromic in nature; roots of the polynomial which lie on the unit circle form a countably infinite set of optimal designs. Palindromic polynomials are finding increasing applications in mechanics [4], and pure and applied mathematics [5], but we are not aware of any other work that relates them to the optimal design of problems governed by hyperbolic field equations.

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Resonance Energy Transfer in Nonlinear Oscillatory Chains: From Small to Large Systems

Leonid Manevitch
Department of Polymer and Composite Materials, Institute of Chemical Physics RAS

Dr. Valeri V. Smirnov
Department of Polymer and Composite Materials, Institute of Chemical Physics RAS

We consider nonlinear oscillatory chain with polynomial potential of interparticle interaction, including quadratic, cubic and quartic terms. This system can be considered as model of a number of mechanical and physical systems. Despite it was a subject of intensive study in the context of Fermi-Pasta-Ulam problem and solitonic excitations, one of the most important aspects of nonlinear dynamics, energy transfer by discrete breathers, remains yet non-clarified one. We present an adequate approach to study of discrete breathers mobility and formulate the conditions of resonance energy transfer along the chain. A special attention is paid to transition from small systems to large ones in which continuum description for the breathers in the terms of modulating functions turns out to be valid. Both general and specific regularities of resonance energy transfer in the systems with different number degrees of freedom are studied in detail. We use for this the conception of limiting phase trajectory, introduced early by one of authors, and new notion of supernormal mode as well as conventional notions of stationary points and separatrix (for modulating variables). In these terms all qualitative transformations of phase plane in relative to amplitudes and asymmetry of potential clarified. We discuss also the conditions of transition from small to large system for which continuum description of the breathers in terms of modulating functions has been formulated. As an example of localized excitation in the large system the breather problem for zigzag chain modeling a plane stress has been solved. The conditions of discrete breathers mobility in large systems are discussed. At last, we consider the energy exchange in the system of weakly coupled FPU chains.

Seismic Protection of Multi-storey Steel Structures through Targeted Energy Transfer

Concetta Tripepi
Doctoral Student
Department of Mechanics and Materials, Mediterranean University of Reggio Calabria, Italy

Francesco Nucera
Postdoctoral Associate
Department of Mechanics and Materials, Mediterranean University of Reggio Calabria, Italy

Alexander Vakakis
Mechanics Division, School of Applied Mathematical and Physical Sciences, National Technical University of Athens

D. Michael McFarland
Research Associate and Professor
Department of Aerospace Engineering, University of Illinois

Lawrence Bergman
Department of Aerospace Engineering, University of Illinois

The aim of this work is to show that is possible to apply the Nonlinear Energy Sink (NES) concept to protect full scale seismically excited steel structures through Targeted Energy Transfer (TET). We consider, as primary (linear) systems, several multi-storey shear frames with beams sufficiently rigid so that the frame can reasonably be considered as shear-type. To each frame, we connect one or more NESs which can be either smooth or non-smooth, the latter a vibro-impact device (VI-NES). We study the performance and the robustness of the augmented structures excited by a set of historical earthquakes through a set of previously defined evaluation criteria and show that it is possible to drastically reduce the peak structural responses in sufficiently fast time scale to effectively control the parameters related to structural damage.

Targeted Energy Transfer in 3D of System: Coupled Oscillators with Close Frequencies Attached to Nonlinear Energy Sink

Oleg Gendelman
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Yuly Starosvetsky
Department of Mechanical Engineering, Technion, Israel Institute of Technology

System under investigation in present study is comprised of two weakly coupled linear oscillators with close natural frequencies and nonlinear energy sink (NES) attached to one of the linear oscillators. Linear subsystem (system of two weakly coupled oscillators) is subject to impulse excitation. Targeted energy transfer (TET) from the linear subsystem to the NES is studied analytically and numerically.

Main difference between current system and majority of systems with TET studied before is that since the frequencies of the linear subsystem are close, the NES interacts with beats of the linear subsystem, rather than with each linear frequency separately. Thus the motion which corresponds to 1:1:1 resonance should be studied. Analysis of such process requires investigation of dynamics in 5D state space of the averaged problem; it is much more complicated that 3D motion typical for common TET.

Present studies have revealed that for relatively high excitation values the transient part of the system response resembles a strongly modulated response (SMR). The TET in the system is realized via finite number of NES excitation cycles. Singular asymptotic analysis enables us to predict analytically the number of relaxation cycles done by the system and also to estimate the required amount of initial energy that should be supplied to the linear subsystem to invoke the transient relaxation. In order to predict the existence of the transient cycles the two dimensional mapping diagrams are constructed. Influence of various system parameters on the existence of the transient relaxations is also studied by the developed analytical and numerical methods.

Targeted Energy Transfer Phenomena in Acoustics, Experimental, and Numerical Results

Romain Bellet
PhD Student
Laboratoire de Mécanique et d'Acoustique, CNRS

Bruno Cochelin
Professor
Laboratoire de Mécanique et d'Acoustique, CNRS

Pierre-Olivier Mattei
Research Associate
Laboratoire de Mécanique et d'Acoustique, CNRS

Philippe Herzog
Research Associate
Laboratoire de Mécanique et d'Acoustique, CNRS

The association of a nonlinear oscillator to a linear primary system allows to observe the so-called targeted energy transfer phenomena in mechanics [1,2,3,5]. This presentation focuses on the application of this concept in acoustics as a new technique of passive sound control. The system considered is an acoustic medium (as the linear primary system) associated to an essentially nonlinear mechanical oscillator. An academic experimental set-up has been developped using the air vibrating on the first mode of a tube for the acoustic linear system, a thin circular visco-elastic membrane for the essentially cubic oscillator and the air inside a box as a weak coupling of those two elements [4]. A simple model based on the set-up has been also elaborated. This presentation deals with both experimental and numerical results about nonlinear localization and targeted energy transfer phenomena in acoustics. In the time domain and under harmonic forced excitation, we observe three different regimes depending on the amplitude of the source. For low and strong excitation amplitudes two periodic regimes are observed. The first one, obtained for low excitation amplitude, is localized on the acoustic medium and the other on the nonlinear oscillator. They correspond to two nonlinear modes of the system. In a limited range of moderate excitation amplitude, the vibratory regime is quasi-periodic and we can observe a repeated irreversible transfer of energy from the acoustic medium to the nonlinear oscillator. This targeted energy transfer phenomenon, also called energy pumping, is also visible on the free oscillations of the system. Indeed, above a threshold of initial excitation, the sound extinction in the tube follows a quasi-linear decrease that is much faster than the usual exponential one and during which the energy is irreversibly transfered to the membrane. Frequency responses have been also studied and between the same limited range of excitation levels, a clipping of the first resonance peak of the tube occurs. The membrane acts then as a sound limiter. Up to a certain threshold, whatever the excitation level, the sound level in the tube can not exceed a certain ceiling. Targeted energy transfer phenomena give then a good prespective in the sound limitation field in the high levels and low frequencies domains.

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Theoretical Understanding of Targeted Energy Transfers for Suppressing Aeroelastic Instabilities in a Nonlinear Aeroelastic Test Apparatus

Young Lee
Postdoctoral Research Associate
Department of Aerospace Engineering, University of Illinois

D. Michael McFarland
Research Associate Professor
Department of Aerospace Engineering, University of Illinois

Gaetan Kerschen
Department of Aerospace and Mechanical Engineering, University of Liege

Alexander Vakakis
Professor
Divison of Mechanics, National Technical University of Athens

Lawrence Bergman
Department of Aerospace Engineering, University of Illinois

Since a mechanism of triggering aeroelastic instability (or limit cycle oscillations; LCOs) in a 2-degree-of-freedom (DOF) rigid wing was investigated [1], a series of papers have been devoted to demonstrating applicability of passive, broadband targeted energy transfers (TETs) through a nonlinear energy sink (NES) to suppressing aeroelastic instability [2]; and to examining robustness enhancement of such suppression mechanisms by utilizing multi-DOF NESs [3]. Furthermore, experimental demonstration of LCO suppression mechanisms was performed in a nonlinear aeroelastic test apparatus (NATA) at Texas A&M University [4]. In this paper, we analytically study the LCO triggering of the NATA, based on which one can understand how the TET mechanisms observed in experiments worked out by attaching an NES to the wing structure. Utilizing a numerical continuation method, bifurcation analysis of LCOs is performed. Unlike the mathematical model, the experimental system involves friction at joints or contacts. Effects of such friction present for both structural modes (i.e., heave and pitch modes) are investigated in detail. By comparing friction effect to TET efficiency, we conclude that the aeroelastic instability occurred in the NATA was mitigated significantly due to TET activation, rather than due to friction.

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Wave Propagation in a Two-Dimensional Nonlinear Periodic Structure: A Perturbation Approach

Raj Kumar Narisetti*
Research Assistant
School of Aerospace Engineering, Georgia Institute of Technology
rajknarisetti@gatech.edu

Michael J. Leamy
School of Mechanical Engineering, Georgia Institute of Technology

Massimo Ruzzene
School of Aerospace Engineering, Georgia Institute of Technology

Wave propagation in a nonlinear two-dimensional periodic structure subjected to a point harmonic displacement is studied. The infinite lattice considered is modeled as a spring-mass system having linear and cubic (nonlinear) stiffness. Hard and soft nonlinear springs are considered. Response is captured by phase-constant contours dependent on excitation amplitude and the nonlinearity parameter. Within the pass band there is a frequency band termed the "caustic band" where the response is characterized by the appearance of caustics which give rise to low response regions or "dead zones" [1]. For a two-dimensional lattice having asymmetric nonlinearity, it is shown that these caustic bands are highly dependent on the excitation amplitude, unlike the linear model. A first order dispersion relation is obtained using a Lindstedt-Poincare' perturbation analysis. This approximate, closed-form solution is verified via comparisons to response generated using a time-domain simulation of a finite one-dimensional nonlinear chain. A Perfectly Matched Layer (PML) is appended to the finite system in order to simulate waves in the far-field. Results obtained are in very good agreement with those approximated by the perturbation analysis.

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Vibration-Based Energy Harvesting Based on Essential Nonlinearities

D. Dane Quinn
Department of Mechanical Engineering, The University of Akron

Angela A. Triplett
Student
Department of Mechanical Engineering, The University of Akron

Lawrence A. Bergman
Department of Department of Aeronautical and Astronautical Engineering, University of Illinios

Alexander F. Vakakis
Department of Applied Sciences, National Technical University of Athens

The capability to convert ambient mechanical energy to usable electrical energy offers a unique opportunity to develop a self-renewing source of energy that power applications, including portable electronics and inaccessible devices such as wireless sensors. Current research in energy harvesting seeks to increase the efficiency and performance of these devices, as measured by the power that can be obtain from external vibration sources. However, to achieve acceptable performance conventional vibration-based energy harvesting devices based on elements must be specifically tuned to match environmental conditions such as the frequency and amplitude of the external vibration. As the environmental conditions vary under ambient conditions the performance of these linear devices is dramatically decreased.

This work focuses on the use of essentially nonlinear components as the basis for vibration-based energy harvesting. Such components, which have no linear stiffness, have in the past served as the basis for passive damping through irreversible targeted energy transfer. In the present application their use allows for broadband harvesting of energy from ambient vibrations, thus reducing the need for tuning that is so prevalent with linear harvesters. These systems are studied using the method of averaging and their performance is compared to the corresponding mistuned linear systems.

Complex Fluids

ORGANIZER:

Paulo E. Arratia, *Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania*

SYMPOSIUM
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Transport and Collective Dynamics in Suspensions of Swimming Microorganisms

Michael Graham
Professor
Chemical and Biological Engineering, University of Wisconsin, Madison

A suspension of swimming organisms is an example of an "active" complex fluid. At the global scale, it has been suggested that swimming organisms such as krill can alter mixing in the oceans. At the laboratory scale, experiments with suspensions of swimming cells have revealed characteristic swirls and jets much larger than a single cell, as well as causing increased diffusivity of tracer particles. This enhanced diffusivity may have important consequences for how cells reach nutrients, as it indicates that the very act of swimming toward nutrients alters their distribution. The enhanced diffusivity has also been proposed as a scheme to improve transport in microfluidic devices and might be exploited in microfluidic cell culture of motile organisms or cells.

The feedback between the motion of swimming particles and the fluid flow generated by that motion is thus very important, but is as yet poorly understood. In this presentation we describe theory and simulations of hydrodynamically interacting microorganisms that shed some light on the observations. In the dilute limit, simple arguments reveal the dependence of swimmer and tracer velocities and diffusivities on concentration. As concentration increases, we show that cases exist in which the swimming motion generates dramatically enhanced transport in the fluid. This transport is coupled to the existence of long-range correlations of the fluid motion. Furthermore, the mode of swimming matters in a qualitative way: microorganisms pushed from behind by their flagella are predicted to exhibit enhanced transport and long-range correlations, while those pulled from the front are not. A physical argument supported by a mean field theory sheds light on the origin of these effects. These results imply that different types of swimmers have very different effects on the transport of nutrients or chemoattractants in their environment; this observation may be related to the evolution of different modes of swimming.

A Multiscale/Stabilized Finite Element Method for Incompressible Non-Newtonian Fluid Flows

Arif Masud
Associate Professor
Civil and Environmental Engineering, University of Illinois

JaeHyuk Kwack
Civil and Environmental Engineering, University of Illinois

We present a variational multiscale method for developing multiscale/stabilized finite element formulation of the Navier-Stokes equations for application to non-Newtonian fluids. Salient mathematical attributes of the method are highlighted. The multiscale formulation [1] possesses the superior properties of the state-of-the-art stabilized formulations, namely the SUPG and the GLS method. The new method can accommodate a variety of nonlinear models for viscosity, namely the power law [2], Casson [3], Cross [4], modified Cross [5], Carreau [5], Carreau-Yasuda [5] and Zhang model [3]. A comparative study of the performance of various commonly used nonlinear viscosity models is presented. Standard benchmark problems employing various element types show the superior numerical accuracy and convergence properties of the proposed finite element method. Test problems showing the application of the new method to bio-rheological fluids is also presented.

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Microfluidic Device with Coupled Confocal Imaging to Probe Viscoelastic Properties of Bacterial Biofilms

Michael Solomon
Chemical Engineering, University of Michigan

Dan Hohne
Chemical Engineering, University of Michigan

John Younger
Department of Emergency Medicine, University of Michigan

We characterize the viscoelasticity of bacterial biofilms by means of a microfluidic device. The biofilms are comprised of *Staphylococcus epidermidis* and *Klebsiella pneumoniae*. The presence of implanted foreign bodies such as central venous catheters is a key risk factor for infection by bacteria of this kind. To develop a model of therapeutic value that can predict bacterial floc development and fate in flowing blood, fundamental understanding of biofilm mechanical properties is required. Because of the sensitivity of biofilm properties to environmental conditions (such as degree of hydration), characterization of the mechanical properties of micron scale flocs that are of the actual size implicated in infection is desired. Thus, we developed a microfluidic device that uses the response of a flexible, deforming membrane to characterize the viscoelasticity of the test material. Attributes of the device are its simple fabrication and operation as well as its ability to accept biofilms grown at biologically relevant shear rates in the microfluidic environment. We find that the static and temporal responses of the valve membrane correlate well with the viscoelastic properties of a model gellan gum as simulated by finite element modeling. Measurement of steady-state deformation yields the linear elastic response of the biofilms as well as their yield strains. We also study the transient response of the PDMS membrane coupled to the biofilm when the system is subjected to a step stress of varying magnitude. By means of time-resolved confocal laser scanning microscopy we track the membrane deformation and thereby extract the viscoelastic relaxation time of the soft biological solid.

Non-invasive Biomechanical Assessment of Low-Reynolds Undulatory Swimming

Paulo Arratia
Assistant Professor
Department Mechanical Engineering & Applied Mechanics, University of Pennsylvania

Prashant Purohit
Department Mechanical Engineering & Applied Mechanics, University of Pennsylvania

Josue Sznitman
Department Mechanical Engineering & Applied Mechanics, University of Pennsylvania

Nematodes, such as *C. elegans*, achieve locomotion by using the bending motion of their body to propagate traveling waves along their length. While these low-Reynolds number swimmers (~1mm long) have long been described by theoretical fluid models (e.g. slender body theory), the implementation of such has been largely confined to prescribed analytical profiles of the animal body (i.e. traveling wave pattern). In the present work, we compute force and moment signals of C. elegans swimming at low-Reynolds numbers from image analysis using resistive force theory coupled with force and moment balances for the slender body. By combining experimentally obtained kinematic data and assuming the animal to be modeled as an elastic slender filament immersed in a viscous fluid, we investigate biomechanical properties (i.e. Young's modulus) of *C. elegans* which govern its bending motion.

Modeling the Inhomogeneous Response of Steady and Transient Flows of Entangled Micellar Solutions

Gareth McKinley
Professor
Mechanical Engineering, MIT

Lin Zhou
Visiting Professor
Mathematical Sciences, University of Delaware

L. Pamela Cook
Professor
Mathematical Sciences, University of Delaware

Surfactant molecules can self-assemble in solution into long flexible structures known as wormlike micelles. These structures entangle, forming a viscoelastic network similar to those in entangled polymer melts & solutions. However, in contrast to "inert" polymeric networks, wormlike micelles continuously break and reform leading to an additional relaxation mechanism and the name "living polymers." Observations in both classes of entangled fluids have shown that steady and transient shearing flows of these solutions exhibit spatial inhomogeneities such as shear-bands at sufficiently large applied strains. In the present work, we investigate the dynamical response of a class of two-species elastic network models [1, 2] which can capture, in a self-consistent manner, the creation and destruction of elastically-active network segments, as well as diffusive coupling between the microstructural conformations and the local state of stress in regions with large spatial gradients of local deformation. These models incorporate a discrete version of the micellar breakage and reforming dynamics originally proposed by Cates and capture, at least qualitatively, non-affine tube deformation and chain disentanglement. The "flow curves" of stress and apparent shear rate resulting from an assumption of homogeneous deformation is non-monotonic and linear stability analysis shows that the region of non-monotonic response is unstable. Calculation of the full inhomogeneous flow field results in localized shear bands that grow linearly in extent across the gap as the apparent shear rate increases. Time-dependent calculations in step strain, large amplitude oscillatory shear (LAOS) and in start up of steady shear flow show that the velocity profile in the gap and the total stress measured at the bounding surfaces are coupled and evolve in a complex non-monotonic manner as the shear bands develop and propagate. The model is able to capture many of the spatiotemporal features observed in recent detailed experimental measurements.

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Instabilities, Pattern Formation, and Mixing in Active Particle Suspensions

David Saintillan
Assistant Professor
Mechanical Science and Engineering, University of Illinois

Michael J. Shelley
Professor
Courant Institute of Mathematical Sciences, New York University

Suspensions of self-propelled particles, such as swimming microorganisms, are known to undergo complex dynamics as a result of hydrodynamic interactions. To elucidate these dynamics, a kinetic theory is developed and applied to study the linear stability and the non-linear pattern formation in these systems [1]. The evolution of a suspension of self-propelled particles is modeled using a continuity equation for the particle configurations, coupled to a mean-field description of the flow arising from the stress exerted by the particles on the fluid. Based on this model, we first investigate the stability of both aligned and isotropic suspensions. In aligned suspensions, an instability is shown to always occur at finite wavelengths, a result that extends previous predictions by Simha and Ramaswamy [2]. In isotropic suspensions, we demonstrate the existence of an instability for the active particle stress, in which shear stresses are eigenmodes and grow exponentially at long scales. Non-linear effects are also investigated using numerical simulations in two dimensions. These simulations confirm the results of the stability analysis, and the long-time non-linear behavior is shown to be characterized by the formation of strong density fluctuations, which merge and break up in time in a quasi-periodic fashion. These complex motions result in very efficient fluid mixing, which we quantify by means of a multiscale mixing norm.

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Electric Field Induced Self-Assembled Adjustable Monolayers

Nadine Aubry
Professor and Department Head
Mechanical Engineering, Carnegie Mellon University

Pushpendra Singh
Professor
Mechanical Engineering, New Jersey Institute of Technology

Muhammad Janjua
Mechanical Engineering, New Jersey Institute of Technology

Sai Nudurupati
Mechanical Engineering, New Jersey Institute of Technology

As chips further shrink toward smaller scales, fabrication processes based on the self-assembly of individual particles into patterns or structures are often sought. A popular technique used for two-dimensional assembly is based on capillary forces experienced by particles floating at fluid-fluid interfaces. However, capillarity-induced clustering has its limits: it is restricted to relatively large particles (with a radius greater than ~10m), the resulting lattice has defects and lacks long range order, and the distance between the particles cannot be adjusted (particles touch other). In this presentation, we will report recent work showing that these issues can be addressed by applying an external electric field normal to the interface[1]. The resulting self-assembly is capable of controlling the lattice spacing in either a static or a dynamic fashion, generating nearly defect-free monolayers, and using a variety of particle sizes and types such as nano-particles and electrically neutral particles. We will also explore the fundamental physics underlying such a phenomenon by presenting a simple model where both fluids and particles are assumed to be perfect dielectrics[2]. Specifically, we analyze the forces involved which are found to be of two kinds, capillary and electrical, and deduce an expression for the lattice spacing under equilibrium condition. We also investigate the dependence of the latter upon the various parameters of the system, such as the radius of the particles, the dielectric properties of the fluids and particles, the particles' vertical position within the interface, the particles' buoyant weight and the applied voltage. For (large) particles whose buoyant weight is much larger than the vertical electrostatic force, it is found that the equilibrium distance increases with electric field strength. However, for submicron sized particles whose buoyant weight is negligible, the distance decreases with increasing electric field. In between (namely, for intermediate sized particle), the distance first increases and then decreases with increasing electric field strength.

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Phase-Locking in the Transport of Suspended Particles through Periodic Systems

German Drazer
Assistant Professor
Chemical and Biomolecular Engineering, Johns Hopkins University

We investigate the transport of suspended species moving through a periodic array of solid obstacles under the action of a constant external force. The trajectory followed by both finite-size spheres as well as tracer particles at high Peclet numbers exhibit become locked into periodic trajectories with an average orientation that coincides with one of the lattice directions and is, in general, different from the direction of the driving force. Differences in the locking angle for different species could lead to vector separation for certain orientations of the external force. We investigate the possibility of separation by means of numerical simulations, simple theoretical models and macroscopic experiments.

Stretching Rod-Like Molecules in Microfluidic Devices

Prashant Purohit
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

Rod like macromolecules such as actin, DNA etc., are most commonly stretched using optical tweezers. However, it has been demonstrated that these molecules can also be stretched using drag forces exerted by flowing fluids. In this presentation we will describe the mechanics of short rod like molecules in tension. The mechanics is dominated by the competition between tensile forces (exerted by fluid flow, or by a device, such as, optical tweezers) and the thermal fluctuations of the molecule. For molecules whose contour length is comparable to the persistence length we show that the boundary conditions play major role in determining the mechanical behavior. We use the equipartition theorem of statistical mechanics to obtain expressions for the amplitude of the transverse fluctuations of the molecule and its force-extension relation for various boundary conditions [1]. We then apply our theory to an experiment on short fluctuating actin filaments trapped by AC dielectrophoresis. We estimate the tension in these filaments by fitting our theory to the measured values of transverse fluctuations as a function of the position along the filament. In this way we demonstrate that measurement of transverse fluctuations (instead of the end-to-end extension) can be used as a reliable method for estimating the tension in short rod like molecules.

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The Colloidal Glass Transition in Tight Spaces

Eric Weeks
Associate Professor
Physics, Emory University

Kazem Edmond
Physics Department, Emory University

Are glasses merely extremely slow liquids, and if so, why are they many orders of magnitude slower than conventional liquids? We study concentrated colloidal suspensions, a model system which has a glass transition. These are suspensions of small solid particles in a liquid, and exhibit glassy behavior when the particle concentration is high; the particles are roughly analogous to individual molecules in a traditional glass. We view the motion of these colloidal particles in three dimensions by using an optical confocal microscope. This allows us to directly study the microscopic behavior responsible for the macroscopic viscosity divergence of glasses. In particular, we study how confinement changes the particle dynamics [1]. We confine a colloidal suspension between two parallel walls, and find that in thin sample chambers the particle motion is greatly slowed. This suggests that confinement causes the onset of the glass transition to happen "sooner", at particle concentrations which are not normally glassy.

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A Minimal Model for Kinetic Arrest

Corey O'Hern
Associate Professor
Mechanical Engineering and Physics, Yale University

Prasanta Pal
Mechanical Engineering, Yale University

Jerzy Blawzdziewicz
Associate Professor
Mechanical Engineering and Physics, Yale University

Eric Dufresne
Assistant Professor
Mechanical Engineering and Physics, Yale University

To elucidate slow dynamics in glassy materials, we introduce the Figure-8 model in which N hard blocks undergo Brownian motion around a circuit in the shape of a figure-8. This system undergoes kinetic arrest at a critical packing fraction, and below this critical value long-time diffusion is controlled by rare, cooperative `junction-crossing particle rearrangements. We find that the average time between junction crossings and hence the structural relaxation time, does not simply scale with the configurational volume of transition states, because the structural relaxation time also depends on the time to complete a junction crossing. The importance of these results in understanding cage-breaking dynamics in glassy systems is also discussed.

Hydrodynamics of Colloidal Dispersions: Microscale Structure and Bulk Phenomena

Jeff Morris
Professor
Levich Institute and Chem Engineering, City College of New York

Colloidal dispersions composed of solid particles in a viscous liquid are encountered in a range of settings. These include natural muds and mining sludges, as well as paints, coatings and a range of personal care products. The flow properties of these mixtures include a variety of nontrivial rheological responses and a great deal of study has been devoted to them. However, the hydrodynamic or fluid mechanical behavior of these mixtures is not well-established because they exhibit two-phase phenomena, particularly particle migration, which is not completely understood. Here, we focus on the simplest of colloidal dispersions, that of hard-spheres.

Hard-sphere dispersions are characterized by their solid volume fraction, Φ, and the ratio of shearing motion to Brownian motion known as the Peclet number, $Pe \sim \eta\gamma a3/kT$; here η and γ are the suspending fluid viscosity and the shear rate, respectively, a is the particle size (radius) and kT is the thermal energy. We will discuss the microstructure of dispersions, meaning the arrangement at the particle scale, under shearing flow and the impact this has on the rheology. This is relatively well-established, except in regard to the quantity termed the "particle pressure" denoted Π. The quantity Π is the nonequilibrium continuation of p, the equilibrium (thermal) osmotic pressure which for hard spheres satisfies $\pi = nkT[1+ g(2)]$ where n is the particle number density and $g(2)$ is the contact value of the pair distribution function, $g(r)$. Theory, experiment and analysis of Π will be briefly described to establish the general behavior of this function, which critically scales as $\eta\gamma$ (times a function of Φ at large Pe and thus Π/π can easily be several orders of magnitude for colloidal particles of 100 nm to micron scale.

The relevance of Π to bulk flow phenomena will be shown to mirror that of π, i.e. it serves as the driving force for a particle flux which relaxes the state of the system. The connection of this behavior to established nonequilibrium thermodynamics (note that π is thermodynamically well-defined) as well as the implications for migration phenomena in bulk flows in simple (viscometric flows and straight channels or tubes) as well as more complex conduit shapes will be described.

An Experimental Study of Dispersion of Solid Particles in Grid-Generated Turbulent Flow

Medhat Hussainov*
Institute of Physics, University of Tartu
medhat.hussainov@ttu.ee

Alexander Kartushinsky
Faculty of Science, Laboratory of Multiphase Media Physics, Tallinn University of Technology

Ylo Rudi
Faculty of Science, Laboratory of Multiphase Media Physics, Tallinn University of Technology

Sergei Tisler
Faculty of Science, Laboratory of Multiphase Media Physics, Tallinn University of Technology

Igor Shcheglov
Faculty of Science, Laboratory of Multiphase Media Physics, Tallinn University of Technology

Particles dispersion in turbulent flows takes place in various natural phenomena and industrial processes. For example, it is a major factor for powdered-coal combustion, motion and precipitation of particles in dust filters etc. Main objectives of the investigation is to study influence of gravity and particles inertia on their dispersion in turbulent gas flow. Experiments were carried out in horizontal 200 x 400 mm channel. Mean flow velocity was 5.1 m/s. Turbulence of gas flow was generated by the grid of 16 mm mesh size. 36, 56 and 128 mkm spherical glass particles were ejected into the flow by means of 0.6 mm tubule. The particles dispersion was determined by the measuring technique applied the high-speed digital cameras, which registered the paths of particles in two flow planes (y, x) and (z, x). The distributions of the averaged and fluctuation components have been obtained for the particles velocity. The present study covered not only the long-time [1, 2], but also the short-time dispersion, and it was revealed that the short-time particles dispersion had been conditioned by the initial velocity slip between gas and solid particles. It was obtained that the particles dispersion occurred in the gravity direction had been larger than in the direction perpendicular to gravity. The experiments showed that the increase of the particles size resulted in reducing of the short-time dispersion.

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Novel Inks for Direct-Write Assembly of Functional Materials

Jennifer Lewis
Professor
Materials Research Laboratory, University of Illinois

The ability to pattern functional materials in planar and three-dimensional forms is of critical importance for several technological applications, including photonics, sensors, microfluidics, and tissue engineering scaffolds. Direct ink writing enables one to rapidly design and fabricate materials in arbitrary shapes without the need for expensive tooling, dies, or lithographic masks. Recent advances in the design of concentrated inks composed of colloidal, polyelectrolyte, and organometallic building blocks with tailored rheological properties will be highlighted with an emphasis on patterning 3D structures at the microscale

Formation of Nanofibers by Capillary-Driven Thinning of Drying Viscoelastic Filaments

Jerome Crest
Mechanical Engineering, Hatsopoulos Microfluids Laboratory, Massachusetts Institute of Technology

Jean-Christophe Nave
Instructor of Applied Mathematics
Mathematics, Massachusetts Institute of Technology

Gareth H. McKinley
Professor
Mechanical Engineering, Hatsopoulos Microfluids Laboratory, Massachusetts Institute of Technology

Recent experiments have shown that it is possible to self-assemble very uniform polymeric nanofibers by exploiting elastocapillary thinning of macroscopic liquid bridges [1]. We develop a model of this process that describes the simultaneous visco-elasto-capillary thinning and drying of cylindrical filaments of polymer solutions. A one dimensional formulation is developed using a slender body approximation to the inertialess equations of motion. The evolution in the kinematics, stress and composition of differential material elements are computed by numerical simulation on a fixed mesh using an explicit Eulerian scheme. The polymer rheology is described by a single mode Giesekus model with a concentration-dependent shift factor that accounts for compositional dependence of the zero shear rate viscosity and relaxation time of the fluid. The numerical simulations are compared to capillary break-up extensional rheometer (CABER) experiments using high molecular weight poly(methyl methacrylate) solutions in cholorobenzene with mass fractions spanning both the semi-dilute entangled and concentrated regimes. The power law scaling of the rheological properties with concentration is determined experimentally with an ARG2 shear rheometer. Very large radius reductions—spanning three to four orders of magnitude—are attainable by careful control of the mass transfer rate, the extensibility of the dissolved polymer and the elasto-capillary thinning dynamics. Simulations show that the nanofiber formation process can be conveniently parameterized by two dimensionless parameters which compare, respectively, the rate of capillary thinning, the rate of elastic stress relaxation and the rate of solvent evaporation [2].

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Harmonic Regelation

Joe Goddard
Department of Mechanical and Aerospace Engineering, University of California, San Diego

The early works of Faraday and the Thomson brothers mark the beginning of a sustained scientific fascination with "regelation", the pressure-induced thawing and refreezing of ice at solid boundaries. This phenomenon has been invoked to explain various processes such as basal melting of glaciers, ice-skating, and a well-known classroom experiment involving the passage without trace of a solid wire through a block of ice.

Nye [1] provides an elegant mathematical theory for the movement of a circular wire, with speed controlled by a lubrication-type flow in an interfacial liquid layer, together with conduction of heat through wire, water layer and surrounding ice. He also derives an analytical solution to the problem, based on the angular symmetry of the associated harmonic temperature and pressure fields, Subsequent careful experiments, e.g. of [2], show close agreement with Nye's theory in some cases but not in others.

After a brief review of theory and experiment, it is shown here that Nye's is a special case of a more general theory admitting analytical solutions for the translation and rotation of symmetrical bodies such as elliptic cylinders and general ellipsoids. This provides a generalization of the "Stokes-law" proposed by Nye for the virtual motion of one rigid body through another. The current theory also suggests a simpler regelation experiment with measurement of torque required for the slow rotation of an elliptic cylinder in ice.

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Rheological Response of Concentrated Latex Suspensions in Relaxation and Aging Conditions

Gregory McKenna
Professor
Chemical Engineering, Texas Tech University

Tetsuharu Narita
Chercheur CNRS
PPMD UPMC-ESPCI-CNRS UMR7615, E.S.P.C.I.

Francois Lequeux
Directeur CNRS
PPMD UPMC-ESPCI-CNRS UMR 7615, E.S.P.C.I.

There is considerable interest in the use of colloidal suspensions as model systems for glass-forming substances. Here we examine the isochronal stress-strain behavior of colloidal suspensions of 200 nm diameter latex particles and compare it with the behavior of polymeric glasses. Similarities and differences are described. In addition, it is widely considered that colloidal suspensions can be "shear melted" to an effective temperature that, upon cessation of the shear treatment, leads to aging of the colloidal suspension. Here we examine the "aging" response of the latex suspensions and make comparisons with the aging behavior of polymeric glasses subjected to temperature-jump conditions rather than shear melting conditions. Again, similarities and differences are described. The discussion and focus of the talk centers on the view that colloidal glasses, while showing some similarities to structural glasses (as represented by polymers in this case), are not necessarily good model systems for the glass transition phenomenon itself.

Fluid-Structure Interaction

ORGANIZERS:

Daniel J. Bodony, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Philippe H. Geubelle, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

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A 3D Multiscale/Stabilized Formulation of the Incompressible Navier-Stokes Equations for Moving Domain Problems

Arif Masud
Associate Professor
Civil and Environmental Engineering, University of Illinois

Ramon Calderer
Civil and Environmental Engineering, University of Illinois

We present a 3D multiscale / stabilized finite element method for the incompressible Navier-Stokes equations [1,2] written in arbitrary Lagrangian-Eulerian (ALE) frame of reference for moving boundary flows and fluid-structure interaction. The structure of the stabilization terms in the new method is derived based on the Variational Multiscale ideas. A significant feature of the new formulation is that the definition of the stabilization tensor appears naturally via the solution of the sub-grid scale problem. We propose a computationally economic scheme to evaluate the advection part of the stabilization tensor. The formulation is integrated with a 3D mesh moving scheme for solving problems that involve moving and deforming spatial fluid domains [3,4]. Several benchmark problems are presented to show the accuracy and stability of the new formulation.

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A Cartesian Mesh Method for Flow-Structure Interactions with Finite Solid Deformation

Hong Zhao
Postdoc Research Associate
MechSE, University of Illinois

Jonathan B. Freund
Professor
MechSE, University of Illinois

Robert D. Moser
Professor
Mechanical Engineering, University of Texas at Austin

A fixed-mesh algorithm is proposed for simulating flow—structure interactions such as those occurring in biological systems, in which both the fluid and solid are incompressible and the solid deformations are large [1]. Several of the well-known difficulties in simulating such flow—structure interactions are avoided by formulating a single set of equations of motion on a fixed Eulerian mesh. The solids deformation is tracked to compute elastic stresses by an overlapping Lagrangian mesh. In this way, the flow—structure interaction is formulated as a distributed body force and singular surface force acting on an otherwise purely fluid system. These forces, which depend on the solid elastic stress distribution, are computed on the Lagrangian mesh by a standard finite-element method and then transferred to the fixed Eulerian mesh, where the joint momentum and continuity equations are solved by a finite-difference method. The constitutive model for the solid can be quite general. For the force transfer, standard immersed-boundary [2] and immersed-interface methods [3] can be used and are demonstrated. We have also developed and demonstrated a new projection method that unifies the transfer of the surface and body forces in a way that exactly conserves momentum; the interface is still effectively sharp for this approach. The spatial convergence of the method is observed to be between first- and second-order, as in most immersed-boundary methods for membrane flows. The algorithm is demonstrated by the simulations of an advected elastic disk, a flexible leaflet in an oscillating flow, and a model of a swimming jellyfish.

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A Newton-Schur Type Finite Element Formulation for Navier-Stokes with Applications in Nonlinear Fluid Structure Interaction

Daniel Z. Turner
CSE Fellow
Civil and Environmental Engineering,University of Illinois

Kalyana B. Nakshatrala
Postdoctoral Research Associate
Civil and Environmental Engineering, University of Illinois

Keith D. Hjelmstad
Professor
Civil and Environmental Engineering, University of Illinois

Recent advances in coupling algorithms for fluid-structure interaction problems have highlighted the need for robust monolithic schemes. The instabilities that arise from staggered coupling schemes require the treatment of the fluid and solid equations in simultaneously integrated fashion, particularly when dealing with incompressible flows. To facilitate monolithic coupling in the finite element context for highly nonlinear problems, we present a Newton-Raphson type solution procedure for the Incompressible Navier-Stokes equations capable of quadratic convergence and very well suited for integration with nonlinear solid formulations that employ an iterative Newton update equation. We also incorporate the Schur's complement form to decrease computational cost and improve parallel performance. To explore further the relationship between consistent and fixed-point type approaches, we compare the performance of the Newton-Schur formulation with an equivalent fixed point iteration strategy for low and moderate Reynolds numbers. As expected, for low-Reynolds flows, the Newton-Schur strategy converges in much fewer iterations. For moderate Reynolds flows (Re = 5,000), the fixed-point strategy diverges while the Newton-Schur approach converges in three iterations. This work lays the foundation for advanced solution techniques, such as arc-length or homotopy methods that require the nonlinear weak form of the governing equations, which is not available for methods that employ fixed-point linearization.

Effects of Mesh Motion on the Accuracy and Stability of ALE-based Formulations for the Navier-Stokes Equations

Arif Masud
Associate Professor
Department of Civil and Environmental Engineering, University of Illinois

Flow equations are invariably written in an arbitrary Lagrangian-Eulerian (ALE) frame of reference for the modeling of Fluid-Structure Interaction (FSI) problems. There are several other problem classes, namely, free surface flows and advancing front flows where the governing equations are expressed in an ALE frame. Numerical treatment of these problems involves controlled motion and deformation of the underlying computational grids. There has been an outstanding issue in these problems that can be posed as follows: "Can an arbitrary motion of the fluid mesh in an arbitrary Lagrangian-Eulerian framework destabilize an otherwise stable formulation?" Employing functional analysis techniques we present a mathematical proof of the deleterious effects of arbitrary mesh motion on the accuracy and convergence properties of an otherwise stable scheme for the advection-diffusion equation [1]. The proof is then extended to linearized Navier-Stokes equations that are written in an ALE frame for application to moving boundary flows and fluid-structure interaction. We explicitly show that the advection dominated case in moving mesh problems is susceptible to growth in the error in the computed solution because of the motion of the computational grid. If the mesh motion, which can otherwise be arbitrary, causes the norm of the relative velocity to grow, then the bound on the error norm is lost. This has negative effects especially on the implicit time integration schemes where the growing numerical error engendered by the mesh convective effects eventually makes the computed solution unstable. Some numerical examples that highlight the effects of mesh motion are also presented.

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Computing Both the Flow and Elastic Deformations on Cartesian Grids

Haoxiang Luo
Assistant Professor
Department of Mechanical Engineering, Vanderbilt University

Rajat Mittal
Professor
Department of Mechanical and Aerospace Engineering, George Washington University

A new numerical approach for modeling a class of flow-structure interaction problems typically encountered in biological systems is presented. In this approach, a previously developed, sharp-interface, immersed-boundary method [1] for incompressible flows is used to model the fluid flow and a new, sharp-interface Cartesian grid, immersed boundary method [2] is devised to solve the equations of linear viscoelasticity that governs the solid. The two solvers are coupled to model flow-structure interaction. This coupled solver has the advantage of simple grid generation and efficient computation on simple, single-block structured grids. Multigrid methods and domain-decomposition based parallel algorithms can be easily incorporated into the solvers. In addition, it is possible that the discrete equations for the flow and those for the solid are assembled in a single linear or nonlinear algebraic system to be solved simultaneously for both the flow and solid, therefore enabling strong coupling between the two solvers. The numerical method has been implemented for both two- and three-dimensional problems. We will demonstrate its application for modeling the laryngeal aerodynamics and vocal fold vibration during the human voice generation process.

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Computational Tools for the Study of Intracranial and Abdominal Aneurysms: An Introduction to the Fluid-Solid-Growth Framework

Carlos Alberto Figueroa
Engineering Research Associate
Department of Bioengineering, Stanford University

Seungik Baek
Department of Mechanical Engineering, Michigan State University

Charles A. Taylor
Department of Bioengineering, Stanford University

Jay D. Humphrey
Department of Biomedical Engineering, Texas A&M University

We introduce a new computational framework that combines together advances in the fields of computational biosolids [1],[2] and biofluids [3],[4] mechanics to understand better the mechanobiology and pathophysiology of aneurysms. This framework tries to provide the computational foundation for a new class of problems that we will refer to as Fluid-Solid-Growth problems (FSG) [5].

In this work, we concentrate our efforts in the hemodynamic characterization of intracranial and abdominal aneurysms. These aneurysm types result from different underlying disease processes and exhibit different rupture potentials, but they share many histopathological and biomechanical characteristics. We will discuss in deeper detail some of the computational tools used in the biofluids part of this FSG framework for these types of aneurysms.

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Compressible Turbulence-Structure Interaction Using AMR-based Large-Eddy Simulation

Ramji Kamakoti
Postdoctoral Research Associate
Mechanical Science and Engineering, University of Illinois

Kostas Karagiozis
Postdoctoral Research Associate
Mechanical Science and Engineering, University of Illinois

Fehmi Cirak
University Lecturer
Department of Engineering, University of Cambridge

Carlos Pantano
Assistant Professor
Mechanical Science and Engineering, University of Illinois

The increasing interest on the effect of high-speed flows on the outer-skin panels of aircraft, missiles, aerospace vehicles and lately in the design of entry-decent-landing methodologies has advanced research into developing sophisticated hybrid CFD and FEA models to describe the fluid-structure interaction (FSI) of systems with complex geometries. We utilize a three-dimensional compressible fluid solver with low numerical dissipation based on a conservative finite difference approach. Large-eddy simulation (LES) models unresolved turbulence scales using the stretched-vortex subgrid model. The overall flow solver is based on a hybrid methodology, wherein a centered difference scheme is used in turbulent flow regions whereas a weighted-essential non-oscillatory (WENO) scheme is employed to capture discontinuities in the flow field, such as shocks. The structural model is based on finite-element approach using the Kirchhoff-Love theory for thin shells allowing for large shell deformation and small strains. A subdivision scheme is used to generate smooth deformed shapes from triangulation of an arbitrary nodal point set. The FSI is modeled only near the interface of the fluid-solid regions. An implicit geometry coupling methodology that embeds the structural system into a fixed Cartesian fluid mesh and continuously exchanges coupling data on the topological surface of the flexible structure between the fluid and solid solver components is employed. The computational environment is based on adaptive mesh refinement (AMR) using the object-oriented C++ (AMROC) framework. The FSI model is used to investigate the response of planetary exploration decelerator structures for various flow regimes. The main purpose of these structures is to aide in the entry and decent of space vehicles into the thin Martian atmosphere. The interaction between turbulent wakes and shocks and its interaction with the structure will be discussed.

A Simulation Model for Red Blood Cell Flow in Microcirculation

Amir H. G. Isfahani
Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Hong Zhao
Postdoctoral Research Associate
Department of Mechanical Science and Engineering, University of Illinois

Luke Olson
Department of Computer Science, University of Illinois

Jonathan B. Freund
Departments of Mechanical Science and Engineering and Aerospace Engineering, University of Illinois

Multi-cellular hydrodynamic interactions are important for much of the phenomenology of microcirculation. For example, leukocyte margination as a physiological response to inflammation[1], and detachment and metastasis of cancer cells appear to depend directly upon interactions with flowing red cells. We have developed a simulation model capable of representing large numbers of red cells interacting in the complex geometry confinement of capillaries. The cells are modeled as elastic shell membranes with strong resistance to surface dilatation and relatively small but finite resistance to bending. Their surface is discretized by marker points in a referential configuration. These points are interpolated by global spectral basis functions: Fourier modes in two dimensions and spherical harmonics in three, yielding optimal efficiency for a given accuracy. More importantly, it offers a rigorous treatment of de-aliasing without adding any numerical dissipation, a necessary component to stable integration of nonlinear terms. Stokes flow provides a realistic model for both the blood plasma and the red cell cytoplasm. An O(NlogN) smooth particle-mesh Ewald method[2,3] is employed to decompose the periodic Green's functions of the Stokes operator into singular short-range and smooth long-range interactions. A process of parameter selection to optimize computational efficiency for a desired accuracy is presented. Mismatched viscosity between the concentrated solution of hemoglobin inside red blood cells and the plasma on the outside gives rise to an implicit system, which benefits from iterative solution techniques. The impact of different physical configurations on the performance and efficiency of several iterative strategies will be outlined. The vessel walls are modeled using a penalty-like method that enables simulation of complex geometries using free-space (in a sense) periodic Green's functions. This representation is then used to study the forces exerted on a cancer cell, modeled as a hump attached to the vessel wall, in flow configurations which differ in hematocrit, hump radius, and vessel diameter.

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Computational Modeling of Fluid-Structure Interaction in Surgically Altered Vocal Folds

Rajat Mittal
Professor
Department of Mechanical and Aerospace Engineering, The George Washington University

Qian Xue
Department of Mechanical and Aerospace Engineering, The George Washington University

Xudong Zheng
Department of Mechanical and Aerospace Engineering, The George Washington University

Steve Bielamowicz
Professor
Department of Surgery, The George Washington University

Phonation is a biomechanical process that requires the two vocal folds to be medialized such that air forced through the vocal folds sets them into self-sustained vibrations. Some stroke patients suffer unilateral vocal fold paralysis that leads to an inability to medialize the paralyzed vocal fold resulting in loss of voice production. Medialization laryngoplasty is a surgical procedure that is designed to correct this pathology [1]. In this procedure a rigid implant is inserted into the larynx in such a way that it medializes the paralyzed vocal fold thereby restoring voice function. However, the outcome of the surgery is highly dependent on the precise shape and placement of the implant and furthermore, the implant can also modify the voice quality of the patient. It would therefore be highly desirable to model the process of voice production and the effect of the implant on phonation since this could lead to improvement in surgery planning and outcome. In the current effort, we have developed a unique fluid-structure interaction solver for modeling the vibration of the vocal folds and we are using this solver to gain insight into the biophysics of phonation in surgically modified larynges.

In the current solver, the glottal aerodynamics is simulated using an accurate sharp interface immersed boundary method solver [2] and this is coupled with a three-layer finite-element anisotropic tissue model to model the FSI problem in vocal folds. The simulation is based on a cover-ligament-body vocal folds model with rigid false vocal folds, which is reconstructed from high-resolution CT scans. Simulation results show that self-sustained vibrations of the vocal folds can be achieved and the vibration mode as well as frequency is very close to the experimental data. The effects of medialization laryngoplasty on vocal folds eigen frequencies has been investigated. We also examine the vibratory characteristics of a larynx where one of the vocal folds is normal and the other one is surgically altered.

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Coupled Fluid-Structure Simulation of Acoustic Damping

Hady Joumaa
Mechanical Engineering, University of Illinois

Philippe Geubelle
Professor
Aerospace Engineering, University of Illinois

Daniel Bodony
Assistant Professor
Aerospace Engineering, University of Illinois

Acoustic loads play an important role in the design of a variety of aerospace structures as they may lead to the fatigue failure of thin-walled panels. Usually, the acoustic loads on an aircraft structure are obtained through a one-way coupled analysis of the fluid/structure interaction. However, as an acoustically loaded thin-walled structure vibrates, it radiates acoustic energy to the surrounding fluid medium in a phenomenon often referred to as acoustic damping. The accurate simulation of this phenomenon necessitates a two-way coupling between the fluid and solid domain. The development, implementation and validation of a coupled structural/acoustic solver constitute the primary objectives of this research project. The focus of this presentation is the 2-D version of the coupled solver. After a brief overview of the finite difference fluid solver and the finite element solid solver, we describe a set of test problems adopted to verify the individual and coupled solvers. One of these problems involves a thin cylindrical shell surrounded by an acoustic medium and subjected to an initial radial displacement. This verification problem is solved analytically in the Laplace domain and asymptotically in the time domain, allowing for the extraction of a closed-form expression of the acoustic damping coefficient. Excellent agreement is achieved with the numerical solution provided by the coupled structural/acoustic solver. The coupled solver is then used to analyze the structural/acoustic response of a baffled and unbaffled cantilever beam. As shown experimentally, the presence of a rigid separation between the upper and lower sides of the beam (baffled configuration) strongly affects the acoustic response of the structure, leading to a much larger value of the acoustic damping coefficient than that of the unbaffled configuration, for which the fluid domain located above the structure is in contact with that located below. Transient simulations performed with the structural/acoustic solver demonstrate how this different acoustic response is associated with radically different fluid flow patterns in the vicinity of the vibrating beam.

Porous Melt Flow Analysis Using Coupled Finite Element Method

Taehyo Park
Professor
Civil Engineering, Hanyang University

Moonho Tak
Graduate Student
Civil Engineering, Hanyang University

George Z. Voyiadjis
Professor
Civil & Environmental Engineering, Louisiana State University

In order to analyze melt flow, many methods such as DEM (distinct element modeling), SPH (smoothed particle hydrodynamics) based on particle scope and FEM (Finite element method) have been introduced for many decades. However, these methods cannot easily be applied to complex porous melt flow analyses because of the need for large CPU time and constitutive equations that should consider rheological interactions. In order to overcome these difficulties, numerical techniques have been proposed using stability analysis. However, numerical accuracy and stability problems have not been able to address the real phenomena involved in this problem.

In this work, a new coupled finite element method is proposed in order to resolve the above mentioned shortcomings of the numerical analysis. In this algorithm, multi time step for numerical stability and remeshing scheme for numerical accuracy are introduced with sub iteration method which helps address the procedures on equilibrium condition. In addition, this scheme is performed in each different finite element description. Namely, the Lagrangian motion analysis is used for the solid phase in the porous media while the Eulerian description is used for the fluid phase. For the special case of porous flow use is made of the Eulerian description. Each constituent is superposed with the interaction analysis for the sub iteration. In summary, this provides an easy method to approach complex mechanisms in porous melt flow using the difference finite element descriptions.

For verification, the proposed method is compared with analytical solutions and the solutions obtained using the ABAQUS software for one-, and two- dimensional porous melt flow models such as for fresh concrete or magma flow.

Sensitivities Studies of the Influence of Viscoelastic Material Property on Flutter Speeds

Harry H. Hilton*
Professor Emeritus of Aerospace Engineering and NCSA Senior Academic Lead for Structural/Solid Mechanics
Aerospace Engineering and NCSA/TRECC, University of Illinois
h-hilton@uiuc.edu

Daniel H. Lee
Research Assistant
Aerospace Engineering and NCSA/TRECC, University of Illinois

Bending and torsion flutter is investigated for a flexible linear viscoelastic wing. Parametric studies are conducted for a number of ratios of the instantaneous (elastic) modulus to the fully relaxed one and for various values of the largest relaxation times of these moduli. Computer simulations show that the flutter velocity reaches a maximum after which increases in relaxation times lead to diminished flutter velocities. This pattern is due to the ever-changing phase relations between inertia forces, unsteady lift and viscoelastic internal bending and shear stresses. The latter, of course, are dependent on the idiosyncrasies of the chosen viscoelastic constitutive relations, which define the material. It is apparent from these studies that increased damping may stabilize or destabilize viscoelastic lifting surfaces. For the combinations of parameters considered in the simulations, viscoelastic flutter speeds reached higher values than those for equivalent elastic wings. However, different parametric combinations could readily drive the viscoelastic flutter velocities to lower than elastic values [1–3]. In other words, additional material damping and/or increased stiffness do not necessarily produce higher viscoelastic flutter velocities. Since viscoelastic materials are heavily temperature dependent, these conclusions are of importance to flight vehicles with high polymer composite lifting surfaces operating in distinct climates. While primarily intended for full-sized flight vehicles, UAVs and MAVs the analysis is equally applicable to suspension bridges, tall buildings and computer disk drives.

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Aeroelastic Limit Cycle Oscillations in High Performance Aircraft

Earl H. Dowell
Department of Mechanical Engineering and Materials Science, Duke University

An overview is presented of limit cycle oscillations (LCO) that occur due to the nonlinear aeroelastic response of high performance aircraft. Both theoretical/computational and experimental work including wind tunnel andflight test data are discussed.

Primary emphasis is on (1) computational/experimental correlation and (2)recent developments in constructing rapid solution methods for computational models that retain state of the art high fidelity accuracy.

Results for a High Altitude Long Endurance (HALE) configuration, a fighter aircraft and a morphing (folding) wing illustrate the state of the art and also demonstrate the sensitivity of flutter and LCO prediction that may occur due to modest changes in key system parameters.

Integrating Structure and Chemistry in Biomedical Imaging

ORGANIZER:

Rohit Bhargava, *Department of Bioengineering, University of Illinois at Urbana-Champaign*

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Nonlinear Optical Properties of Gold Nanowires

Hyun Min Kim
Department of Chemistry, University of California

Xiang Chengxiang
Department of Chemistry, University of California

Reginald Penner
Department of Chemistry, University of California

Eric O. Potma
Assistant Professor Chemistry
School of Physical Sciences, University of California

We have investigated the nonlinear optical properties of gold nanowires. These nanowires, having a rectangular cross-section, a precisely-defined thickness, and millimeter-scale length, were prepared using the lithographically patterned nanowire electrodepostion (LPNE) technique. The precise scaling of the nanowire system allows for a detailed study of nonlinear optical properties as a function of the structure's dimensions. It is found that the optical properties of the wire are dominated by the transverse surface plasmon resonance. The strong plasmon resonance gives rise to enhanced coherent emission in the form of second harmonic generation (SHG) and coherent anti-Stokes scattering (CAS), in addition to two-photon-excited luminescence (TPEL) form the gold. We have examined the dependence of these nonlinearly driven emission processes on the dimensions of the nanostructure.

FTIR Micro-spectroscopy Identifies Symmetric Phosphate Modifications as a Marker of the Putative Stem Cell Region of Human Intestinal Crypts

Michael Walsh
Department of Biological Sciences, Lancaster University

Francis L. Martin
Department of Biological Sciences, Lancaster University

Cellular biomolecules absorb in the mid-infrared (λ = 2-20 μm) giving rise to vibrational spectra associated with structure and function [1]. We employed Fourier transform infrared (FTIR) micro-spectroscopy to "biochemically-fingerprint" cells along the length of human small and large intestinal crypts. Paraffin-embedded slices of normal human gut were sectioned (10-μm thick) and mounted to facilitate infrared (IR) spectral analyses. IR spectra were collected employing globar (15 μm × 15 μm aperture) FTIR microspectroscopy in reflection mode, synchrotron (≤10 μm × 10 μm aperture) FTIR microspectroscopy in transmission mode, or near-field photothermal micro-spectroscopy (PTMS). Dependent on the location of crypt interrogation, clear differences in spectral characteristics were noted. Epithelial-cell IR spectra were subjected to principal component analysis to determine whether wavenumber-absorbance relationships expressed as single points in "hyperspace" might on the basis of multivariate distance reveal biophysical differences along the length of gut crypts. Following spectroscopic analysis, plotted clusters and their loadings plots pointed towards symmetric (ν_s) PO_2^- (1080 cm^{-1}) vibrations as a discriminating factor for the putative stem cell region; this proved to be a more robust marker than other phenotypic markers such as β-catenin or CD133. This pattern was subsequently confirmed by image mapping and points to a novel approach of non-destructively identifying a tissue's stem cell location. $\nu_s PO_2^-$, probably associated with DNA conformational alterations, might facilitate a means of identifying stem cells, which may have utility in other tissues where the location of stem cells is unclear [2].

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Fourier Transform Infrared Microspectroscopy and Nanoindentation Study of the Age Effect in Swine Cortical Bone

Iwona Jasiuk
Professor
Mechanical Science and Engineering Department, Bioengineering Department, University of Illinois

Liang Feng
PhD Student
Mechanical Science and Engineering Department, Bioengineering Department, University of Illinois

Rohit Bhargava
Professor
Mechanical Science and Engineering Department, Bioengineering Department, University of Illinois

Bone has a complex hierarchical structure. At the nano scale the main two components of bone are collagen fibrils which are reinforced by mineral crystals, mainly hydroxyapatite (HA). The chemical composition and properties of bone at this scale are affected by age [1]. The Fourier Transform Infrared (FTIR) spectroscopy is a well-established and well-understood technique, which is very useful for studing biological materials. For example, this technique can detect the changes in the collagen to mineral ratio, crystal size, perfection of bone apatite crystals, collagen cross-linking, and other parameters which influence bone quality [2, 3]. In this study, we propose to investigate the age effects in cortical bone on its chemical composition by using the FTIR microspectroscopy and the mechanical properties by nanoindentation. The experimental specimens are obtained from femurs of three groups of healthy swines of different ages: six months, one year old and three and half years old. The cortical bone sections are fixed with 70% ethanol and dehydrated in series of acetone before they are embedded in polymethylmethacrylate (PMMA). These embedded bone samples are then sectioned into 5m thickness thin slices and placed between two barium fluoride windows for FTIR microscopy study. The left over unsectioned samples are used for the scanning electron microscopy (SEM) imaging and the nanoindentaion testing to measure the local modulus and hardness at micro scale. One important contribution of this project includes the coupling of the information obtained from the FTIR and SEM microscopy with the results from the nanoindentation testing. It allows us to obtain a fuller understanding of bone's local structure and chemical composition and infer correlations between the mechanical properties and the chemical structure. This information will serve as a valuable input in the analytical and computational micromechanics models which will be used to predict the elastic modulus, strength and fracture toughness of cortical bone.

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Towards Automated Breast Histopathology with Mid-IR Spectroscopic Imaging

Frances Pounder
Graduate Student
Bioengineering, University of Illinois

Rohit Bhargava
Assistant Professor
Bioengineering, University of Illinois

Automated techniques for molecular evaluation of tissue could improve the accuracy and efficiency of breast cancer diagnosis. Fourier transform infrared (FT-IR) molecular spectroscopy, extensively used in chemical analysis, may be applicable for breast pathology. An IR spectrum gives a quantitative measurement of breast tissue molecular composition, which can then be numerically related to histopathology. Recent advances in instrumentation permit the combination of FT-IR molecular spectroscopy with optical microscopy to rapidly obtain spatial and spectral information with FT-IR imaging. This technique produces tissue image datasets containing extensive morphological and biochemical information without the use of molecular probes or contrast agents [1]. FT-IR tissue datasets are then automatically classified by a modified Bayesian supervised pattern recognition method to provide false-color images comparable to hematoxylin and eosin (H&E) and immunohistochemical (IHC) staining used for conventional breast cancer diagnosis [2,3]. This study employs tissue microarrays (TMAs), which offer a high-throughput approach to collect data and build a prediction algorithm from a large selection of cancer and normal tissue samples. The classification accuracy is then assessed by quantitative receiver operating characteristic analysis and qualitative validation on biopsy surgical resections. This computerized technique for breast histopathology is robust and non-destructive, and is applied directly to fixed tissue sections prepared for H&E or IHC staining [4,5]. Results demonstrate accurate tissue histology classification and progress towards identification of breast tumors. This study helps establish FT-IR imaging as a novel technology for breast cancer diagnosis and research.

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Modeling, Analysis, and Instrumentation in Scanning Probe Microscopy

ORGANIZER:

Srinivasa M Salapaka, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

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Contact Resonance Atomic Force Microscopy for Viscoelasticity

Philip Yuya
Engineering Mechanics, University of Nebraska, Lincoln

Donna C. Hurley
Materials Reliability Division, National Institute of Standards and Technology

Joseph A. Turner
Professor
Engineering Mechanics, University of Nebraska, Lincoln

We present a quantitative method for determining the viscoelastic properties of materials with nanometer spatial resolution. The approach is based on the atomic force acoustic microscopy (AFAM) technique that involves the resonant frequencies of the AFM cantilever when its tip is in contact with a sample surface. We derive expressions for the samples viscoelastic properties in terms of the cantilevers frequency response and damping losses. We demonstrate the approach by obtaining experimental values for the storage and loss moduli of a poly methyl methacrylate (PMMA) film using a polystyrene sample as a reference material. Experimental techniques and system calibration methods to perform materials-property measurements are also presented.

Investigation of Interface Properties by Nanoscale Elastic Modulus Mapping

Doron Shilo
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Haika Drezner
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Avraham Dorogoy
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Variations in material properties at the vicinity of interfaces have important implications both for interface characteristics and for overall material properties. We present a method for investigating the spatial changes of elastic moduli in a nm-scale vicinity of interfaces. The method is demonstrated on twin walls, a type of interface which is observed in a broad class of materials including ferroelectric, shape memory alloys, and superconducting crystals. Measurements taken from PbTiO3 single crystals reveal that the region near the twin wall is significantly softer than the two domains surrounding it. A comparison with finite element simulations relates this effect to an anelastic relaxation due to point defect accumulation around the twin wall. Local softening around the twin wall can affect the overall elastic modulus in thin films and nanostructured ferroelectric materials, in which the average distance between twin walls is smaller than the thickness of the softer region.

Quantitative Measurement for Lateral Force Microscopy: A Diamagnetic-Levitation Spring System

Qunyang Li
Research Associate
Division of Engineering, Brown University

Kyung-Suk Kim
Professor
Division of Engineering, Brown University

Allan Rydberg
Technical Staff
Division of Engineering, Brown University

From its inception [1], atomic force microscope (AFM) has been widely used for studying nano-scale friction properties [2, 3, 4], which is also known as lateral force microscopy. However, for as long as AFM has been used to study the frictional properties of materials at the nanometer scale, there have been difficulties in measuring the absolute lateral force components involved in the friction process. A novel diamagnetic lateral-force-calibrator (D-LFC) has been developed to directly calibrate AFM cantilever-tip or -bead assemblies [5]. This technique enables an AFM to accurately measure the lateral forces encountered in friction or biomechanical-testing experiments at a small length scale. In the process of development, deformation characteristics of the AFM cantilever assemblies under frictional loading have been analyzed and four essential response variables, i.e. force constants, of the assembly have been identified. Calibration of the lateral force constant and the "cross-talk" lateral force constant, among the four variables, enables the measurement of the absolute lateral force. The D-LFC is composed of four NdFeB magnets and a diamagnetic pyrolytic graphite sheet, which can calibrate the two constants with an accuracy on the order of 0.1%. Preparation of the D-LFC and the data processing required to get the force constants are significantly simpler than any other calibration methods. More importantly, the D-LFC is capable of calibrating both constants simultaneously for AFM tips or beads with any radius of curvature. These capabilities extend the applicability of AFM lateral force measurement to studies of anisotropic multi-scale frictional processes and bio-mechanical behavior of cells and molecules under combined loading. Some application examples on nanotribology are also discussed.

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A New Approach to Achieve Broadband Measurement of Frequency Dependent Viscoelasticity at Nano-scale by AFM

Qingze Zou
Department of Mechanical Engineering, Iowa State University

Zhonghua Xu
Graduate Student
Department of Mechanical Engineering, Iowa State University

A novel nanoscale broadband viscoelastic spectroscopy approach is proposed. The proposed approach utilizes the recently developed model-less inversion-based iterative control (MIIC) technique to achieve rapid measurement of rate-dependent mechanical properties of materials using scanning probe microscope (SPM). SPM has become an enabling tool to quantitatively measure the mechanical properties of a wide variety of materials. Current SPM-based force measurement, however, is limited by the slow operation of SPM: Current force measurement using SPM is too slow to measure the rate-dependent phenomena, and large measurement (temporal) errors can be generated when dynamic evolution of the sample is involved during the measurement. Such low-speed operation of SPM is due to the challenge in accounting for the adverse effects including the hysteresis of the piezo actuator (used to position the probe relative to the sample), the vibrational dynamics of the piezo actuator and the probe along with the mechanical parts in between, and the dynamics uncertainties caused by the probe variation and the probe-sample interaction. In the proposed NBVS approach, the MIIC technique is used to compensate for these adverse effects and thereby enable rapid measurements of rate-dependent material properties. The proposed NBVS method is illustrated by implementing it to measure the viscoelasticity of poly(dimethylsiloxane) (PDMS) over a broad frequency range of 3 orders (10~Hz to 6~KHz).

Extending the SPM Operating Range from 100 microns to 10 mm: XY Nanopositioner Design Challenges and Potential Solutions

Shorya Awtar
Department of Mechanical Engineering, University of Michigan

Gaurav Parmar
Research Assistant
Department of Mechanical Engineering, University of Michigan

There has been a long-standing need for compact desktop-size nanopositioners that can provide motion range of the order of several millimeters and yet achieve nanometric precision, resolution, and accuracy [1-2]. With the current instrumentation technology, Scanning Probe Microscopy and Scanning Probe Lithography have to be carried out in the "step and scan" mode if the desired range exceeds a few hundred microns.

We will discuss a first of its kind large-range high-precision XY nanopositioner that eliminates the need for 'step and scan' and the stitching errors associated with it. This promises a significant increase in the throughput of scanning probe based imaging and nanofabrication.

Technological challenges in achieving large range and high precision simultaneously include bearing stage design, sensor and actuator choice, structural dynamics and controls, thermal management, and drive and controller electronics [3]. The proposed XY nanopositioner overcomes these challenges by employing a unique flexure bearing geometry to offer unprecedented motion performance—10 x 10 mm motion range; nanometric motion resolution, repeatability and accuracy; low cross-axis coupling and parasitic rotation errors; and, low sensitivity to temperature fluctuations and manufacturing tolerances—all in a cost-competitive single-stage compact package.

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Real-Time Detection and Reduction of Probe-Loss in Atomic Force Microscopy

Pranav Agarwal
Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis

Murti Salapaka
Department of Electrical and Computer Engineering, University of Minnesota, Minneapolis

In this presentation, a real-time methodology is developed to determine regions of dynamic atomic force microscopy based image where the cantilever fails to be an effective probe of the sample. Probe-loss is more pronounced during high speed imaging operations. A quantitative measure called reliability index is proposed as a diagnostic measure for determining probe-loss. It is experimentally demonstrated that probe-loss affected portion of the image can be unambiguously identified by a signal termed the reliability index signal that can be determined in real-time. The reliability index signal, apart from indicating the probe-loss affected regions, can be used to minimize such regions of the image. Controllers implemented on FPGA that employ reliability index to tune their behavior will be elucidated. It is experimentally demonstrated that by using such a scheme, probe-loss area can be reduced by a factor of 4, suggesting a possible increase in imaging bandwidth by the same factor. Improvement in on-sample performance will be presented.

Two-Degree-of-Freedom Designs for Nanopositioning Systems: Fundamental Limitations, Control Design, and Related Trade-Offs

Chibum Lee
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

This paper studies and analyzes fundamental trade-offs between positioning resolution, tracking bandwidth and robustness to modeling uncertainties in two-degree-of-freedom (2DOF) control designs for nanopositioning systems. The analysis of these systems is done in optimal control setting with various architectural constraints imposed on the 2DOF framework. In terms of these trade-offs, our analysis shows that the primary role of feedback is providing robustness to the closedloop device whereas the feedforward component is mainly effective in overcoming fundamental algebraic constraints that limit the eedback-only designs. This paper presents (1) an optimal prefilter model matching design for a system with an existing feedback controller, (2) a simultaneous feedforward and feedback control design in an optimal H1 mixed sensitivity framework and 3) a 2DOF optimal robust model matching design. The experimental results on applying these controllers show a significant improvement, as high as 330% increase in bandwidth for similar robustness and resolution over optimal feedback-only designs. Other performance objectives can be improved similarly. We demonstrate that the 2DOF freedom design achieves performance specifications that are analytically impossible for feedback-only designs.

A Non-raster Approach to Scanning Force Microscopy

Sean Andersson*
Assistant Professor
Mechanical Engineering, Boston University
sanderss@bu.edu

Peter Chang
Graduate Research Assistant
Mechanical Engineering, Boston University

Atomic force microscopy (AFM) and its many variants are invaluable tools for the study of systems with nanometer-scale features. In recent years, the technology is increasingly being used to study the dynamics of such systems. Images are built pixel-by-pixel and the time to form a single frame is typically on the order of seconds. This is far slower than the time scale of many important phenomena, severely restricting the applicability of the technology. As a result, there is great interest in improving the effective temporal resolution of the instrument. We will present our recent efforts on the use of non-raster methods to study dynamics in nanometer-scale systems. By utilizing the data coming from the microscope to adjust the measurement process itself, measurements can be made where they are most effective, such as where the sample has spatially or temporally varying features. We will outline the general approach and describe our efforts on applications in AFM and magnetic force microscopy (MFM).

Removal of Artifacts for Better Nanoscale Normal and Lateral Force Imaging in Atomic Force Microscopy

Srinivasa Salapaka
Department of Mechanical Science and Engineering, University of Illinois

A. Shegaonkar
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

C. Lee
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

This work presents a feedback scheme that simultaneously corrects, in real time, for the imaging artifacts caused by cantilever and photosensor misalignments as well as misinterpretations in relative lateral position of the tip with respect to the sample due to the tip-sample stick in atomic force microscopy (AFM). The optical beam bounce method, typically used in AFM for imaging, is sensitive to inaccuracies of cantilever geometry and the relative misalignment of the laser source, cantilever, and the laser sensitive diode from the intended design. These inaccuracies, which contribute to the geometrical crosstalk between the normal and the lateral signals, become prominent at the atomic and sub-nanometer scales, and thereby impediment high resolution imaging studies. The feedback scheme accounts for these artifacts and makes imaging insensitive to, in fact, practically independent of, these inaccuracies. This scheme counteracts the lateral twisting dynamics of the cantilever, and as a result, it avoids the misinterpretation problem of the relative lateral position of the cantilever tip from the sample and therefore the corresponding imaging artifacts that are typically prominent in contact mode Friction Force Microscopy (FFM). The feedback scheme consists of simultaneously regulating the normal as well as the lateral cantilever deflection signal at a set point. This not only removes the imaging artifacts due to geometrical misalignments, mechanical crosstalk and irregular sliding, but the corresponding compensatory control signal gives a more accurate real time measure of the lateral interaction force between the sample and the cantilever as compared to the lateral deflection signal used in FFM. Experimental results show significant improvement, and in some cases practical elimination, of the artifacts.

Non-invasive Diagnostics for Biomechanics

ORGANIZERS:

John Georgiadis, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Michael Insana, *Bioengineering Department, University of Illinois at Urbana-Champaign*

SYMPOSIUM V

Bio-material Evaluation Using Ultrasound Radiation Force

Marko Orescanin
Bioengineering, and Electrical and Computer Engineering, University of Illinois

Kathleen S. Toohey
Bioengineering, and Electrical and Computer Engineering, University of Illinois

Michael F. Insana
Bioengineering, and Electrical and Computer Engineering, University of Illinois

Acoustic radiation force methods facilitate estimation of mechanical properties in sterile 3-D biological cell cultures. These measurements are critical to understanding the role of the extracellular matrix (ECM) microenvironment in cell activity within natural and engineered tissues. Accurate and noninvasive measurements of viscoelastic features of the cellular ECM may help us reveal the essential role of cell-matrix signaling in disease progression and scaffold breakdown in engineered tissues.

We validated the accuracy of an acoustic radiation force technique for non-destructive measurements of rheological properties. Studies are conducted using hydrogels that share a few key structural and mechanical features of engineered tissues. To enhance force coupling between the acoustic field and the hydrogels, a spherical scattering body is embedded. We conducted several experiments to study the displacement of embedded spheres to pulsed acoustic fields. The magnitude of the exerted force depends on the time-averaged energy density of the field and material properties of the scattering object and surrounding medium.

Acoustic force was applied to the samples using a weakly focused (f/4), single element, PZT transducer transmitting at 1 MHz. Spectral Doppler acquisitions with an array transducer were used to estimate velocity of the sphere during and after force application. Square-wave modulated acoustic energy bursts were applied to estimate the viscoelastic impulse response of the hydrogel at relatively low force frequencies. Sinusoidally-modulated acoustic transmissions provided harmonic stimuli for high frequency measurements. In both cases, shear elastic moduli and shear viscosities were estimated. Pulse sequences for the source and Doppler transducers were adapted to match the gel stiffness.

Measured data were fit to a second-order Kelvin-Voigt model in which model parameters were related to viscoelastic properties. Acoustic measurements were verified using independent rheometer measurements. For 3% concentration hydrogels, we estimated a shear elastic modulus 317 Pa using the acoustic radiation force technique and 321(+/–)14 Pa for storage modulus with a rheometer measurement. When measured at low frequencies, the dynamic shear storage modulus can be compared to the shear elastic modulus. For 4% concentration gels, the acoustic radiation force method yielded 681 Pa and rheometer yielded 640(+/–)17 Pa.

While other groups have been examining the application of acoustic radiation force for diagnostic imaging, our group is focused on developing precise basic science tools for discovering the role of the mechanical environment in cellular behavior.

Work supported by NIH/NCI R01 CA082497 and the Beckman Institute at UIUC.

Enhanced Mechanical Characterization of Tissue Response Using Full-Field Deformation Data from 3D Ultrasound

Petr Jordan
School of Engineering and Applied Sciences, Harvard University

Simona Socrate
Department of Mechanical Engineering, Massachusetts Institute of Technology

Todd E. Zickler
School of Engineering and Applied Sciences, Harvard University

Robert D. Howe
School of Engineering and Applied Sciences, Harvard University

Computational models of tissue mechanical response are beginning to play a significant role in modern computerized medicine and have become integral components of image-guided surgery and interventions. Such image-guided tasks require close interplay of computational biomechanical models with preoperative and intra-operative imaging. The development of appropriate models for the mechanical behavior of soft tissues is challenging due to the inherent complexities of the material response, and the limitations on testing protocols associated with in-vivo settings. Current in vivo soft tissue testing is dominated by indentation due to the simplicity of the tool configuration, and low-risk of injury associated with the procedure. Much of the information related to the interplay between shear and bulk compliance in the complex deformation field beneath the indenter is lost when capturing the single (time-displacement-force) output of the tool. Therefore, supplemental experimental methods, such as secondary indentation sensors [1] are necessary for well-conditioned parameter identification. Image-based characterization methods are a promising alternative solution, as they provide the means for noninvasive, in vivo measurement of the tissue response with improved sensitivity and uniqueness of the recovered material parameters. We present a general inverse finite-element modeling approach [2] to identify an appropriate constitutive framework and corresponding model parameters using full-field volumetric deformation data obtained from 3D ultrasound (3DUS). The finite-element model is coupled to full-field visual measurements by regularization springs attached at nodal locations. The free ends of the springs are displaced according to the 3DUS-estimated tissue motion and the normalized potential energy stored in all springs serves as a measure of model-experiment agreement for material parameter optimization. This approach enriches the traditional force-displacement indentation response with the measurement of volumetric deformation and provides good sensitivity to parameters governing the bulk response of the material. These parameters are otherwise not observable in conventional indentation. We demonstrate good accuracy of estimated parameters and consistent convergence properties on synthetically generated data. We present constitutive model selection and parameter estimation for perfused porcine liver in indentation. The proposed method is independent of imaging modality and constitutive law, suggesting potential applications for other tissues and scales (i.e. nanoindentation, confocal microscopy, etc.).

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Imaging Microenvironmental Factors of Breast Cancer: Ultrasonic Elasticity Imaging of Tissue pH

Rebecca Yapp
Graduate Student
Department of Bioengineering and Beckman Institute of Advanced Science and Technology, University of Illinois

Rohit Bhargava
Department of Bioengineering and Beckman Institute of Advanced Science and Technology, University of Illinois

Michael Insana
Department of Bioengineering and Beckman Institute of Advanced Science and Technology, University of Illinois

The microenvironment of breast cancer tumor cells differs from that of normal tissue both mechanically and chemically. Diseased cells interact via signaling pathways with the surrounding extracellular matrix (ECM) to induce tissue responses such as desmoplasia, edema, and acidic conditions. Each of these microenvironmental factors can destabilize cell behavior to increase metastatic potential and reduce responses to traditional therapies. Our goal is to develop medical imaging modalities that can sense the mechano-chemo-microenvironment of tumors. These types of images help us detect and accurately diagnose tissues as well as monitor the responses to treatment.

The focus of this report is on pH imaging, where ultrasonic methods are applied to image viscoelastic features of breast tissues and tissue-like hydrogels. Changes in extracellular pH can strongly affect the ultrastructure of type I collagen being formed in the extracellular matrix (ECM) of breast stroma. As the ECM structure is varied, so are the viscoelastic (VE) features. A small force (< 5N) is applied to the medium under study and held constant (quasi-static compression) while ultrasonic echo data are acquired to image strain. From the echo data, a time series of strain images is formed to visualize tissue creep as functions of both time and space. Creep curves are fit to rheological models to estimate VE parameters and form images of the elastic compliance as well as time constants associated with viscous creep. We and others have observed significant changes in breast patient data that are specific to the diagnosis. However, the complexity of breast tissue structures in vivo makes it difficult to explain the sources of the contrast observed. To understand why there is tissue-specific contrast, we study tissue-like gelatin hydrogels.

Gelatin is a reasonable physical model for breast stroma. To model physiological acidosis we added a linear track of acid to the gelatin during polymerization. This pH-induced contrast was analyzed to determine the sensitivity of the measurement, and then compared to traditional rheological measurements to validate for accuracy. The results in hydrogels are then compared to patient studies to help us understand sources of tumor contrast. We find that pH greatly affects the instantaneous elastic strain by altering the collagen fibers and their cross-linking structure. However, the VE time constants were not significantly changed, suggesting that pH affects the VE response very little. To better understand the molecular-scale events responsible for the observed mechanical responses, we also monitored compression tests with Fourier Transform Infrared (FTIR) spectroscopy. FTIR methods explain the thermodynamic changes responsible for the elastic response during deformation. Through a combination of these experimental methods, a theory of VE tumor contrast is beginning to emerge.

Layered Metal Nano Probes for Ultra-sensitive Biomolecular Surface-Enhanced Spectroscopic Imaging

Anil K Kodali
Graduate Student
Mechanical Science and Engineering, Micro and Nanotechnology Lab, University of Illinois

Megan Koop
Undergraduate Student
University of Illinois

Laura Jane Elgass
Undergraduate Student
University of Illinois

Margie Mathewson
Undergraduate Student
University of Illinois

Rohit Bhargava
Assistant Professor
Bioengineering,
Beckman Institute, University of Illinois

Detection of multiple molecular species is significant in a range of biomedical analyzes from functional imaging to disease detection, diagnosis and prognosis. Biomolecular imaging using nanoparticle probe based optical detection technologies is especially attractive due to simple (cheap) and widely available instrumentation involved. The level of sensitivity however is often not high enough for molecular detection. Here we propose the design and fabrication of layered nanoscale metal particle probes with tunable intense optical responses reproducibly. The enhancement in the optical signals is due to the surface plasmon effect of metal. We demonstrate this tunability and enhancement using light scattering calculations based on classical electromagnetic theory. We further discuss an approach for optimization of configuration parameters like size, shape and properties for desired optical response. The design of the probes with specific reference to probes for imaging techniques based on vibrational spectroscopy, light scattering spectroscopy etc is presented. Controllable fabrication of such probes using organic/biomolecular linkers is also discussed. We finally report the proof of concept of fabrication of probes in aqueous suspensions.

Intrinsic Indicators of Pathological States: Refractive Index Maps and Membrane Fluctuations in *P. falciparum* Infected Human Red Blood Cells

YongKeun Park
Graduate Student
Health Science, & Technology (HST), Harvard-MIT

Monica Diez-Silva
Postdoctoral Associate
Department of Materials Science and Engineering, MIT

Gabriel Popescu
Assistant Professor
Department of Electrical and Computer Engineering, University of Illinois

George Lykorafitis
Postdoctoral Associate
Department of Materials Science and Engineering, MIT

Wonshik Choi
Postdoctoral Associate
G. H. Spectroscopy Lab., MIT

Michael S. Feld
Professor
Physics, MIT

Subra Suresh
Professor
School of Engineering, and Harvard-MIT Division of Health Science and Technology, MIT

Pathogenesis of malaria induces by *Plasmodium falciparum* is characterized by structural, biochemical, and mechanical modifications to the host RBCs [1-2]. In order to study these modifications, we investigate two intrinsic indicators: the refractive index maps and membrane fluctuations in P. falciparum infected human red blood cells. We report the first experimental connections between these intrinsic indicators and pathological states. Employing two novel optical techniques (tomographic phase microscopy and diffraction phase microscopy) [3-4], three dimensional maps of refractive index and nanoscale cell membrane fluctuations in individuals red blood cells are quantitatively and non-invasively characterized. Our systemic experiments cover all intra-erythocytic stages of parasite development under body and febrile temperatures. These findings offer potential new avenues for identifying, through cell membrane dynamics, pathological states that could result in human diseases.

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Magnetic Resonance Measurement of Transient Shear Waves *In Vivo*

Philip V. Bayly
Hughes Professor of Engineering
Departments of Mechanical, Aerospace, and Structural Engineering, and Biomedical Engineering, Washington University

Panagiotis G. Massouros
PhD
Department of Mechanical, Aerospace, and Structural Engineering, Washington University

Efty Christoforou
PhD
Department of Mechanical, Aerospace, and Structural Engineering, Washington University

Arash Sabet
MS
Department of Mechanical, Aerospace, and Structural Engineering, Washington University

Guy M. Genin
Department of Mechanical, Aerospace, and Structural Engineering, Washington University

Imaging the effects of rapid loading on soft tissue is a persistent biomechanics challenge. We have developed a system that estimates dynamic strain fields in bulk specimens and in vivo through tagged magnetic resonance imaging (MRI) [1-2] synchronized to periodic impact excitation. The MRI sequence imparts magnetic gradients upon a specimen that translate with material particles, enabling estimation of an array of distributed displacement and strain measurements. In our implementation [3] we have obtained high spatial (here 5 mm) and temporal (6 ms) resolution. We will present validation of the approach on shear waves traveling through gelatin, and show examples of its application to non-invasive measurement of dynamic shear waves in brain tissue during angular acceleration of the skull.

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MRI-based Finite Element Modeling of Mild Head Trauma

Ying Chen
Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Marcus Slavenas
Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Martin Ostoja-Starzewski
Department of Mechanical Science and Engineering, University of Illinois

This paper reports work on a model simulating human head under impact loading with resolution down to a millimeter. The model is based on a finite element (FE) mesh developed from a structural magnetic resonance image (MRI) set. We discuss: (i) acquisition of T1 and a T2 images, their processing via FSL (a library of MRI analysis tools) to produce a set of image files that designate each voxel as either scalp, skull, cerebral spinal fluid (CSF), grey matter, white matter, or non-object; (ii) creation of a FE mesh based upon the FSL tissue identification and the image geometry; (iii) mesh smoothing; (iv) choice of material constitutive parameters for all the tissues involved; and (v) simulations of frontal impact of human head. The numerical results were found to agree well with previous cadaver test data, and are currently being validated using dynamic imaging on live patients in the MRI tunnel. The agreement indicates the potential use of our MRI-based FE model for understanding mechanics of head trauma injuries.

Extraction of Skeletal Muscle Microstructure and Mechanics from Diffusion MRI Signal

Dimitrios C. Karampinos
Department of Mechanical Science and Engineering, University of Illinois

Bradley P. Sutton
Department of Bioengineering, University of Illinois

Kevin F. King
General Electric Healthcare, Global Applied Science Laboratory

John G. Georgiadis
Department of Mechanical Science and Engineering, University of Illinois

Diffusion Tensor Imaging (DTI) MRI unique non-invasive microstructure probing capabilities and it constitutes a valuable tool in the study of fiber orientation in skeletal muscles. By implementing a DTI sequence with highly sensitive directional encoding to quantify in vivo the microarchitectural properties of the calf muscles of a healthy volunteer at rest, we report that the secondary eigenvalue is significantly higher than the tertiary eigenvalue, a fact corroborated by prior DTI findings. In order to explain this observation, we propose a composite medium model that accounts for water diffusion in the space within the muscle fiber and the extracellular space. The muscle fibers are abstracted as infinite cylinders with an elliptical cross section, which closely approximates microstructural features well documented in prior histological studies of excised muscle. The values of fiber ellipticity predicted by our model agree with prior studies, and the spatial orientation of the cross-sectional ellipses is consistent with local muscle strain fields and the putative direction of lateral transmission of stress between fibers. Since myocyte shape adapts to stress, this orientation can ostensibly coincide with the direction of lateral transmission of stress between fibers. In the medial gastrocnemius, for example, this orientation is consistent with the strain non-uniformity found in other studies. We conclude that DTI combined with model-based analysis can give useful clues about in vivo intramuscular force transmission. As a metric, fiber cross-sectional ellipticity may be useful for quantifying morphological changes in skeletal muscle fibers with aging, hypetrophy, or following physical exercise.

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Experimental Multiscale Mechanics

ORGANIZERS:

Samantha Daly, *Department of Mechanical Engineering, University of Michigan*

Julia Greer, *Department of Materials Science, California Institute of Technology*

SYMPOSIUM
W

Plastic Flow in Amorphous Metals: Insight From *In Situ* Tests in a TEM and MD Simulations

Evan Ma
Professor
MS&E, Johns Hopkins University

The metals and alloys we are familiar with are all crystalline and well understood. In contrast, their amorphous counterparts, i.e., "bulk metallic glasses" (BMGs), pose new challenges to the materials science community. Here even the basic issues, such as why they are such easy glass formers, how atoms pack inside, and how plastic deformation proceeds in the absence of well-defined dislocations, have not been fully resolved.

We report in situ nanocompression and nanotensiton tests of metallic glasses (MGs) in a transmission electron microscope. This new technique is capable of spatially and temporally resolving the plastic flow in MGs. The observations reveal the intrinsic ability of monolithic MGs to sustain large plastic strains (in some cases with gradual necking in tension as known for ductile crystalline metals), which would otherwise be pre-empted by catastrophic instability in macroscopic samples and conventional tests. The high ductility in volume-limited MGs, and the sample size effects in suppressing the rapid failure common to glasses, is explained by considering the evolution of the collectivity of flow defects towards localization.

MD modelling efforts will also be reported, which provide physical understanding of the initiation of plastic flow in amorphous metals. In particular, we describe the structural processes involved in shear transformations, and the effects of alloy composition on the local structure and dynamics, and hence the propensity for plastic relaxation.

In Situ Tensile-Creep Characterization of Structural Alloys

Carl Boehlert
Associate Professor
Chemical Engineering and Materials Science, Michigan State University

Sara Longanbach
Graduate Student
Chemical Engineering and Materials Science, Michigan State University

A technique has been developed to acquire secondary electron and backscattered electron detector images and electron backscattered diffraction (EBSD) orientation maps during tensile-creep deformation at temperatures as high as 76°C. The EBSD observations during deformation proved to be useful for quantifying the types of grain boundaries which have preferentially cracked. Details and limitations of this testing technique and the results obtained on advanced structural alloys (titanium-, nickel-, and cobalt-based) will be presented.

In particular, a cobalt-based superalloy, Udimet alloy 188, was subjected to grain boundary engineering involving thermomechanical processing in an attempt to improve the creep performance and to determine how creep deformation processes are affected. Udimet alloy 188 is a cobalt-based superalloy with good creep and fatigue strength and oxidation resistance up to 1093°C [1,2]. The as-received sheet was cold rolled to either 10%, 25%, or 35% reduction per pass followed by a solution treatment. This sequence was repeated four times and the resultant microstructure and the grain boundary character distribution were described using electron backscatter diffraction. A significant amount of grain boundary cracking was observed both on the surface and subsurface of deformed samples, but surface cracks were greater in number and size than those within the bulk. The cracking behavior was similar both in vacuum and air environments, indicating that grain boundary cracking was not caused by environment. To assess the mechanisms of crack nucleation, in-situ scanning electron microscopy was performed during elevated-temperature tensile-creep deformation using an Ernest Fullam tensile stage. Details of this apparatus and testing technique can be found elsewhere [3-7]. From such experiments, the deformation in the form of cracking was observed at the FCC grain boundaries. Sequential secondary electron imaging and EBSD orientation mapping were performed in-situ to allow the evolution of crack nucleation and linkage to be followed. Cracking occurred preferentially along general high-angle grain boundaries and less than 15% of the cracks were found on low-angle grain boundaries and coincident site lattice boundaries. Thus there is evidence that the special boundaries in this alloy are resilient to cracking during creep. The findings of this work have significant implications regarding grain boundary engineering of this alloy and potentially for other alloy systems.

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Direct Measurements of Microstructure and Micromechanical State at Several Length Scales via Synchrotron X-Ray Diffraction

Joel Bernier
Postdoctoral Fellow
Engineering Technologies Division, Lawrence Livermore National Laboratory

The availability of intense, high-energy synchrotron x-rays has revolutionized experimental mechanics for polycrystalline materials. When combined with the large, position-sensitive area detectors and flexible configurations provided by many user facilities, synchrotron x-ray diffraction has spurred the development of several novel methods for multi-scale, in situ characterization of microstructure and micromechanical state. In this talk, techniques for quantitative strain/stress analysis at three length scales are presented: mesoscopic, grain-averaged, and intragranular.

The mesoscopic technique is analogous to quantitative texture analysis [1]. It provides orientation-dependent intergranular stresses in the form of tensor fields over the orientation space for each phase in the material. Statistically representative volumes (~300-1000 μm^3) are interrogated and micromechanical stress states may be correlated with texture components. Two examples are presented for specimens deformed in situ: the co-evolution of stress states for several texture components in a rolled and re-crystallized Cu sample, and stress partitioning between the (HCP) and (BCC) phases in a Ti-6Al-4V sample. The latter showcases a particular strength of the mesoscopic technique.

The grain-averaged technique—referred to as 3DXRD [2]—provides the average orientation, strain tensor and size of each grain in a small neighborhood (~50-300 μm^3). It enables in situ observations of complex processes such as twinning and phase transformations at the grain scale. Results from in situ observations of tensile twinning in Mg AZ31 alloy as well as local stress evolution in a neighborhood of Ti-7Al grains are shown.

Lastly, the intragranular technique—referred to as Laue micro- and nanodiffraction [3]—provides spatially resolved measurements of lattice orientation and strain tensor components in volumes as small as ~1 μm^3. This facilitates calculation of orientation and strain/stress gradients, towards understanding the micromechanical environment near grain boundaries and regions of high GND densities. Preliminary results from line indented single-crystal Cu and Al specimens are presented, and future applications with respect to understanding plasticity in complex microstructures are discussed.

This ensemble of techniques comprise an experimental analog to multi-scale modeling frameworks. The data they provide is critical for verification and validation across the various length scales. Integration of these data with the modeling frameworks is discussed with emphasis on current developments and future goals.

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Recrystallization in a 304L Steel during Dynamic Deformation at High-Temperatures

Bo Song
Sandia National Laboratories

Bonnie Antoun
Sandia National Laboratories

Weinong Chen
Professor
School of Aeronautics & Astronautics and School of Materials Engineering, Purdue University

To investigate the recrystallization in a 304L stainless steel deforming at high rates and high temperatures, a split Hopkinson pressure bar (SHPB) was modified to compress the specimen dynamically at different temperatures and then quenched at different times after high-rate plastic deformation. The shapes of the loading pulses were controlled such that the specimen deformed under dynamic equilibrium at constant strain rates. A furnace was used to heat specimen to 1500—1700 F before dynamic loading. The specimens were quenched 6 and 15 seconds after the dynamic loading to facilitate the investigation of recrystallization and other microstructural changes in the plastically deformed specimens.

Hypervelocity Impact: Damage Mechanics and Material Response

Leslie Lamberson
Graduate Research Assistant
Department of Aeronautics, California Institute of Technology

Ares J. Rosakis
Professor and Director of Graduate Aeronautical Laboratories
Department of Aeronautics, California Institute of Technology

Marc A. Adams
Principal Engineer
Jet Propulsion Laboratory, California Institute of Technology

Hypervelocity impact is a rising concern in spacecraft missions where man-made debris in low Earth orbit and micrometeoroids are capable of compromising or depleting the structural integrity of a vehicle. This high-energy-density phenomenon gives rise to pressures in the Mbar range and strain rates up to 10^{11} $1/D^s$ that can alter vehicle trajectory and structural, thermal, optical, and/or electrical properties [1]. While numerous computational models are utilized for risk mitigation of hypervelocity impacts [2], little is actually understood regarding the mechanisms responsible for damage incurred during a hypervelocity strike [1]. Depending on impact velocity and material choices, damage mechanisms can include melting and vaporization, dissociation, ionization, plasma formation, fracture and fragmentation, and mixed phase flow, to name a few [3]. Integrated experiments performed at Caltech/JPL's Small Particle Hypervelocity Impact Range (SPHIR), a two-stage light gas gun capable of launching projectiles in vacuum at speeds ranging from 1 to 10 km/s, use optical diagnostics and high-speed photography to investigate dynamic material behavior. Projectiles are small spheres and cylinders 0.25-2.5 mm in diameter with aspect ratios, L/D, of 1-2. Materials selected for the study include nylon and tantalum projectiles, and Homalite, tantalum and aluminum 150 mm diameter target discs. Photoelasticity and coherent gradient sensing, a shearing interferometry technique, are utilized to capture target deformations in-situ. High speed photography is used to capture projectile velocity, spectral flash, ejecta, and in some case, plasma formation. Using microtomy, tantalum projectile grain structures are examined pre- and post-impact. Various scaling effects of projectile to impact size and resulting damage zone, implications on vehicle shielding, and validation of numerical simulations are discussed.

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Effect of Loading Rate and Surface Conditions on Tensile Strength of Borosilicate Glass

Weinong W. Chen
Departments of MSE and AAE, Purdue University

Xu Nie
Research Assistant
Department of MSE, Purdue University

Andrew A. Wereszczak
Oak Ridge National Laboratory

Borosilicate glass has been used in windows for resisting blast and impact loading. It is of significant interest to develop quantitative understanding of the dynamic deformation, damage, and failure behavior of the glass. Recent research on the dynamic compressive response of borosilicate glass showed that the glass is capable of bearing up to 1.5 GPa uniaxial compression stress before cracks propagate extensively in the specimen [1]. The dynamic deformation and fracture behavior of this glass under multiaxial compression was studied with the specimens confined by steel collars in a split Hopkinson pressure bar [2]. However, in window applications, the thickness of the glasses plates is limited and that introduces the potential initiation of damage effects caused by deflection. Under ballistic impact loading conditions, it has been shown that the most dominant and vital failure modes are spalling and bending induced tension on the backside of the plate [3], which points to the need for determining the dynamic failure behavior under high-rate tension loading. Under tensile or flexural loading, glass strength is typically limited by surface defects introduced by after-manufacturing handling, but rarely by bulk defects [4]. Therefore, for the glasses in blast-resisting window applications, it is important to understand the loading rate and surface condition effects on the tensile or flexural strength. In this study, (uniaxial) flexural strength testing is performed because uniaxial tensile strength testing of glasses is very difficult to validly conduct experimentally, so reported flexural strength values are used to make inferences to the (uniaxial) tensile strength of glass. Flexural strength is experimentally conducted here and comparisons and interpretations are made in reference to their values; however, it is a tensile stress produced during flexural loading that initiates fracture, so the authors will refer to the fracture response as being due to flexural and tensile loading.

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High Strain-Rate Compression and Shear Response of Polycarbonate

Jason G. Vogeler
Graduate Research Assistant
Engineering Mechanics, University of Nebraska, Lincoln

Ruqiang Feng
Associate Professor
Engineering Mechanics, University of Nebraska, Lincoln

Mehrdad Negahban
Associate Professor
Engineering Mechanics, University of Nebraska, Lincoln

Polycarbonate is a tough, transparent engineering thermoplastic that has been widely used in critical applications such as impact-resilient eyewear, aircraft window, and transparent armor. Characterization of its behavior over the strain rate, strain and temperature ranges relevant to these applications is an important need. To investigate the effect of confinement on the high-rate flow stress response of polycarbonate, we have developed an experiment using a modified Kolsky torsion bar device. The experimental technique permits the sample material to be preheated and compressed to desired temperature and stress states and then tested under impulsive high strain-rate shear loading. Experiments with this new technique have been carried out on LEXAN9034, a polycarbonate manufactured by General Electric, for initial temperatures from the room temperature up to 100 degrees Celsius, initial compressive stresses up to 20 MPa, and dynamic shear loadings with shear rates from 500 1/s to 2500 1/s. The results will be presented and discussed in comparison with the data from high stain-rate compression or shear only experiments as well as low strain-rate experiments on the same material in terms of strain rate and stress invariants and with those reported in the literature.

Blistering and Delamination in High Temperature Polymer Matrix Composites Due to Rapid Heating

Alan Zehnder*
Department of Theoretical and Applied Mechanics, Cornell University
atz2@cornell.edu

Michael Czabaj
Graduate Research Assistant
Department of Theoretical and Applied Mechanics, Cornell University

Due to their high glass transition temperatures, polyimide matrix composites (PiMCs) extend the role of composite materials into extreme temperature environments [1, 2]. As PiMCs are likely to be used only in applications where their high-temperature properties are truly needed, understanding their high-temperature performance is critical. Many PiMCs can absorb up to 1% moisture by weight. If laminates are heated rapidly, the moisture will vaporize developing high internal pressures that can lead to plasticization[3, 4], initiate void nucleation, delaminate pre-existing flaws, and ultimately result in laminate failure [1, 3]. To date, little effort has been given to the study of steam-induced damage, since most PMCs operate at moderate temperatures where the relatively low water vapor pressure is insufficient to cause internal damage.

A new method to predict initiation of steam-pressure induced damage for rapidly heated polyimide neat resin and composites is proposed. This method entails use of a simple theory to calculate the internal steam pressure. Using a thermal mechanical analyzer it is shown that the onset of steam-induced damage can be detected by the point of rapid expansion of moisture-saturated specimens. Optical microscopy is used to visualize initiation and evolution of damage in neat resin and laminates. Data from tests performed over a range of heating rates and initial moisture saturations are used to develop a critical pressure-temperature envelope. With this envelope we show the dependence of damage on initial moisture content and heating rate and describe the application of the envelope to failure prediction and design of laminates subjected to rapid heating.

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Toughening of Polymeric Materials by Dispersion of Nanoparticles

Amit Kaushik
Mechanical Engineering, University of Michigan

Paul Podsiadlo
Chemical Engineering, University of Michigan

Ellen M. Arruda
Professor
Mechanical Engineering, University of Michigan

Ming Qin
Chemical Engineering, University of Michigan

Anthony M. Waas
Professor
Aerospace Engineering, University of Michigan

Nicholas A. Kotov
Associate Professor
Chemical Engineering, University of Michigan

Harish Iyer
Mechanical Engineering, University of Michigan

Eugene Kheng
Aerospace Engineering, University of Michigan

The dispersion of nanoparticles into polymers provides an opportunity to synthesize materials that can challenge the advanced materials found in nature. However, dispersion of these nanoparticles, especially in high volume fractions is a challenge and often results in their aggregation. Here, we demonstrate that, using a layer-by-layer (LBL) manufacturing technique, it is possible to not only disperse these nanoparticles in the polymer matrix even at very high volume fractions but also controlling their spatial orientation[1]. The incorporation of nanoparticles (clay nanoparticles) in the polymer (polyurethane) matrix exhibits a substantial improvement in the stiffness, yield strength, ultimate strength and toughness of the polymer (polyurethane). The nanoscale control in the LBL technique allows us to conduct well-controlled experiments to examine the toughening mechanisms in nanoparticle-reinforced polymers at nanoscale and design polymer-clay nanocomposites with enhanced toughness and other mechanical properties.

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Thermal Response of Sol-Gel Derived Lead Zirconate Titanate (PZT) Thin Films

Thomas Berfield
Department of Mechanical Engineering, University of Louisville

Nancy Sottos
Department of Material Science and Engineering, University of Illinois

Ferroelectric properties of electroceramic thin films are influenced by residual stresses related to thermal processing. Two methods are used to monitor the evolution of mechanical response for a blanket PZT sol-gel thin film (c.a. 40 nm thickness) as the film is heated from 30°C to 300°C. Wafer curvature measurements are made to estimate the residual stress, and a fluorescence-based digital image correlation method (DIC) is used to measure the development of in-plane strains. Thin film specimens are fabricated through solution deposition of a 0.25M PZT stock onto a $Pt/Ti/SiO_2/Si$ substrate. A suspension of silica nanoparticles (c.a. 140 nm diameter) in ethanol is spincast onto the sample surface to provide the random speckle pattern necessary for performing DIC strain measurements.

For comparison, the stress and strain development within thin film line features patterned via a mediated octadecyltrichlorosilane (ODS) monolayer is also presented. Within the patterned line features, tensile stress and strain parallel to the line direction are found to be similar to the constrained blanket film case, and reduced in the direction perpendicular to the line feature.

An Electrical Technique to Measure *In Situ* Contact Area during Instrumented Indentation and Its Application of Characterizing Materials That Pile Up

Lei Fang
Graduate Student
Department of Engineering Science and Mechanics, Pennsylvania State University

Christopher Muhlstein
Department of Materials Science and Engineering, Pennsylvania State University

James Collines
Graduate Student
Department of Materials Science and Engineering, Pennsylvania State University

Amber Romasco
Graduate Student
Department of Materials Science and Engineering, Pennslyvania State University

Lawrence Friedman
Department of Engineering Science and Mechanics, Pennslyvania State University

One of the primary tools for mechanical characterization of materials is instrumented indentation using the Oliver-Pharr data analysis method. The resulting mechanical properties such as the (reduced) elastic modulus and hardness are described as force per area; however, the Oliver-Pharr method lacks a direct in-situ measurement of contact area between the indenter and sample. The indirect measurement of contact area via Oliver-Pharr confounds instrumented indentation tests when characterizing dynamic properties, thin films, and materials that "pile-up" around the indenter. Indenting annealed copper, an electrical technique is demonstrated to continuously measure the in-situ contact area and hardness by relating non-linear electrical contact current-voltage (I-V) curves to the instantaneous contact area. The electrical instrumented indentation technique is then applied to characterize work-hardened copper that exhibits "pile-up".

Small-Scale Mechanical Properties of Chromium Carbide-Based Composites

Irina Hussainova
Department of Materials Engineering, Tallinn University of Technology

Iwona Jasiuk
Department of Mechanical Science and Engineering, University of Illinois

High- resolutions measurements of mechanical properties of the constituent phases of multi phase materials are of immerse importance in design of new composites. Measuring the intrinsic properties of each phase separately gives the information on the special heterogeneity in local material properties and serves as a guide to process engineering and advanced materials design. In this study, the nanoindentation, X-ray analysis and microstructural SEM investigations have been used to reveal the properties and structural features of ceramic-metal composites with respect to chromium carbide based cermets of different binder composition. The results indicate that sintering process influences the microstructural parameters such as grain size, residual porosity and thermal stresses; however, nano-hardness and Young's module of constituent phases remains less affected. Phase-specific mechanical properties are measured and correlated with bulk behavior. Furthermore, hardness of the binder metal is detected to be higher in cermet as compared to the bulk hardness of metal. It is shown that the indentation laod or depth of penetration should be carefully chosen to extract the in situ properties of the constituent phases. The results demonstrate the information required for any micromechanical model that would predict composition-based mechanical performance of a given composite materials.

Measuring the Constitutive Behavior of Viscoelastic Solids in the Time and Frequency Domain Using Flat Punch Nanoindentation

Erik Herbert
MTS Nano Instruments Innovation Center

Warren C. Oliver
MTS Nano Instruments Innovation Center

Arnold Lumsdaine
MTS Nano Instruments Innovation Center

George M. Pharr
Department of Materials Science and Engineering, University of Tennessee, Oak Ridge National Lab

The purpose of this work is to further develop experimental methodologies using flat punch nanoindentation to measure the constitutive behavior of viscoelastic solids in the frequency and time domain. The reference material used in this investigation is highly plasticized polyvinylchloride (PVC) with a glass transition temperature of -17 C. The nanoindentation experiments were conducted using a 983 μm diameter flat punch. For comparative purposes, the storage and loss modulus obtained by nanoindentation with a 103 μm diameter flat punch and dynamic mechanical analysis are also presented. Over the frequency range of 0.01 to 50 Hz, the storage and loss modulus measured using nanoindentation and uniaxial compression are shown to be in excellent agreement. The creep compliance function predicted from nanoindentation data acquired in the frequency domain is also found to be in excellent agreement over two decades in time with the creep compliance function measured using a constant stress test performed in uniaxial compression. A constraint factor of 1.55 is found to overlay the creep compliance function measured by nanoindentation in the time domain with the creep function measured in uniaxial compression. Time-temperature superposition of nanoindentation data taken at 5, 10, 15, and 22 C show the sample is not thermorheologically simple and thus the technique cannot be used to expand the mechanical characterization of this material. Collectively, these results clearly demonstrate the ability of flat punch nanoindentation to accurately and precisely determine the constitutive behavior of viscoelastic solids in the time and frequency domain.

Peeling of Extensible Elastic Adhesive Tapes

Christopher Kovalchick
Graduate Aeronautical Laboratories, California Institute of Technology

Alain Molinari
Professor
Laboratoire de Physique et Mécanique des Matériaux, Université de Metz

Guruswami Ravichandran
Professor
Graduate Aeronautical Laboratories, California Institute of Technology

The measurement of interface mechanical properties between an adhesive layer and a substrate is significant for optimization of a high-quality interface [1]. A common method for measuring these properties is the peel test. Although analytical models exist for peeling of elastic tapes from smooth surfaces, there is a need for rigorous experiments in this area. Furthermore, several assumptions are made in the models regarding the mechanical and material properties of the tape as well as the testing conditions [2]. A common assumption is the inextensibility of the tape, which requires that the elastic energy term in the energy balance of the peel process be neglected [3]. However, this term can become significant for elastomers at small peel angles [4], in which case the tape is considered as an extensible linear elastic medium.

The peel force at varying angles is determined for several commercial tapes, including 3M Scotch(TM) MultiTask tape and 3M Super 33+ Electrical tape. Tests are conducted using a newly-developed peel arrangement capable of peel angles from 0 to 180 degrees. The influence of extensibility on adhesion is examined, and results are compared to a model which accounts for the extensibility of the tape.

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Reversible Elasticity and Structural Damping of Individual Multi-walled Carbon Nanotubes in Radial Direction

Majid Minary-Jolandan*
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois
mminary2@uiuc.edu

Min-Feng Yu
Department of Mechanical Science and Engineering, University of Illinois

Carbon nanotubes (CNTs) exhibit great promising application as light-weight and extremely strong fiber components as well as structural damping elements in high performance composites and films [1, 2]. Despite their extremely high tensile strength and the Young's modulus in axial direction [3], CNTs are shown to be rather soft in transverse (radial) direction to the extent that van der Waals interaction between two adjacent CNTs can induce radial deformation [4]. We probed elastic and damping properties of individual multi-walled carbon nanotubes (MWCNTs) in radial direction using nanoindentation with atomic force microscope (AFM). Static force-deformation with AFM revealed that MWCNTs show reversible radial deformation up to the complete flattening (~60% deformation). The exact number of walls (thus the shell thickness) in MWCNTs, often uncertain in previous studies, was also uniquely determined in this study. This allowed application of a continuum shell model to obtain an effective elastic modulus of E ~16 GPa in radial direction. Furthermore, an improved method was introduced to obtain the tangent modulus (loss modulus/storage modulus) vs. indentation depth in continuous dynamic nanoindenation with AFM. Using this method, dynamic nanoindentation was conducted on individual MWCNTs in transverse direction to obtain their structural damping characteristics. The results revealed that individual MWCNTs show a tangent modulus of ~ 0.055, which is comparable to common polymers such as high density polyethylene.

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Nanoscale Meniscus Effects in Nanowire-Substrate Adhesion and Friction

Aman Haque
Assistant Professor
Mechanical & Nuclear Engineering, Penn State University

Mohanprasad Manoharan
Graduate Student
Mechanical & Nuclear Engineering, Penn State University

The micro-scale analysis of friction involves a normal load, which in conjunction with adhesion, gives rise to the friction force. The dominance of adhesive forces at the nanoscale implies that significant friction forces can manifest at the interface even with zero externally applied normal load. This effect is pronounced if one of the contacting bodies is compliant such as nanotubes and nanowires, which is the central theme of this paper. We have designed and nanofabricated an adhesion-friction force sensor to characterize friction in zinc oxide nanowires on silicon substrates. Experimental results show static friction coefficients for zero externally applied normal load can be as high as 45. This behavior is observed to be strongly influenced by the ambient conditions and we propose that the presence of molecularly thin moisture layers is responsible for the observed pseudo-static friction. Accordingly, we measure the shear strength of this layer to about 1 MPa. The findings of this study will provide valuable input to nanoscale interfacial systems such as nanowires and nanotube based sensors and nanocomposites, where the contact is primarily due to adhesion, and strong adhesion-friction coupling is needed to maintain device performance and integrity.

Multiscale Modeling of Defects in Solids

ORGANIZERS:

Kaushik Dayal, *Department of Civil and Environmental Engineering, Carnegie Mellon University*

Vikram Gavini, *Department of Mechanical Engineering, University of Michigan*

SYMPOSIUM Y

Multimillion-to-Billion Atom Molecular Dynamics Simulations of Shear Deformation, Fracture, and Nanoindentation in Silica Glass

Rajiv Kalia
Professor
Collaboratory for Advanced Computing and Simulations, University of Southern California

Aiichiro Nakano
Professor
Collaboratory for Advanced Computing and Simulations, University of Southern California

Priya Vashishta
Professor
Collaboratory for Advanced Computing and Simulations, University of Southern California

Cavitation is a ubiquitous form of damage in the ductile fracture of metallic alloys. However, recent Atomic Force Microscopy studies of stress corrosion cracking and molecular dynamics (MD) simulations of dynamic fracture reveal that the key damage mechanism during crack extension in "brittle" glasses also involves cavitation, albeit at the nanometer scale. In this talk, I will present results of our multimillion-to-billion atom MD simulations on: (1) nucleation, growth and coalescence of damage nanocavities in dynamic fracture of amorphous silica (a-SiO_2); (2) deformation and breakup mechanisms for nanovoids in shearing silica glass; and (3) defect migration and recombination in nanoindentation of a-SiO_2.

The Formation Volume and Formation Energies of Point Defects in Crystals

Krishna Garikipati
Associate Professor
Mechanical Engineering, & Michigan Center for Theoretical Physics, University of Michigan

Brian Puchala
Graduate Student Research Assistant
Materials Science and Engineering, University of Michigan

Michael L. Falk
Associate Professor
Materials Science and Engineering, Johns Hopkins University

We discuss the roles of continuum linear elasticity and atomistic calculations in determining the formation volume and the strain energy of formation of a point defect in a crystal. Our considerations bear special relevance to defect formation under stress. The elasticity treatment is based on the Greens function solution for a center of contraction or expansion in an anisotropic solid. It makes possible the precise definition of a formation volume tensor and leads to an extension of Eshelbys result for the work done by an external stress during the transformation of a continuum inclusion (Proc. Roy. Soc. Lond. Ser. A, 241, 376, 1957). Parameters necessary for a complete continuum calculation of elastic fields around a point defect are obtained by comparing with an atomistic solution in the far field. However, an elasticity result makes it possible to test the validity of the formation volume that is obtained via atomistic calculations under various boundary conditions. It also yields the correction term for formation volume calculated under these boundary conditions. Using two types of boundary conditions commonly employed in atomistic calculations, a comparison is also made of the strain energies of formation predicted by continuum elasticity and atomistic calculations. The limitations of the continuum linear elastic treatment are revealed by comparing with atomistic calculations of the formation volume and strain energies of small crystals enclosing point defects. Our studies also reveal the role of distortion-dependent elastic moduli in controlling the rate of convergence of atomistic calculations.

Peridynamics for Multiscale Modeling of Defects in Solids

Richard Lehoucq
Applied Mathematics and Applications, Sandia National Labs

Stewart Silling
Multiscale Dynamic Materials Modeling, Sandia National Labs

Peridynamics (Silling 2000) is a continuum theory that employs a nonlocal model of force interaction in order to describe long-range material interaction. This is accomplished by replacing the classical stress/strain relationship by an integral operator that sums forces seperated by a finite distance. This integral operator is not a function of the deformation gradient, and so allows for a more general notion of deformation than classical elasticity. The purpose of peridynamics is to provide a more general framework than the classical theory for problems involving discontinuities or other singularities in the deformation. Peridynamic's effectiveness has been demonstrated in several applications, including fracture and failure of composites, nanofiber networks, fracture of polycrystals, and crack instability.

Our presentation presents a (brief) overview of peridynamics and introduces the force flux, and associated stress tensor that are generalizations of contact forces, and the first Piola-Kirchoff stress tensor, respectively. We also explain how peridynamics converges to the classical theory as the region of nonlocality decreases to zero, and a relationship with molecular dynamics. This suggests that peridynamics is a viable mechanical theory for length scales ranging from molecular dynamics to those of classical elasticity.

Coupling Quasicontinuum and Quantum Mechanics

Ellad Tadmor
Professor
Aerospace Engineering and Mechanics, University of Minnesota

Viacheslav Sorkin
Postdoctoral Fellow
Aerospace Engineering and Mechanics, University of Minnesota

Noam Bernstein
Center for Computational Materials Science, Naval Research Laboratory

Gabor Csanyi
Professor
Centre for Micromechanics, Engineering Department, University of Cambridge

Computing mechanical and structural properties of materials can require an atomistic description of a chemically complex defect, for example a dislocation or a crack tip, while simultaneously describing the long range stress fields that couple to the defect. The former requires a quantum-mechanical model of interatomic bonding, while the latter is most efficiently treated with a continuum elasticity method such as finite elements. We present an implementation of the quasicontinuum method [1-2], which couples continuum elasticity with atomistic simulations, that uses a quantum-mechanical description of bonding in the core of the atomic resolution region. The method for combining the quantum-mechanical (QM) and interatomic potential (IP) descriptions of bonding [3] conserves energy, gives accurate forces with minimal effects from the interface between the QM and IP regions, and relies on fewer assumptions about the nature of bonding and the chemical species involved than QM/MM methods used in quantum chemistry. We compare results using this method with previously implemented approaches [4] for for several systems, including a crack tip and a dislocation in Al and Si.

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Hamiltonian-Based Concurrent Molecular Dynamics and Finite Element Simulation

Robin Selinger
Professor
Liquid Crystal Institute, Kent State University

Badel Mbanga
Research Assistant
Liquid Crystal Institute, Kent State University

Wilder Iglesias
Research Assistant
Liquid Crystal Institute, Kent State University

We present a method for multi-scale modeling of solids in three dimensions via concurrent molecular dynamics and finite element simulation. Here we build on the remarkable series of papers [1-4] by Abraham et al who developed a concurrent multi-scale modeling technique to simulate mode I fracture in Si. In their approach, the crack-tip region is modeled at the atomic scale with tight binding interactions; the plastic zone is modeled via classical molecular dynamics; and the rest of the sample is modeled at the continuum level using the finite element method. They define a Hamiltonian that includes contributions from each region with "hand-shaking" procedures at the boundaries. In the present work, we focus on the finite element part of the Hamiltonian, which Abraham et al formulated in two dimensions and with the caveat that it is valid only in the limit of small rotations. These limitations greatly restrict the usefulness of their multi-scale approach, e.g. it cannot be used to model crack propagation in mode III, or any other process requiring finite rotation and mechanics in three dimensions. To overcome those limitations, here we formulate an improved finite element Hamiltonian valid for rotations of arbitrary size, and extend the method to three dimensions. These additions allow the multi-scale approach to be applied to a far broader class of applications. We demonstrate that single-scale finite element simulation using this method conserves energy to high precision, and show it can be used to model elastodynamics of soft materials [5]. We further show that the same method can be extended to a broad class of elastic potential energy functions. Lastly we discuss applications of the multiscale method to problems in friction and fracture.

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An Effective Interaction Potential Model for Single Crystals of the Shape Memory Alloy AuCd

Ryan Elliott
Professor
Aerospace Engineering and Mechanics, University of Minnesota

Venkata Guthikonda
Graduate Student
Aerospace Engineering and Mechanics, University of Minnesota

Solid-to-solid martensitic phase transformations are responsible for the remarkable behavior of shape memory alloys (SMAs). There is currently a need for shape memory alloys with improved corrosion, fatigue, and other properties. The development of new accurate models of martensitic phase transformations based on the materials atomic composition and crystal structure would lead to the ability to computationally discover new improved SMAs.

This talk explores the Effective Interaction Potential (EIP) method for modeling the material behavior of SMAs. In particular, an extensive parameter study of the Morse pair potential model of the stress-free B2 cubic crystal is performed. Results for the stability, instantaneous bulk modulus, and the two instantaneous cubic shear moduli are presented and discussed. It is found that an Effective Interaction Potential model based on the Morse potential is appropriate for modeling transformations between the B2 cubic structure and the B19 orthorhombic structure, but is not likely to be capable of simulating the B2 cubic to B19 monoclinic transformation found in the popular SMA NiTi.

Accordingly, a procedure is developed to fit a Morse EIP model for the SMA AuCd, which is known to undergo a B2 to B19 transformation. The procedure matches the atomistic model to relevant material properties for the constituent elements and for the austenite phase (but not for the martensite phase) of the alloy. These properties include the lattice parameters, elastic moduli, coefficients of thermal expansion, and heat capacities. The resulting model is investigated, via branch-following and bifurcation (BFB) techniques, and it is found that a B2 to B19 transformation is indeed predicted by the model.

Chemomechanics of Defect Kinetics at Far-from-Equilibrium Interfaces

Krystyn Van Vliet
Professor
Materials Science and Engineering, MIT

The mechanical behavior of structurally complex materials are governed in large part by the thermodynamics and kinetics of point, line, and planar defects. For materials that are processed or utilized under far-from-equilibrium conditions, the concentration and motion of these defects play a critical role in material strength but are difficult to quantify experimentally. Here, we discuss multiscale modeling of such defect chemomechanics in three distinct materials: amorphous solids with high surface area, supersaturated alloys, and biomolecular complexes. In each system, long timescale dynamics and metastability present challenges and opportunities for predictive computational simulations of material mechanics.

Multiscale Model for Electrical and Optical Effects of Dislocations in III-V Semiconductors

Harley Johnson
Associate Professor
Mechanical Science & Engineering, University of Illinois

Jeong Ho You
Postdoctoral Research Associate
Caltech

Dislocations provide strain relief in GaN and GaAs, but they also affect optical and electronic properties due to electron trapping by dangling bonds, and the bandstructure shift due to the dislocation strain field. Here we develop a multiscale atomistic-continuum model that accounts for these factors and quantitatively predicts the reduction in photoluminescence intensity and electron mobility with increasing dislocation density, the presence of dislocation-related radiative recombination, and the difference in dislocation sensitivity in various materials. The model uses first principles atomistic calculations to determine the charged state of the dislocation core, and then classical electrostatics to model the line charge nature of the dislocation, both in the context of a classical scattering model used to understanding electrical effects, and a finite element based quantum mechanical model used to predict optical properties.

Revisiting Quantum Notion of Stress

Pradeep Sharma
University of Houston

Ravi Maranganti
University of Houston

Existing notions of stress in a quantum mechanical framework are reviewed and discussed. Notwithstanding early fundamental work in this area since 1930's, the increasing availability of computational tools to perform ab initio quantum mechanical calculations with high accuracy and efficacy has renewed interest in this field especially in the context of computational mechanics and materials science. Although some unresolved issues remain, the subject has evolved considerably in the past two decades with various authors offering their own unique viewpoint. In the present review, we summarize the debate over the "definition" of stress in a quantum mechanical setting and discuss some controversial issues such as the uniqueness of the stress. Finally, we provide our own perspective.

Electronic Structure Calculations at Macroscopic Scales

Vikram Gavini
Assistant Professor
Mechanical Engineering, University of Michigan

Electronic structure calculations (first-principle, quantum-mechanical calculations), especially those using density-functional theory have provided many insights into various materials properties in the recent decade. However, the computational complexity associated with electronic structure calculations has restricted these investigations to periodic geometries with cell-sizes consisting of few atoms (200 atoms). But, material properties are influenced by defects in small concentrations (parts per million). A complete description of such defects must include both the electronic structure of the core at the fine (sub-nanometer) scale and also elastic and electrostatic interactions at the coarse (micrometer and beyond) scale. This in turn requires electronic structure calculations at macroscopic scales, involving millions of atoms, well beyond the current capability.

This talk presents the development of a seamless multi-scale scheme, quasi-continuum orbital-free density-functional theory (QC-OFDFT) to perform electronic structure calculations at macroscopic scales [1]. This multi-scale scheme has enabled for the first time a calculation of the electronic structure of multi-million atom systems using orbital-free density-functional theory, thus, paving the way to an accurate electronic structure study of defects in materials. The key ideas in the development of QC-OFDFT are (i) a real-space variational formulation of orbital-free density-functional-theory [2], (ii) a nested finite-element discretization of the formulation, and (iii) a systematic means of adaptive coarse-graining retaining full resolution where necessary, and coarsening elsewhere with no patches, assumptions or structure. Rigorous proofs of convergence of the finite-element approximation using the variational notion of Gamma-convergence will be presented. The accuracy of QC-OFDFT scheme and the physical insights it offers into the behavior of defects in materials are highlighted by the study of vacancies in aluminum.

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Atomistic Simulations of Deformation Mechanisms in Nano-twinned Metals

Yashashree Kulkarni
Postdoctoral Researcher
Department of Structural Engineering, University of California, San Diego

Robert J. Asaro
Department of Structural Engineering, University of California, San Diego

Nanocrystalline metals and alloys have been shown to possess attractive combinations of properties including ultra-high strength, superior fatigue and wear resistance which are attributed to the transition in deformation mechanisms and mobility of grain boundaries as the grain size falls within the nanocrystalline domain (~100 nm). However, the ductility of these nanostructured metals is limited to only a few percent. On the other hand, nano-twinned metals, such as copper, are shown to exhibit very high ductility in addition to high strength. In order to understand this extraordinary behavior of nano-twinned materials, we performed finite temperature atomistic simulations of nanoindentation and shear tests on nano-twinned copper. In this talk, we will present some results of this study focusing on the mechanism of dislocation nucleation and propagation through twin boundaries and its effect on the strength of nano-twinned metals.

Peridynamic Models for Heat Conduction and Thermoelastic Fracture

Florin Bobaru
Department of Engineering Mechanics, University of Nebraska, Lincoln

Monchai Duangpanya
PhD Candidate
Department of Engineering Mechanics, University of Nebraska, Lincoln

Heat transfer at the atomistic scale is a nonlocal phenomenon. In earlier studies, the parabolic equations of transient heat-transfer have been replaced by nonlocal and hyperbolic equations that result in a finite speed of propagation of heat. When thermal processes take place over small spatial and temporal regions, these nonlocal formulations give more accurate results than the classical heat transfer models. There is, however, another important case where nonlocality of the heat transfer equations is important, namely in fracture and fragmentation of thermoelastic or thermoplastic solids. Recently it has been shown that peridynamics is capable of predicting the crack speed and path in challenging problems in dynamic crack propagation, such as crack branching in thin brittle plates. To extend the formulation to thermoelastic fracture, for example, we develop the transient heat conduction equations in peridynamics and couple it with the peridynamic formulation for microelastic materials. We show convergence results to the classical (local) solutions of steady-state and transient heat conduction and discuss future developments of the method for thermoelastic fracture.

A Framework for Continuum-Atomistic Simulations of Dislocations

Robert Gracie*
Mechanical Engineering, Northwestern University
rgracie@northwestern.edu

Ted Belytschko
Professor
Mechanical Engineering, Northwestern University

Multiscale continuum-atomistic models of crystal plasticity have to potential to overcome one of the salient drawbacks of dislocation dynamics simulations—the large number of rules and empirical laws needed to account for short range interactions. However, to date multiscale simulations continue to suffer from one significant limitation. As these simulations progress, more and more of the simulation domain is converted from continuum to atomistics in order to accommodate the evolution of dislocations. In this presentation we will describe a continuum-atomistic framework for modeling dislocations which allows one to retain atomic resolution in the near core region, without significantly increasing the number of degrees of freedom in the system.

The framework combines the Bridging Domain Method (BDM) of Xiao and Belytschko [1] with the eXtended Finite Element Method (XFEM) of Moës et al. [2]. The BDM is a hierarchical overlapping domain decomposition scheme where compatibility between the atomistic and continuum domains is enforced using Lagrange Multipliers. Material far from dislocations cores is modeled as a continuum using the XFEM, whereas Molecular Mechanics is used to resolve the near core behavior and dislocation reactions. The XFEM-BDM framework allows the coarse-graining of both regions where the atomistic displacements are homogeneous and where they are discontinuous by replacing large portions of the atomistic domain along the glide planes by the XFEM dislocation approximation developed by Gracie et al. [3,4]. The framework will be compared to several direct numerical simulations and its advantages and limitations will be discussed.

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On the Nonlocal Nature of Dislocation Nucleation during Nanoindentation

Ronald Miller
Department of Mechanical And Aerospace Engineering, Carleton University

David Rodney
Laboratoire SIMap/GPM2, INP Grenoble, Domaine Universitaire

Plasticity is governed by the motion, interaction and multiplication of dislocations during deformation. A fundamental mechanism of plastic flow is the nucleation of new dislocations, but a complete understanding of the mechanical conditions which lead to nucleation has remained elusive. A number of dislocation nucleation criteria have been proposed, but none appear to accurately describe the phenomenon. The goal of the current work is to develop a criterion that is accurate and at the same time practical for use in larger-scale models like Discrete Dislocation Dynamics.

The presentation will focus on the test problem of a spherical, frictionless indenter pressed into an initially defect-free single crystal, which is studied using molecular dynamics and statics with empirical interatomic potentials. The simulations provide a full understanding of the details of the nucleation mechanism and the mechanical conditions within a crystal just prior to nucleation.

Next, each of the existing nucleation criteria will be examined in turn, demonstrating that they neither correctly describe the phenomenon nor accurately predict the nucleation of a dislocation. Finally, a new criterion will be presented that is a successfully predictive model.

The new criterion is based on a stability analysis of sub-matrices from the dynamical matrix of the atomistic crystal. It accurately predicts the load level at which a defect nucleates and correctly determines both the location and the type of defect that forms. The presentation will conclude with a discussion of the remaining challenges to be confronted before the criterion can be practically applied in larger-scale models.

Nucleation and Kinetics of Phase Boundaries in Peridynamics

Kaushik Dayal
Assistant Professor
Civil and Environmental Engineering, Carnegie Mellon University

Kaushik Bhattacharya
Professor
Mechanics and Materials Science, California Institute of Technology

Understanding the nucleation and kinetic behavior of phase boundaries is critical for predicting hysteresis and dynamic behavior in active materials. This is challenging as the dynamics of defects including phase boundaries in the classical theory requires material information beyond the stress-strain relation, in the form of a nucleation criterion and a kinetic relation [1]. Further, computation is difficult as one needs to track these defects. Phase field type models get around this by involving strain gradient and viscosity, but these add to the computational complexity. We report on an alternative approach using the peridynamic theory [2,3]. This is a nonlocal formulation of continuum mechanics that uses only the displacement field, and not its spatial derivatives such as strain and strain gradients. Hence there are no requirements on the smoothness. This makes it attractive to model defects such as phase boundaries and cracks. We show that extra nucleation and kinetic information is not required in this theory. We find that phase boundaries may be viewed as traveling waves in this theory, and their propagation induces a kinetic relation. We derive a nucleation criterion by examining the dynamic stability of a nominally single phase displacement field. The results of this analysis show good agreement with the boundary-value calculations. This provides a new perspective on nucleation as a dynamic instability and phase boundaries as traveling waves in microscopic theories. We exploit the computational efficiency of this method to attack a two dimensional problem of a phase boundary impinging on a defect. Our numerical simulation reveals an unusual mechanism that allows the phase boundary to bypass the defect without requiring large distortions. As the acoustic waves leading the phase boundary interact with the stress field of the defect, they nucleate a new phase boundary that then propagates, as the original phase boundary comes to rest. Some results are reported in [4].

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Towards a Consistent Internal State Variable Theory of Inelasticity

Douglas Bammann
Department of Mechanical Engineering, Mississippi State University

A structure for an internal state viable description of inelastic deformation of crystals is developed. The deformation gradient is multiplicatively decomposed into an elastic deformation resulting from externally applied loads and the deformations associated with each density of defects to be included as internal state variables. The deformations associated with these defects or foreign atoms such as diffusing species, may further be decomposed into elastic and plastic parts depending upon the structure of the defect. In many cases, either the elastic or plastic part of a particular deformation gradient will be negligible, depending upon the situation. The appropriate strain-like variable associated with the defects is included in the free energy resulting in conjugate thermodynamic forces (internal stresses) that must be included in the dissipation inequality. In addition, these forces (stresses) are required to satisfy micro or meso scale linear and angular balance laws. All transport equations (e.g. heat conduction or diffusing species) are derived from a combination of the energy balance and these force balance laws. This is in contrast to classic state variable theories in which only temporal evolution equations were specified for the internal state variables. Constraint equations are required for the extra kinematic degrees of freedom that are introduced. These are based upon the physics of the associated defect density/state variable an example given by the flow rule or plastic velocity gradient based upon the Orowan equation relating plastic strain rate to mobile dislocation density and velocity.

Examples are given for the construction of such theories ranging from simple statistically stored dislocations, coupled transport theories for hydrogen and micropolar type theories for asymmetric defects.

Torsional Buckling of Carbon Nanotubes Using a Non-local Elastic Thin-Shell Model

Nimal Rajapakse*
Professor
Mechanical Engineering, University of British Columbia
Rajapakse@mech.ubc.ca

Farzad Khademolhosseini
Graduate Student
Mechanical Engineering, University of British Columbia

Alireza Nojeh
Assistant Professor
Electrical and Computer Engineering, University of British Columbia

For almost two decades, carbon nanotubes (CNTs) have attracted much attention from scientists and engineers. Their small size and theoretically perfect structure, give rise to outstanding mechanical, thermal and electrical properties. Ever since their discovery, a great deal of effort has been put into the characterization of CNT properties. Various approaches have been used to this end, ranging from computationally expensive ab-initio and semi-empirical methods to continuum models and experimental observations. Continuum models are computationally efficient for the investigation of large systems. However, at the nano-scale, quantum effects become significant, making the applicability of classical continuum mechanics questionable. Unlike classical continuum models, the non-local elasticity theory assumes that the stress at a reference point in a body depends not only on the strains at that point, but also on strains at all other points of the body [1]. At the nano-scale, non-local effects become significant [2], and non-local continuum mechanics provides a useful tool in the characterization of CNT properties. Non-local continuum models have been used to study CNT vibrations, buckling of CNTs under axial and radial loads, and propagation of waves in CNTs [3-5]. In this study, we develop a non-local thin-shell model to investigate the torsional buckling of CNTs. We perform molecular dynamics (MD) simulations to determine the value of the non-local parameter for our continuum model. Results from MD simulations and the non-local thin-shell model are compared.

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Post-buckling Behavior of Graphene Sheets

J. Patrick Wilber
Department of Theoretical and Applied Mathematics, The University of Akron

Graphene is a single-atom thick sheet of carbon atoms. In the last several years techniques have been developed for isolating individual graphene layers from bulk graphite. These layers exhibit fascinating mechanical and electronic transport properties. We study a basic mechanical problem for a graphene sheet over a rigid substrate. We model the sheet as an elastica subject to a body force that arises from the van der Waals interaction between the atoms on the sheet and the atoms on the substrate. We present numerical results that describe the post-buckling behavior of the sheet and explore how this behavior depends on the length of the sheet and the resistance to bending. The post-buckling behavior includes some interesting secondary bifurcations. Our results also indicate some of the limits of continuum modeling of nanoscale structures like graphene.

A Model for Magnetoelastic Plates in a Stationary Applied Field

David Steigmann
Department of Mechanical Engineering, University of California

Matthew Barham
Graduate Student
Department of Mechanical Engineering, University of California

Daniel A. White
Senior Scientist
EE-ETD Computational Electromagnetics Group, Lawrence Livermore National Laboratory

Robert E. Rudd
Senior Scientist
Lawrence Livermore National Laboratory

Michael McElfresh
Department of Physics, University of California

We descibe the development of a model for the bending and stretching of magneto-sensitive elastic plates in an applied magnetic field. This is based a through-thickness expansion of the field equations which is truncated at a level that accounts for the effects of combined bending and stretching. The model is applied to the study of the stability of the plate in the presence of an applied field of specified strength and distribution.

Investigation of the Growth Mechanism during Plasma-Assisted Deposition of a-C:H

Cristian Ciobanu
Assistant Professor
Division of Engineering, Colorado School of Mines

Bhavin Jariwala
Department of Chemical Engineering, Colorado School of Mines

Sumit Agarwal
Assistant Professor
Department of Chemical Engineering, Colorado School of Mines

Abstract: We have employed classical molecular-dynamics (MD) simulations to study the structure and properties of hydrogenated amorphous carbon (a-C:H) thin films. The structure and properties of these films are defined by the sp2-to-sp3 hybridization ratio and the H content. In particular, interaction of H generated in the plasma results in local and overall transformations due to reactions such as, insertion into C-C bonds, surface H abstraction, bulk diffusion, and hydrogen-induced etching. In this presentation, we will discuss the mechanism and energetics of these reactions and show how they affect the film structure.

To study the radical-surface interactions, we have developed a procedure for creating realistic a-C:H thin films starting with diamond(001) slabs. Due to the density difference between a-C:H (1.7-2.2 g/cm^3) and diamond (3.52 g/cm^3) a certain number of atoms were randomly removed from the diamond(001) slab. The resulting structure was amorphized at 1000 K, hydrogenated, relaxed and then thermalized at 700K to create the a-C:H films. We have also formulated a scheme to characterize the sp2-to-sp3 hybridization ratio of these films based on the coordination number and the dangling bonds for each carbon atom, and the values obtained agree well with the range of values reported in the literature for experimentally deposited a-C:H films. Furthermore, the sp2-to-sp3 hybridization ratio and the H content in these films can be varied by tuning their initial density. H-induced reactions were observed by impinging H atoms on the surface of these realistic a-C:H films at 700 K. The detailed energetics of the various reaction pathways along with the structure and energies of the corresponding equilibrium and transition-state configurations will be presented.

Understanding Stress at the Atomic Scale

Alan M. Rosenwinkel
PhD Candidate
Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

John L. Bassani
Richard H. and S. L. Gabel Professor of Mechanical Engineering
Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania

The ability to construct and manipulate nanoscale structures has renewed interest in understanding the concept of stress at the atomic scale. In particular, in the setting of molecular dynamics, one would like to compute stress given a description of interatomic potentials along with atomic coordinates and momenta as a function of time. Key concepts leading to the so-called Virial Stress were introduced by Clausius in 1870 in a study of the "effective force of heat" and have been adopted, more or less consistently, since then. Nevertheless, a rigorous derivation of atomic-level stress and a clear demonstration of its validity have been somewhat elusive. Of particular interest is the extent to which the atomistic expression can be localized in time and space while maintaining a meaningful connection to the continuum definition of stress.

Using the principle of virtual work we present a derivation of stress in a discrete, dynamical medium that yields an expression comprising three terms: the two well known terms of the Virial Stress and one that vanishes by the virial theorem. To understand the significance of each term and to establish the validity of this atomic-level stress, we have carried out a series of molecular dynamics simulations for heating of both harmonic and anharmonic crystals, with and without constraint. The calculated stresses are shown to agree both with physical intuition and continuum limits. Localization of the atomic stress is investigated, both from a theoretical perspective and by molecular dynamics simulation of both space- and time-varying stress fields.

Simulation of the Motion of Defects in Solids by Objective Molecular Dynamics

Richard James
Department of Aerospace Engineering and Mechanics, University of Minnesota

Kaushik Dayal
Department of Civil and Environmental Engineering, Carnegie Mellon University

We describe a method of doing exact molecular dynamics that relies on a (neglected) time-dependent invariant manifold of the equations of molecular dynamics. The method has links to some of the most important motions of continuum mechanics, like the viscometric flows of Newtonian or Non-Newtonian fluids and the large-scale bending and twisting of beams. It also seems well adapted to study the formation and motion of defects in solids. For example it is well adapted to study the failure of carbon nanotubes under conditions of constant strain rate. Results of such simulations will be presented. It also has other interesting links to the kinetic theory of gases and the fundamental laws of continuum mechanics, which we briefly describe.

An Inverse Method for Establishing Traction-Separation Relations for Void Growth

Huck Beng Chew*
Department of Engineering, Brown University
Huck_Beng_Chew@brown.edu

Kyung-Suk Kim
Department of Engineering, Brown University

Cohesive zone laws for predicting semi-brittle fracture, for which the rapid failure process with limited plastic deformation is localized along a narrow zone, have been well established. However, the exact relationship between traction-separation distributions and ductile fracture process where substantial plastic dissipation is involved in the background remains relatively unexplored. One method to identify the crack-tip cohesive zone relations from the elastic far-fields is the inverse-problem solution termed the "field projection method" [1]. In this symposium, the field projection method, together with equilibrium field regularization, is used to extract crack-tip cohesive zone laws from an elastic-plastic porous solid. To this end, we deploy a single row of void-containing cell elements directly ahead of a crack in an elastic-plastic medium subjected to a remote K-field loading [2]; the macroscopic behavior of each cell element is governed by the Gurson porous material relation, extended to incorporate vapor pressure effects [3, 4]. A thin elastic strip surrounding this fracture process zone is introduced, from which the cohesive zone variables can be accurately extracted using field projection. Results show that the cohesive zone law for void growth has a distinctively convex shape. The convexity of this traction-separation relationship also increases with the material's initial porosity. Constant vapor pressure induced by high moisture content in the micropores reduces both the cohesive traction and energy, and also the convexity of the traction-separation relationship. These effects of constant vapor pressure are exacerbated when the material's initial porosity is high. These observations are consistent with experimentally determined cohesive-zone laws in HIPS and PMMA [5].

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Multiscale Simulation of Nanomaterial Formation during Crystallization

Xiupeng Wei
Mechanical and Industrial Engineering, The University of Iowa

Jun Ni
Associate Professor
Radiology, The University of Iowa

Shaoping Xiao
Assistant Professor
Mechanical and Industrial Engineering, The University of Iowa

Nanomaterials formation involves complex physical and chemical processes occurring over a multiple time and length scales. In order to control and predict nanomaterials final desirable properties and special functions, it is necessary to simulate a whole process of materials formation. This paper presents a multiscale method to simulate nanomaterial formation during crystallization. The method is used to simulate multi-time scales and multi-length scales coupled by stage to stage transition. At the microscale, a molecular dynamics method is used for simulating the nucleation and growth of material crystal. The interfacial topology for microscopic structure is also obtained to predict the properties of material. The micromodel is coupled with a finite element method solution of the macroscale transport phenomena. This method is employed to investigate ice crystallization process and predict the properties of ice. Comparison of the simulation predictions with experimental and numerical results is also presented.

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Modeling and Simulation of Crack Propagation through an Atomistic Field Theory

Liming Xiong*
Mechanical and Aerospace Engineering, University of Florida
lmxiong@ufl.edu

Youping Chen
Assistant Professor
Mechanical and Aerospace Engineering, University of Florida

In this paper, formulation of an atomistic field theory and its finite element implementation are introduced. Dynamic crack propagation in single crystal and nanocrystalline materials are simulated by an atomistic field theory. For single crystal copper, models with initial notches and voids serving as a crack seed are constructed. Stress concentration and dislocation emissions from the crack tips are investigated. Nanostructures of the shear band are characterized. With an average grain size of 10~12 nm, nanocrystalline SiC thin film under uniaxial tension are modeled. Tensile strength and Young's modulus of nanocrystalline SiC with different dopants are measured. Intergranular crack propagations are observed. It is found that the mechanical properties of nanocrystalline SiC are dependent on grain size, thickness and compositions of grain boundaries. With the majority of degree-of-freedoms are eliminated by utilizing the concept of shape function, the atomistic field theory is shown to be able to model and simulate physical phenomenon across multiple length scales.

Evolution of Mechanical and Electronic Properties of Mechanically Deforming Nanotubes Containing Point Defects

Raguraman Kannan
Department of Civil and Materials Engineering, University of Illinois at Chicago

Arif Masud
Department of Civil and Environmental Engineering, University of Illinois

A multiscale computational framework is presented that provides a coupled self-consistent system of equations involving molecular mechanics at the small scale and quasi-continuum mechanics at the large scale. The proposed method permits the analysis of problems that require simultaneous resolution of quasi-continuum and atomistic length scales and the associated displacement fields in a unified manner. Interatomic interactions are incorporated into the method through a set of analytical equations that contain nanoscale based material moduli defined via internal variables that are functions of parameters defining the local atomic configurations. Point defects in nanomaterials perturb the atomic structure locally and generate localized force fields. Formation energy of vacancy is employed in conjunction with the Morse potentials to extract these nanoscale force fields that are then employed in the proposed multiscale method to solve for the localized displacement fields around the point defects.

From the equilibrated localized displacement fields obtained through quasi-continuum model the new bond-lengths and bond-angles are evaluated. For axially deforming nanotubes we assume the deformation to be homogenous over the defect-free nanotube and evaluate the electronic properties via the density functional theory. For the case of vacancies that are otherwise assumed to be frozen and repeated periodically over domain of defective nanotubes, the new bond-lengths and bond-angles are obtained. The notion of supercell that encompasses neighboring atoms within the radius of six to seven bond lengths is employed to evaluate electronic properties of defective nanotubes. Representative numerical examples are shown to validate the model and demonstrate its range of applicability.

SYMPOSIUM

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Plasticity and Damage Size Effects at the Micron and Nano Length Scales

ORGANIZERS:

Rashid K. Abu Al-Rub, *Department of Civil Engineering, Texas A&M University*

George Z. Voyiadjis, *Department of Civil and Environmental Engineering, The State University of New York at Buffalo*

Cemal Basaran, *Department of Civil and Environmental Engineering, The State University of New York at Buffalo*

Elasticity and Strength Size Effects in Zinc Oxide Nanowires

Horacio Espinosa
Professor
Mechanical Engineering, Northwestern University

Bei Peng
Graduate Student
Mechanical Engineering, Northwestern University

Ravi Agrawal
Graduate Student
Mechanical Engineering, Northwestern University

Eleftherios Gdoutos
Undergraduate Student
Mechanical Engineering, Northwestern University

Zinc Oxide (ZnO) nanostructures, due to their semiconductive, piezoelectric and biocompatible properties have applications in high performance devices. At nanoscale, the size dependence of these material properties poses a big question on the designing aspect of such devices. Understanding the origin of these size effects in ZnO nanostructures is crucial in employing them as building blocks for devices with reliable and reproducible operations. Performing experiments in this size regime to develop such understanding is not trivial. For example, various studies on elastic properties of Zinc Oxide nanowires have resulted in a range of values for Young's modulus (varying from 20 to 250 GPa). Motivated by the inconsistency in reported values [1-3], we performed an experimental and computational study to unambiguously characterize the Young's modulus of [0001] oriented Zinc Oxide nanowires with diameters ranging from 5 nm to ~400 nm. Experimentally, a MEMS based nanoscale material testing system is used which allows for simple uniaxial tensile testing [4]. Uniaxial tensile loading eliminates many sources of experimental error and simplifies the analysis of the results. The Young's modulus is found to decrease from 160 GPa to 140 GPa as the wire diameter increases from 20nm to 80nm. For larger wires, a Young's modulus of ~140 GPa, consistent with the value for bulk ZnO, is observed. Molecular dynamics simulations are carried out to model the experiments and understand the fundamental origin of this size dependence. ZnO nanowires of diameters ranging from 5 nm to 20 nm were modeled. The computational results demonstrate similar size dependence, confirming the experimental findings, and reveal that the observed size effect is an outcome of surface reconstruction together with long-range ionic interactions. For Zinc Oxide nanowires, surfaces are found to behave differently than metallic nanowires [5]—surfaces are initially in compression leading to overall expansion of the nanowire during relaxation. Also, the effect of surface reconstruction is prominent in ~15% of the wire radius (as opposed to 2-3 atomic layers for metals), which is attributed to long-range coulombic interactions present in ionic compounds.

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Nonlinear Elasticity, Slip, and Mechanical Twinning in Ceramic Crystals

John Clayton
Staff Scientist
Impact Physics, U.S. Army Research Laboratory

A theory is developed for modeling elasticity, plasticity, and twinning in highly anisotropic single crystals subjected to large deformations, deformation rates, and confining pressures. The present work extends a geometrically nonlinear kinematic and thermodynamic framework [1] to account simultaneously for reversible nonlinear elastic and anisotropic thermal deformations, lattice-preserving irreversible deformation associated with dislocation glide, and lattice-altering irreversible deformation associated with mechanical twinning. Strain rates resulting from dislocation glide and deformation twinning are dissipative. Mechanisms of energy storage and hardening associated with dislocation networks, stacking faults, and twin boundaries are considered, leading to size effects.

With regards to ceramic crystals, concepts from atomic scale, discrete lattice statics and continuum crystal plasticity are simultaneously invoked. Driving forces for slip and twinning emerge from consideration of the geometry and energetics of full or partial dislocations associated with each relevant inelastic deformation mode. In particular, the anisotropic Peierls-Nabarro potential [2] for dislocation resistance is known to be of importance for the considered class of crystals featuring covalent and ionic bonding, at low to moderate temperatures and low defect densities [3]. Shearing rates on distinct glide and twinning systems are modeled explicitly, as is the improper lattice rotation across twin boundaries. The model realistically describes the thermomechanical behavior of alumina—the rhombohedral ceramic [4] whose crystals are often referred to as corundum or sapphire—over a range of initial lattice orientations, loading rates, temperatures, and confining pressures. Particular attention is directed towards high rate, high pressure loading scenarios, i.e., shock physics applications [5].

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A Methodology for Studying Hydrogen Embrittlement in a Steel Pipeline

Mohsen Dadfarnia
Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Petros Sofronis
Department of Mechanical Science and Engineering, University of Illinois

Brian P. Somerday
Researcher
Sandia National Laboratories

Ian M. Robertson
Department of Material Science and Engineering, University of Illinois

For the planned hydrogen economy, transmission of hydrogen through steel pipelines at high pressures from central production facilities to refueling stations is the more efficient and economical mode of transport. Among the problems which confront this mode of delivery is the deleterious effect of hydrogen on structural material properties. In an effort to understand the mechanics of hydrogen embrittlement in steel pipelines, we propose a hydrogen transport methodology for the calculation of hydrogen accumulation ahead of a crack tip. In our approach we consider stress-driven transient diffusion of hydrogen and trapping at microstructural defects whose density evolves dynamically with deformation. We investigate the interaction of the transient hydrogen transport with material elastoplasticity in the neighborhood of an axial crack on the inner surface of a pipeline and quantify the hydrogen, stress, and deformation fields in this region. We also explore the development of the same fields through a modified boundary layer (MBL) formulation pertaining to laboratory specimens in which the domain is loaded remotely by the stress intensity factor and the T-stress the real-life pipeline experiences and under the same hydrogen boundary conditions. For all practical purposes, we find that the steady state hydrogen concentration fields in the crack tip region in both real-life pipeline and MBL formulation are nearly the same and independent of the prescribed boundary conditions so long as small scale yielding conditions are prevalent. We conclude that one can study the hydrogen effect on fracture at an axial pipeline crack with the use of laboratory fracture mechanics specimens tested in hydrogen gas.

Prediction of Micro and Nano Indentation Size Effects from Pyramidal and Spherical Indentation

Rashid K. Abu Al-Rub
Assistant Professor
Department of Civil Engineering, Texas A&M University

It is well-known by now that the hardness (or flow stress or yield strength) of the material at the micron, submicron, and nano length scales is dependent on the indent size. The objective of this talk is to present a micromechanical-based model that can be used to predict simultaneously the indentation size effect (ISE) from both micro- and nano-indentations by conical or pyramidal (Berkovich and Vickers) and spherical indenters. This model is based on the evolution of geometrically necessary dislocations (GNDs) beneath the indenter which is nonlinearly coupled to the evolution of statistically stored dislocations (SSDs) through the Taylor's hardening law. It is shown through comparisons with micro and nano-indentation experimental data that the proposed model gives much better predictions of hardness at small indentation depths as compared to the well-known Nix-Gao [1] and Swadener et al. [2] models.

It is also concluded that when using the Taylor's hardening law a simple sum of flow stresses from SSDs and GNDs is more adequate than the simple sum of SSD and GND densities. Besides giving very well predictions of the micro- and nano-indentation size effects, it is shown that this theory gives excellent predictions of the size effect in micro-torsion of thin wires and micro-bending of thin films. Moreover, it is shown that the length scale responsible for the ISE is proportional to the spacing between dislocations and, therefore, it can be taken as a fixed value. It is shown that this length scale is related to the microstructural features (e.g. grain size) and it depends on the course of plastic deformation. Also, it is shown that materials with smaller length scales are harder but exhibit lower size effect.

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Bauschinger Effect in Unpassivated Freestanding Metal Thin Films

Jagannathan Rajagopalan
Mechanical Science and Engineering, University of Illinois

Jong H. Han
Mechanical Science and Engineering, University of Illinois

Taher A. Saif
Professor
Mechanical Science and Engineering, University of Illinois

The mechanical response of unpassivated freestanding metal thin films, subjected to uniaxial tension, was measured during several loading-unloading cycles. The results show that the stress-strain response of these films deviates substantially from linear elastic behavior during unloading, even at large overall tensile stresses. For example, in aluminum films (thickness 200-400 nm, grain size ~ 200 nm) the deviation from elastic behavior, indicative of reverse plasticity, starts at stresses as high as 150 MPa during unloading. As a result of this early Bauschinger effect, the plastic strain in these films after unloading is often less than 50% of the expected value. Similar trends are seen in gold films, but the effect is less pronounced. The current understanding is that only passivated metal films, where reverse deformation is assisted by back stresses from dislocation pile-ups at the film/passivation layer interface, should exhibit Bauschinger effect. The observation of early Bauschinger effect in unpassivated films thus suggests an alternate mechanism, which appears to result from the coupling of small grain size and heterogeneity of the microstructure. During loading, relatively larger grains deform plastically and relax their stresses whereas the stresses in smaller elastically deforming grains keep increasing. During unloading, the smaller grains that are under higher stresses induce reverse plastic deformation in the larger grains to satisfy strain compatibility, leading to early Bauschinger effect. This proposed mechanism is supported by observations from in situ straining experiments in TEM.

A Micromechanical Model for the Nonlinear Viscoelastic-Viscoplastic Behaviors of Hybrid Composites

Anastasia Muliana
Professor
Mechanical Engineering, Texas A&M University
amuliana@tamu.edu

Jeongsik Kim
Graduate Student
Mechanical Engineering, Texas A&M University

This study formulates a micromechanical model for predicting effective viscoelastic-viscoplastic responses of hybrid composite. The studied hybrid composites consist of two reinforcement systems, i.e., fiber reinforced matrix and homogenized particle reinforced polymers. A combined Schapery's viscoelastic integral model and Valanis's endochronic viscoplastic model based on the concept of internal variables is used for the polymer constituents. The fiber and particle constituents are assumed linear elastic. Thus, the overall composite systems can exhibit nonlinear viscoelastic-viscoplastic responses. Detailed 3D finite element (FE) models of the composite's microstructures are generated for composites having long fiber and randomly distributed short fiber embedded in the cubic matrix. The matrix medium is made of solid spherical particle fillers dispersed in polymer resin. A unit-cell model with four particle and polymer sub-cells is generated for the matrix. This unit-cell model is integrated at the material (Gaussian) points of the detailed 3D FE microstructures of fiber reinforced composites. A time-integration algorithm is formulated for solving the nonlinear time-dependent constitutive model for the isotropic matrix sub-cells and nested to the unit-cell model of the particle fillers. This time-integration algorithm is suitable for the multi-scale model of hybrid composites. Experimental data available in the literature and detailed FE models of composite microstructures are used to verify the capability of the above micro-mechanical model in predicting nonlinear effective viscoelastic-viscoplastic behaviors of the hybrid composites.

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Fatigue Damage Evolution and Reliability Assessment of Cu and Solder Interconnects in 3D Integrated Circuits

Leila Ladani
Mechanical and Aerospace Engineering, Utah State University

Need for higher functional capabilities of semiconductor devices drives the manufacturers to 3 dimensional Integrated Circuits (3D ICs). The new technologies such as die bonding and multilayer buried structures are used to connect the ICs vertically [1]. Higher density of these packages is a driving force to have finer copper and solder interconnects with the size of 10 to 40 microns. Due to size effect [2] and processing difference, the mechanical properties of these interconnects are different from bulk materials and are not readily available in literature. Therefore, making the reliability assessment and damage evaluation more complicated tasks. Because of increased heat flux due to decreased dissipation area, these packages experience high performance temperature and thermo-mechanical cyclic loading which causes plastic deformation and damage in both copper interconnects and small solder joints used in Direct Chip Attach (DCA) connections. Fatigue and creep damage in these interconnects is a critical issue that has prevented many manufacturers of 3D ICs from releasing their ICs for high volume production.

This manuscript is focused on developing a technique to include the size effect in fatigue and damage evolution modeling of these small copper and solder interconnects. Energy Partitioning Damage Evolution (EPDE) model [3] developed by the author is used to assess the damage caused by thermo-mechanical cyclic loading for copper interconnects and solder joints. Two different technologies, DCA and thermo-compression bonding, are compared. The residual stress caused by the electroplating and reflow processes, in the case of solder joint, and electroplating and thermo-compression bonding processes, in the case of Cu-Sn interconnects, are taken into account by simulating these processes and mapping the stress distribution into the package. Durability of the copper interconnects (Through Silicon Vias (TSV) and copper pads), solder joints and Cu-Sn connections are evaluated using Finite Element Analysis. A parametric study is conducted to evaluate the size effect on the reliability of the interconnects and results are presented.

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Fractal Pattern Formation at Elastic-Plastic Transition in Heterogeneous Materials

Martin Ostoja-Starzewski
Professor
Mechanical Science & Engineering, University of Illinois

Jun Li
Mechanical Science & Engineering, University of Illinois

It is well known that many ductile materials display fractal characteristics over a finite range of scales. Indeed, the "finite range" aspect has been generating some heated arguments in the science community—see e.g. the discussion by Mandelbrot, Pfeiffer and Biham [1] ending thus: "an intriguing and fundamental question that remains open is, Why are these limited-range fractals so common?" Here we address this question through two inelastic material models set in 2D: (1) a linear-elastic-perfectly-plastic material made of locally isotropic grains with random perturbations in moduli and/or yield points; and (2) a polycrystal made of anisotropic crystalline grains with random orientations. In each case, the spatial assignment of randomness is non-fractal but simply a field of i.i.d. random variables on a square lattice; the flow rule of each grain follows associated plasticity. Square-shaped domains (comprising several hundred grains on a side) are subjected to simple shear loading, increasing through either one of three macroscopically uniform boundary conditions—kinematic, mixed-orthogonal, traction—admitted by the Hill-Mandel condition. For any particular domain of model 1 or 2, we follow the evolution of a set of grains that have become plastic and find that this set is monotonically plane-filling with increasing macroscopic load. The sets fractal dimension tends towards 2, with the response under kinematic loading being stiffer than that under mixed-orthogonal loading, which in turn is stiffer than the traction controlled one. No matter what the degree of randomness in model 1, all the constitutive responses are always bounded from above by that of a homogeneous material. The present results amplify our earlier finding in a somewhat different context [2] that elastic-plastic transitions in disordered media display fractal patterns.

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Strain Gradient Plasticity with Interface Energy Effects Using Consistent Thermodynamics

George Voyiadjis
Department of Civil and Environmental Engineering, Louisiana State University

Babur Deliktas
Department of Civil Engineering, Mustafa Kemal University

For small scaled materials(micro and nano) interface energy plays an important role on the plastic behavior at the small scales. This effect should be considered within the framework of strain gradient plasticity due its mechanisms based on dislocations movements. In this paper small strain and gradient plasticity is developed by introducing state variables associated with interface. It is incorporated along with the Clausius-Duhem inequality and an appropriate free energy definition in a general thermodynamic framework for deriving a three-dimensional kinematical model for plastic deformations of metals. The evolution equations are expressed in terms of the material time derivatives of the elastic strain, and the accumulated plastic strain.

The equilibrium, or so-called microforce balance, between the internal Cauchy stress and the microstresses that are conjugates to the higher-order gradients turns out to be effective stress from there the yield criterion can be simply retrieved by introducing appropriate form of the flow stress. With the assumption of similar situation of the plastic deformation in the bulk materials, thermodynamically consistent plasticity model for bulk behavior are translated into analogous interface models. Nonstandard boundary condition is discussed within variational principles. Complate set of field equations are derived for the boundary value problem and finite element formulation is established. The prediction of the theory with the comparison of the previous theories is presented here as parametric studies.

Role of Size Effects on Plastic Deformation of Freestanding Cu Films

Ashraf Bastawros
Department of Aerospace Engineering, Iowa State University

Shakti S. Chauhan
Graduate Student
Department of Aerospace Engineering, Iowa State University

In this work aims to elucidate the effects of microstructural constraint as well as geometric dimensional constraint on the strength of free-standing Cu films under uniaxial tension. The films are deposited with a controlled microstructure to control the film thickness to grain size ratio. The results show that thickness effects in free-standing films are primarily an outcome of the competing contributions from two distinct dislocation mechanisms i.e. intragranular, Frank-Read (FR) type dislocations and Grain Boundary (GB) dislocations. At large grain sizes, typically ~O(10μm) in bulk materials and foil/plate type specimen, FR dislocations dominate the overall response. Reducing the film thickness leads to a reduction of the effective microstructural constraint. Consequently, prominent thickness dependent weakening is observed. On the other hand, for small grain sizes, ~O(1μm), GB dislocations play an increasingly prominent role. In such cases, reducing grain boundary area per unit specimen volume, with reducing thickness, results in a reduction of the available GB dislocation source density. As a result, plasticity commences under source-limited conditions leading to thickness dependent, source starvation strengthening.

Interface and Surface Effects in the Mechanical Behavior of Crystalline Materials

Marisol Koslowski
Professor
Mechanical Engineering, Purdue University

Abigail Hunter
Mechanical Engineering, Purdue University

Technological applications of materials and devices with nanoscale and microscale features commonly involve metals and alloys in their polycrystalline form. Plastic deformation in crystalline materials is carried by the nucleation and propagation of dislocations and the intricate structures they form. At micron and submicron scales the interaction of dislocations with interfaces such as grain boundaries and free surfaces play a prominent role in the mechanical behavior due to the confinement in the motion of dislocations.

We will present a theory that describes the interaction of dislocations with grain boundaries and interfaces through a set of continuum field equations. The resulting theory and simulations model explicitly the dislocation lines and are able to reproduce size effects in plastic deformation. We compare our simulations with gradient theories of plasticity and derive the dependency of the length scale parameters introduced in those models on the characteristic sample size and dislocation structure.

Strain Localization in Anisotropic Plastic Materials Undergoing Microstructural Evolution

Haizhen Pan*
Mechanical Engineering and Applied Mechanics, University of Pennsylvania
hpan@seas.upenn.edu

J.L. Bassani
Professor
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

In this paper, microstructural evolution is represented in terms of rotations of the orthotropic axes that define plastic anisotropy, and various effects on bifurcation phenomena are analyzed. Phenomenological constitutive relations that describe elastic-plastic response are proposed, including an equation for plastic spin that is constructed using Spencer's (1971) theory of invariants coupled with representations for tensor-valued functions due to Wang (1969) and Smith (1970). History-dependent rotations of the orthotropic axes are shown to have significant effects on overall material response as well as on strain localization. Sheet necking and shear banding are considered in this paper. The effects of microstructural evolution can increase or delay the tendency for localization from uniform states of deformation, depending upon parameters in the equation for plastic spin that determine the direction and degree of rotations as well as the initial degree of anisotropy and the orientation of orthotropic axes relative to the loading direction.

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On the Higher-Order Nonlocal Gradient Plasticity Theory and its Nonclassical Microscopic Boundary Conditions for Size Effects

Rashid K. Abu Al-Rub
Assistant Professor
Zachry Department of Civil Engineering, Texas A&M University

Recently, there have been many nonlocal gradient plasticity and damage theories proposed in the literature with very little emphasis placed on the physical nature of the resulting higher-order boundary conditions and also the physical nature of the incorporated material length scales. In fact, the full utility of the nonlocal gradient-dependent theory hinges on one's ability to determine the magnitude of the material length scale that scales with the strain gradient effect. Moreover, several researchers have argued the failure of the nonlocal gradient theory in explaining the size effect in small scale structures (e.g. thin films, micro pillars) when subjected to macroscopic uniform stressing or straining due to the absence of strain gradients. This misuse of the gradient theory in explaining this type of size effect is due to the lack of physical interpretation of the non-classical higher-order boundary conditions that result from the mathematical consistency when formulating a higher-order gradient theory.

A physically motivated and thermodynamically consistent formulation of small strain higher-order gradient plasticity theory is presented. Based on dislocation mechanics interpretations, gradients of variables associated with kinematic and isotropic hardenings are introduced. This framework is a two nonlocal parameter framework of gradient type that takes into consideration large variations in both the plastic strain tensor itself and in the equivalent (effective) plastic strain. It is demonstrated that the nonlocal yield condition, flow rule, and non-zero microscopic boundary conditions can be derived directly from the principle of virtual power. It is also shown that the local Clausius-Duhem inequality does not hold for gradient-dependent material and, therefore, a nonlocal form should be adopted. The nonlocal Clausius-Duhem inequality has an additional term that results from microstructural long-range energy interchanges between the material points within the body.

A detailed discussion on the physics and the application of proper microscopic boundary conditions, either on free surfaces, clamped surfaces, or intermediate constrained surfaces, is presented. The physical nature of the material length scale and how it relates to the material microstructural feature is also shown. It is shown that there is a close connection between interface/surface energy of an interface or free surface and the microscopic boundary conditions in terms of microtraction stresses. Finally, applications of the proposed theory for size effects in micro and nano metallic systems under various loading conditions are presented. Different expressions for the interfacial energy are also investigated.

An Analysis of the Size Effect in Void Growth in Single Crystals Using Discrete Dislocation Dynamics

Javier Segurado
IMDEA-Materials and Department of Material Science, Polytechnic University of Madrid

Ignacio Romero
Department of Structural Mechanics, Polytechnic University of Madrid

Javier Llorca
IMDEA-Materials and Department of Material Science, Polytechnic University of Madrid

Ductile failure of metals is normally controlled by the nucleation, growth and coalescence of voids, whose size is of the order of microns. Void growth is caused by the plastic flow around the void and there is compelling experimental evidence that size effects in the resistance to plastic flow appear in metals when the dimensions of the specimen or of the zone subjected to plastic deformation are in the range of m [1]. Classical models of void growth have neglected this size effects [2] and this contribution has been addressed recently using strain gradient plasticity models, which introduce a length scale in the analysis.

In this paper, void growth in single crystals is analyzed within the framework of 2D discrete dislocations dynamics developed by Needleman and Van der Giessen [3], which has been extended to account for the effect of dislocations leaving the crystal through a free surface in the case of non-convex domains, in which the intersection of the slip plane with the domain is not a continuous segment. The new method incorporates the displacement jumps across the slip segments of the dislocations that have exited the crystal within the finite element analysis carried out to compute the image stresses on the dislocations induced by the finite boundaries. This is done in a simple computationally efficient way by embedding the discontinuities in the finite element solution [4]

The simulations analyze the growth of a cylindrical void in a square single crystal of a FCC material. Voids with diameters in the range 0.2 to 2 mm are studied and the void growth rate as well as the resistance to plastic flow of the voided crystal are obtained as a function of the crystal characteristics (number and orientation of slip planes, density of sources and obstacles) as well as of the loading path (uniaxial traction, uniaxial deformation and biaxial deformation). Results are compared with the predictions of classical and strain gradient plasticity models to ascertain the influence of void size in the mechanisms of void growth.

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Multiscale Modeling of Covalent Materials through an Atomistic Field Theory

Liming Xiong*
Department of Mechanical and Aerospace Engineering, University of Florida
lmxiong2@ufl.edu

Youping Chen
Department of Mechanical and Aerospace Engineering, University of Florida

This paper presents an atomistic field theory (AFT) and its application in simulations of single crystal and nanocrystalline covalent materials. Formulation of AFT and its finite element implementations are introduced. Coarse-grained simulations are then performed to characterize the mechanical properties of single crystal silicon. Under uniaxial tension, elastic constant and tensile strength are measured. Under uniaxial compression, crystal structure of silicon becomes unstable when the stress approaches to a critical value. Under three-point bending, with the onset of the local amorphization in the silicon specimen, periodic drop in the force-displacement curve is observed. Although the majority of the degree of freedoms has been reduced in the simulation, all of the results and phenomena are shown to be comparable with that obtained through fully atomistic simulation. On the other hand, in order to model the atomic-scale phenomena, the size of finite element mesh is reduced to the atomic scale, single crystal diamond, silicon carbide and nanoclrystalline silicon carbide with dopants are modeled and simulated. Deformation and failure mechanisms at atomic scale are discovered. Results show that AFT is promising to concurrently simulate multiscale materials behavior of single crystal or polycrystalline materials from the atomic to the macroscopic within one theoretical framework.

Rate Effects in the Response of MEMS and Thin Films

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ORGANIZERS:

John Lambros, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Ioannis Chasiotis, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Adhesion at Epoxy Interfaces from Molecular Dynamics Simulation

Sarah-Jane Frankland
National Institute of Aerospace

T.C. Clancy
National Institute of Aerospace

T.S. Gates
NASA Langley Research Center

As polymer composites replace metallic parts in aircraft, the effectiveness of the current adhesives is being evaluated as to how they withstand the different thermo-mechanical and environmental changes of an aircraft's life cycle. A typical adhesive bond joins an epoxy-based adhesive to a carbon fiber composite adherend which is also an epoxy-based resin system. At this bond, solvent influences such as moisture ingression can additionally affect the adhesion. Modeling of the interfacial effects of the different components of the adhesive and adherend systems and how they are affected by moisture requires consideration of the chemical nature of the substituents. Molecular dynamics (MD) simulation is capable of including the different chemical functionalities at the interface. MD can also be used to determine the work of adhesion at the interface and assess the role of solvent in small quantities at the interface. These simulations enable the identification of key molecular-structure property relationships that affect the compatibility of the adhesive with the adherend.

In the present work, the work of adhesion is calculated for interfaces found in an epoxy-based adhesive/adherend system. Molecular structures of the various components found within the adhesive/adherend system are generated with MD. MD simulations of the components in bulk and the interfaces between them are then carried out to obtain the work of adhesion. The work of adhesion is calculated with and without water present at the interfaces. The objective of the present work is to present the simulation methodology, and the results for the work of adhesion, and to qualitatively show the effects of water at the interface.

Determination of the Time-Dependent Response of Ultrathin Polymer Films

Gregory McKenna
Department of Chemical Engineering, Texas Tech University

Paul O'Connell
Department of Chemical Engineering, Texas Tech University

Shanhong Xu
Graduate Student
Department of Chemical Engineering, Texas Tech University

There is considerable interest in the behavior of ultrathin polymer films both because of their use as model systems in the investigation of the impact of size or confinement on the dynamics near to the glass temperature and because these materials are becoming increasingly important in templated nanostructures. Here we present results from our ongoing investigations of the mechanical response of ultrathin polymer films using a novel bubble inflation method developed in our labs. In the work we have shown the capability to measure the biaxial creep compliance of polymer films as thin as 11 nm and at temperatures encompassing the glass temperature. Two major findings have been reported [1-3]: Polymer films show non-universal dynamics as a function of film thickness. Hence, poly(vinyl acetate)(PVAc) shows no decrease in the glass temperature Tg for films as thin as 22 nm, while polystyrene (PS) exhibits up to 50 K reduction in Tg when the film thickness reaches 11 nm. Perhaps more importantly, both the PS and the PVAc lose long-time dynamic modes with the consequence that the "rubbery plateau" modulus stiffens dramatically. This rubbery modulus scales approximately as the inverse square of the film thickness and can be near to 1,000 times greater than the modulus in the macroscopic material. New investigations show that this effect in PVAc and PS cannot be due to surface tension. On the other hand, the material poly(butyl methacrylate)(PBMA), which is significantly less stiff than either the PS or the PVAc, behaves much as would a "soap film" in that its behavior is dominated by the surface tension. Finally, we describe preliminary results from bubble rupture experiments (creep rupture) for thin PVAc films.

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Mechanical Properties of PZT Films and Their Composites for RF-MEMS

Sivakumar Yagnamurthy
Department of Aerospace Engineering, University of Illinois

Ioannis Chasiotis
Department of Aerospace Engineering, University of Illinois

John Lambros
Department of Aerospace Engineering, University of Illinois

Ronald Polcavich
U.S. Army Research Laboratory

Lead Zirconate Titanate (PZT) films are an excellent material for low-power RF-MEMS because of their large actuation forces. However, the mechanical behavior of PZT thin films is not documented. In this paper, the mechanical response of PZT in thin film form has been investigated by microscale uniaxial tension experiments of PZT stacks. A novel method for local strain measurements that allowed 7 orders of magnitude variation in strain rate has been applied to measure the material and composite film stress-strain curves. Due to the difficulty in fabricating individual freestanding PZT films, thin film stacks were fabricated consisting of combinations of Oxide (Ox), Titanium (Ti), Platinum (Pt) and PZT. The specimens were stacks of Ox-TiPt-PZT-Pt, Ox-TiPt-PZT, Ox-TiPt and individual Ox and Pt thin films, with gauge length of 1000 microns and width of 50-100 microns. Full-field strain measurements were conducted with the aid of a fine speckle pattern (1 micron average particle size) generated on the samples and analyzed by digital image correlation (DIC). The composite mechanical properties of the PZT stacks were computed from the stress vs. strain plots, while the mechanical properties of the individual PZT films were computed from those of the PZT stack and individual layer properties of Ox and TiPt thin films by using laminate theory.

Thermo-elastic Damping in Prestressed Resonators

Aman Haque
Assistant Professor
Mechanical & Nuclear Engineering, Penn State University

Sandeep Kumar
Graduate Student
Mechanical & Nuclear Engineering, Penn State University

Deformation results in change in heat content of the body, which gives rise to coupling of elastic fields and thermal fields. In case of vibrating bodies this coupling results in temperature gradient in the body due to strain field. Temperature gradient results in energy losses due heat conduction, which further results in thermo-elastic damping. At micro/nano levels thermo-elastic damping is one of the important energy dissipation mechanism. Thermo-elastic damping results in lowering of Q-factor of MEMS/NEMS resonator devices.

While the literature contains both exact and numerical schemes to quantify it, no technique is available yet to reduce thermo-elastic damping. We address this issue by introducing a secondary elastic field to derive an exact expression that predicts linear reduction in thermo-elastic damping with respect to frequency. The concept is implemented for a flexural resonator undergoing a static axial stress and an exact expression for thermo-elastic damping is developed. Contrary to the current understanding, the new model suggests simultaneous increase in quality factor and resonant frequency under the applied axial stress. It also quantifies the quality factor corresponding to thermo-elastic damping in terms of the vibrating beam geometry and therefore will be useful in design of micro/nano resonators for reduced thermo-elastic damping and quantitative prediction of the increase in quality factor as an axial stress is applied.

Dynamic Fracture of Silicon: Quantization of Crack Speeds and Fracture Instabilities

Markus J. Buehler
Esther and Harold E. Edgerton Assistant Professor
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Dipanjan Sen
Graduate Student
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Large-scale molecular dynamics (MD) has evolved into a valuable tool to understand the mechanics of materials from a fundamental, atomistic viewpoint. Here we review applications of large-scale MD using a new first principles ReaxFF reactive force field approach to describe fracture and deformation of chemically complex materials. We report hybrid multi-scale studies of crack propagation in a silicon single crystal in which the ReaxFF reactive force field is used to treat a region of several thousand atoms near a moving crack tip with quantum mechanical accuracy, while several hundred thousand atoms in the surrounding area are described with a simpler, nonreactive force field (M.J. Buehler et al., Phys. Rev. Lett., 2006, 2007). We have implemented this hybrid multi-scale model in the Computational Material Design Facility (CMDF), a Python based simulation environment capable of integrating simulation paradigms ranging from quantum mechanics to continuum theory. The ReaxFF reactive force field is completely derived from quantum mechanical calculations of simple silicon systems, without using any empirical parameters. We show that our hybrid model is capable of reproducing key experimental results including fracture instabilities and dependence of crack dynamics on crystal orientation. Further, we find that the steady state speed of a crack in silicon does not increase continuously with applied load, but instead jumps to a finite value immediately after the critical load is reached, followed by a regime of slow increase. This observation contradicts existing fracture theories that predict a continuous increase of crack speed with increasing load. Here we show that this threshold crack speed may be due to a localized phase transformation of the silicon lattice from 6-membered rings to a 5-7 double ring at the tip of the crack. Our studies illustrate the significance of the properties of an ensemble of chemical bonds under large deformation, an aspect neglected in most existing fracture theories.

Pull-In and Snap-Through Instabilities in Transient Deformations of Microelectromechanical Systems

Kaushik Das
Department of Engineering Science and Mechanics, Virginia Tech

Romesh C. Batra
Professor
Department of Engineering Science and Mechanics, Virginia Tech

We analyze transient finite electrodynamic deformations of a prefect electrically conducting clamped-clamped beam, a clamped-clamped parabolic and a clamped-clamped sinusoidal arch suspended over a rigid semi-infinite prefect conductor. The pull-in instability in a beam, and the pull-in and the snap-through instabilities in arches due to time-dependent potential difference between the two electrodes have been determined. The potential difference is applied either suddenly or is increased linearly in time to the steady value. Due to the time scale of the transient electric forces being very small as compared to that of the mechanical forces, inertia effects only in the mechanical deformations have been considered. Effects of both material and geometric nonlinearities have been incorporated in the problem formulation and solution. The coupled nonlinear partial differential equations for the mechanical deformations are solved numerically by the finite element method and those for the electric problem by the boundary element method. The Coulomb pressure due to the potential difference between the two electrodes varies with the a priori unknown distance between them. The potential difference that induces either the pull-in instability or the pull-in followed, preceded or accompanied by the snap-through instability in an arch have been computed. Wherever possible these results have been compared with those available in the literature. It is found that with a decrease in the rate of applied potential difference, the pull-in and the snap-through parameters approach that for a static problem. Also, the rate of applied potential difference determines the order in which the pull-in and the snap-through instabilities occur in an arch.

Strain Rate Dependent Behavior of Nanocrystalline Gold Films

Bart Prorok
Department of Mechanical Engineering, Auburn University

This paper reports on the influence of strain rate on the onset of mechanical softening of nanocrystalline gold at room temperature. Micro-tensile testing was performed with applied strain rates on the order of 10^{-4} 1/s to 10^{-6} 1/s. Our results defined a threshold strain rate, whereby plastic deformation at larger rates was dominated by dislocation processes and at smaller rates by one or more other deformation mechanisms. Furthermore, the data suggested that the critical grain size for inverse Hall-Petch behavior was strain rate sensitive.

Mechanical Behavior of Au Films in a Large Range of Strain Rates

Nikhil Karanjgaokar*
Department of Mechanical Science and Engineering, University of Illinois
nkaranj2@uiuc.edu

Krishna Jonnalagadda
Department of Aerospace Engineering, University of Illinois

Ioannis Chasiotis
Department of Aerospace Engineering, University of Illinois

Fernando Stump
Department of Mechanical Science and Engineering, University of Illinois

Metallic films in MEMS and electronic applications are often subjected to large strains near the material elastic limit and over a wide spectrum of strain rates. A comprehensive experimental investigation was carried out by uniaxial tension experiments to extract the strain rate dependent mechanical behavior of thin Au films with thicknesses between 500-2,000 nm and at nine orders of applied strain rate, i.e. 10^{-7} /s to 10 /s. Full-field strain measurements were conducted with the aid of a fine speckle pattern (1 micron particle size) generated on the samples and analyzed by digital image correlation. The microscale tension experiments on nanocrystalline textured Au (38 nm grain size) films pointed out to a monotonic increase of the elastic limit (325-640 MPa), yield stress (635-900 MPa), and ultimate strength (730-940 MPa) with increasing strain rate. Furthermore, there was a decrease in the fracture strain (max 6.3%) of the films with increasing strain rate with sharp transition at 10^{-4} /s, pointing to enhanced creep at rates slower than this rate. The inelastic properties for the Au films, which were generally higher than those reported in literature, had strong thickness dependence at different rates. As expected, the elastic modulus for Au films was not affected by the strain rate (E= 66.1± 2.8 GPa). The failure of nanocrystalline Au films was predominantly ductile with very different damage mechanisms at the slow (surface damage) and fast (film midplane damage) strain rates.

High Loading Rate Response of Au Microbeams

John Lambros
Department of Aerospace Engineering, University of Illinois

Jamie Kimberley
Department of Mechanical Engineering, Johns Hopkins University

Ioannis Chasiotis
Department of Aerospace Engineering, University of Illinois

Ronald Polcawich
Sensors and Electron Devices Directorate, Army Research Lab

Jeffrey Pulskamp
Sensors and Electron Devices Directorate, Army Research Lab

Madan Dubey
Sensors and Electron Devices Directorate, Army Research Lab

Increasing use of MEMS type sensors and actuators in adverse environments, which can include extreme strain rate loading has motivated the study of MEMS response under these conditions. In this study, to achieve acceleration levels on the order of 10^9 g (g-acceleration due to gravity), Au MEMS devices were subjected to impulsive loads 40 ns in duration generated by a high power pulsed laser. This allowed for the MEMS response to be investigated on time scales that were of the order of wave transit times in the substrate and devices. Simple devices, such as cantilever and fixed-fixed beams of constant cross section were used in the experiments in order to facilitate companion finite element simulations. These simulations investigated the effect of loading rate, boundary conditions, beam length, material constitutive response, and viscous damping on the deformation and final shapes of the beams. Simulation results were compared with the experimental observations to gain insight into the mechanisms responsible for impulsive deformation at the microscale. It was found that a contact and momentum transfer mechanism was responsible for the large deformations observed in postmortem inspection. Additionally, viscous damping effects were found to be dominant in determining the final deformed shape of the beams, while rate effects in material response were found to be of lesser importance—although not negligible.

Dynamic Failure of Multilayer MEMS at Intermediate Loading Rates

John Lambros
Professor
Aerospace Engineering, University of Illinois

Jamie Kimberley
Mechanical Engineering, The Johns Hopkins University

Ioannis Chasiotis
Associate Professor
Aerospace Engineering, University of Illinois

Ronald Polcawich
Sensors & Electron Devices Directorate, Army Research Laboratory

Jeffrey Pulskamp
Sensors & Electron Devices Directorate, Army Research Laboratory

Madan Dubey
Sensors and Electron Devices Directorate, Army Research Laboratory

This effort is focused on understanding how loading rate influences failure occurrence and evolution in multilayer MEMS devices. Of particular interest are our results on multifunctional multilayer MEMS, in the form of SiO_2/TiPt/PZT/Pt, that promote additional modes of failure such as interfacial delamination. To generate loading accelerations of the order of 100,000g's that are comparable to those in kinetic penetrator projectiles, we developed an experimental loading technique based on the split Hopkinson pressure bar (SHPB). A number of different specially designed fixtures were placed in the specimen region of the SHPB, and the dynamic loading generated by the projectile impact was channeled into the MEMS devices. Using appropriate fixtures, peak accelerations of 30,000g to 300,000g were achieved in the SHPB. In this loading range the MEMS devices have time to enter a resonant regime in which vibrational effects are possible. A progressive increase in damage was seen as rate increases up to about 200,000g, but less damage was observed as rate was increased further to 300,000g. This phenomenon was investigated using companion FEA simulations and it was found that failure ultimately depends not only on peak acceleration, but also on the details of the loading history. Specifically, failure occurred much later in time in the lower loading cases, which changed the details of load history to which those MEMS had been subjected.

(Thermo) Mechanical Fatigue of Advanced Materials

SYMPOSIUM
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ORGANIZERS:

John Lambros, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Huseyin Sehitoglu, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

High Temperature Low Cycle and Thermal-Mechanical Fatigue Behavior of Cast Irons

Karl-Heinz Lang
Institut fuer Werkstoffkunde I, Universitaet Karlsruhe (TH)

Andreas Uihlein
Institut fuer Werkstoffkunde I, Universitaet Karlsruhe (TH)

Detlef Loehe
Institut fuer Werkstoffkunde I, Universitaet Karlsruhe (TH)

Cylinder heads of diesel engines for power plants, ships or heavy vehicles are predominantly made of cast irons. A stress analysis of these components show two main loadings: on the one hand a low frequent thermal-mechanical loading induced by unsteady and inhomogeneous temperature fields inside the components and on the other hand a higher frequency isothermal loading caused by the pulsating combustion pressure and mechanical vibrations. To investigate the deformation and the lifetime behavior and to identify usable damage parameters three typical cast irons were tested under such loading conditions. Depending on the test temperature cast irons display a complex lifetime and cyclic deformation behavior. Especially dynamic strain ageing effects in the temperature range between 300°C and 400°C may cause cyclic increasing stresses, decreasing plasticity and a maximum in life-time. For different grades of cast iron these effects may appear in a different extent and at different temperatures influencing the cyclic deformation behavior and/or the lifetime [1, 2].

Isothermal low-cycle-fatigue (LCF) tests were carried out at different temperatures to obtain basic cognitions about the lifetime and the deformation behavior. The investigations show, that the lifetime behaviour of isothermal LCF-tests is dominated by the induced stresses. Due to plastic deformation behaviour and strain ageing effects the stresses are increasing with increasing number of cycles. If the stresses reach a characteristic stress level failure appears. This stress level depends on the material and the temperature. Additionally, thermal-mechanical fatigue (TMF) tests with maximum temperatures in the same range as the temperatures of the LCF tests were performed. These tests show that the TMF lifetime depends also on the induced stresses but the induced stresses are additionally affected by the plastic deformability of the material. Higher plasticity induces higher tensile stresses at minimum temperature.

The investigations show that the different cast irons obey different deformation and failure principles. Neither their cyclic deformation behavior nor their lifetime behavior can be described uniformly.

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Cyclic Deformation and Life Modeling of a Notched Directionally Solidified Nickel-Base Superalloy

Richard W. Neu
Department of Mechanical Engineering, Georgia Institute of Technology

Zachary L. Moore
Department of Mechanical Engineering, Georgia Institute of Technology

Robert A. Kupkovits
Department of Mechanical Engineering, Georgia Institute of Technology

Directionally-solidified (DS) nickel-base superalloys are used in high temperature gas turbines because of their high yield strength at extreme temperatures and excellent low cycle fatigue (LCF) and creep resistance in the longitudinal (i.e., grain growth) direction. Turbine blade life modeling is complicated by the presence of notches, time-dependent dwells, high temperatures and temperature gradients, and highly anisotropic material properties. This presentation provides approaches for predicting the cyclic deformation and life of the hot sections of a directionally-solidified gas turbine blade material taking into consideration orientation, time-dependent deformation, and notch effects. High temperature LCF tests were performed on smooth and notched round-bar specimens in both longitudinal and transverse orientations with and without dwells. Experimental results are used to develop and validate an analytical life prediction model. The analytical model based on a multi-axial Neuber approach predicts the local elastic-plastic stress-strain response at the notch. This approach captures anisotropy through a multiaxial generalization of the Ramberg-Osgood relation using a Hills type criterion. For input to the analytical model, the pseudo elastic notch response is determined using an anisotropic elastic finite element analysis (FEA). The limitations of the simpler analytical life-modeling method are discussed in light of FEA using a more computationally expensive anisotropic elastic-crystal viscoplastic material model.

Multiscale Analysis of Fatigue Crack Growth Using Digital Image Correlation

Jay Carroll
Research Assistant
Mechanical Science and Engineering, University of Illinois

John Lambros
Professor
Aerospace Engineering, University of Illinois

Huseyin Sehitoglu
Professor
Mechanical Science and Engineering, University of Illinois

Christos Efstathiou
Research Assistant
Mechanical Science and Engineering, University of Illinois

Brett Hauber
Air Force Research Laboratory, U.S. Air Force

Michael Spottswood
Air Force Research Laboratory, U.S. Air Force

Ravinder Chona
Air Force Research Laboratory, U.S. Air Force

The dependence of fatigue crack growth on stress intensity range, DK, was established by Paul Paris in the early 1960's. Since the discovery of plasticity induced crack closure by Wolf Elber, several modifications have been proposed to the Paris law in the form of defining an effective stress intensity range, DKeff. Defining DKeff has proven to be a challenge due to the inherent scatter in fatigue data and the indefinite nature of the crack-opening process. The optical technique of digital image correlation (DIC) allows quantitative full-field measurements to be made throughout the specimen lifetime. These measurements can facilitate efforts to define DKeff thereby improving the fidelity of fatigue crack growth predictions. In this work, DIC is used to measure near-tip displacement fields throughout a typical cycle of Paris regime fatigue crack growth in titanium. Full-field displacements (from images at a magnification of 3.9um/pixel) are used to calculate effective stress intensity factors that account for the crack closure effect. These results are then compared to measurements from high magnification (0.33um/pixel) DIC displacement gages on the crack flanks. This comparison gives insight into the crack opening process and selection of the appropriate stress intensity factor range.

Multiscale Deformation Measurements in Polycrystalline Titanium

Christos Efstathiou
Department of Mechanical Science and Engineering, University of Illinois

Jay Carroll
Department of Mechanical Science and Engineering, University of Illinois

John Lambros
Department of Aerospace Engineering, University of Illinois

Brett Hauber
Structural Mechanics Branch, Air Force Research Lab

Mike Spottswood
Structural Mechanics Branch, Air Force Research Lab

Ravi Chona
Director
Structural Sciences Center, Air Force Research Lab

Full-field strain measurements of a particular sample area were obtained at multiple length scales to reveal how the strain fields evolve as the optical resolution is increased. A comparison of the strain fields at low, medium, and high optical magnification (1.6x–50x) revealed that increased optical magnification results in larger strain gradients, and a more detailed description of the strain field. Although measurements obtained at low optical magnification do not illustrate fine details along grain boundaries, the overall strain heterogeneity is consistent with the high magnification results. The local average strain at every optical magnification was in agreement with the nominal applied strain estimated from the cross-head displacement.

Measurements obtained at micrometer length scales revealed significant strain heterogeneities concentrated primarily along grain boundaries inclined ± 45 degrees to the tensile axis, and at grain boundary triple points. These strain heterogeneities span several grain diameters, and often extend into neighboring grain interiors. They resemble networks mesoscopic slip bands.

The strain fields obtained at medium and high optical magnifications were subsequently used to calculate a RVE (representative volume element) size based on the residual plastic strain. The calculation was based on the standard deviation of the average plastic residual strain. The estimated RVE size, based on the high magnification results, was approximately 95 μm which is nearly three times the average grain size. Based on the medium magnification results, the RVE size was estimated as 70 μm. This smaller RVE size is an effect due to the "smeared" strain fields caused by the low measurement resolution at low optical magnification. Additionally, RVE size estimates were shown to be deformation dependent. The estimated RVE size increased with increased plastic residual strain.

Autonomic Materials and Structures

ORGANIZERS:

Scott White, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Nancy Sottos, *Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign*

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Multi-physics Optimization of Biomimetic Microvascular Materials

Alejandro M. Aragón
Graduate Research Assistant
Department of Civil and Environmental Engineering, University of Illinois

Brendan J. O'Rourke
Research Assistant
Department of Computer Science, University of Illinois

Kyle J. Smith
Research Assistant
Department of Aerospace Engineering, University of Illinois

Philippe H. Geubelle
Professor
Department of Aerospace Engineering, University of Illinois

Scott R. White
Professor
Department of Aerospace Engineering, University of Illinois

Recent advances in the manufacturing of polymeric materials have enabled the creation of microvascular materials that mimic features found in a variety of living organisms. These materials, which are being considered for self-healing, self-cooling and self-sensing applications, are constructed by embedding a microvascular network written by a fugitive ink in a polymeric matrix. The void space left by the ink structure after applying heat to the resulting material forms the microvascular network that is responsible for driving the healing/cooling/sensing agent. The large number of variables and constraints makes the design of the topology of the network a problem for which no optimal solution can be obtained in polynomial time with current state-of-the-art algorithms. The design of biomimetic polymers then involves the optimization of simplified mathematical models to a set of objectives and constraints using heuristics to find an optimal (or quasi optimal) set of designs. Earlier work [1] has focused in the optimization of these structures using multi-objective genetic algorithms for flow efficiency and void volume fraction as objective functions. In this work, we extend this initial work to the multiphysics optimization problem of a self-cooling microvascular network using a combination of genetic algorithm optimization and generalized finite element solutions. The presentation will include a discussion of the enrichment functions needed to solve the thermal problem and of the optimized networks associated with various thermal loadings.

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Direct Writing of Biomimetic Networks for Optimal Flow Efficiency

Willie Wu
Department of Material Science and Engineering, University of Illinois

Christopher J. Hansen
Department of Materials Science and Engineering, University of Illinois

Alejandro Aragon
Department of Civil Engineering, University of Illinois

Scott R. White
Department of Aerospace Engineering, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

Phillippe H. Geubelle
Department of Aerospace Engineering, University of Illinois

Jennifer A. Lewis
Department of Materials Science and Engineering, University of Illinois

Engineering networks of microvascular channels in a matrix is of considerable interest in self-healing[1], self-cooling, cell scaffolds[2], and microfluidic applications.[3,4] Recently, self-healing polymers with an embedded 3-D periodic network fabricated with fugitive direct ink writing have been shown to be capable of repeated healing using a coating-substrate design.[4] Next generation multi-functional self-healing materials will exhibit biomimetic architectures for optimizal flow efficiency and fluid distribution. Here, we demonstrate the fabrication of biomimetic networks with computationally optimized flow efficiency. Characterization of hydraulic resistance and flow behavior is performed on bifurcating structures and show agreement with computational models.

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Active Cooling of Polymer Structures Using Microvascular Networks

Brian Kozola
Graduate Research Assistant
Aerospace Engineering, University of Illinois

Vinay Natrajan
Graduate Research Assistant
Mechanical Science and Engineering, University of Illinois

Kenneth Christensen
Professor
Mechanical Science and Engineering, University of Illinois

Scott White
Professor
Aerospace Engineering, University of Illinois

Microvascular materials with interconnected three-dimensional networks offer an efficient method for active thermal control. Utilizing networks at the microscale offers significant advantages in convective cooling since the heat transfer coefficient scales inversely with channel diameter. In this study we examine microvascular networks created in a bulk polymer material via direct-write assembly [1]. Thin fin polymer specimens were fabricated with embedded microvascular networks consisting of 200 and 410 m diameter channels in both single layer and four layer 3-D architecture.

Fin samples were heated along the bottom edge to a constant temperature of 80 ^{o}C while the top and sides were open to the environment. After the samples reached steady state, water was pumped through the material over a range of flow rates between 0.5 and 10 ml/min and surface temperature of the fin was monitored using an infrared camera. Actuation of flow reduced the surface temperature a maximum of 31.5^{o}C at 10 ml/min flow rate and steady state cooling was reached in approximately 90 sec. All experimental conditions showed notable cooling over solid fin controls. Higher flow rates resulted in shorter cooling times and lower steady state temperatures as expected.

Flow analysis was carried out using micro-PIV. At higher flow rates all channels are activated and have steady flow. However, flow rates below 2.5 ml/min exhibited a sharp decrease in cooling efficiency due to channel blockages preventing access to portions of the network. Incomplete network perfusion was accentuated in 3-D networks.

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Three-Dimensional Biologically Inspired Microvascular Systems

Nicholas Fang
Department of Mechanical Science and Engineering, University of Illinois

Chun Guang Xia
Research Assistant
University of Illinois

Ho Won Lee
Research Assistant
University of Illinois

From venation of leaves to the blood vessels and tracheae of insects, 3D filamentous branching networks are a common pattern in all higher organisms. These busy "highways" supply the tissue with nutrition and oxygen, expel waste and heat, as well as conduct immune reactions and other signal pathways. These microvascular networks are also essential for effective response of external stimuli in some sensitive plants, such as Venus flytrap and Mimosa pudica. Nowadays 3D imaging capability such as functional MRI and microCT already unveil the sophisticated tissue structures down to micron resolution. However, challenges remain as how to replicate these highly interconnected tubular network with engineering approaches.

In this talk, we present a novel three dimensional microfabrication technology, the projection microstereolithography[1] to design and fabricate artificial microvascular networks with essential biological functions of nutrient transport and signal transduction. In our preliminary works[2], a set of poly(ethylene glycol) microstructures are demonstrated with sub-micron resolution, sufficient to reproduce the intricacy of the smallest capillaries in the vascular bundles. We observed for the first time the precisely controlled capillary spacing can regulate the metabolism and growth of yeast cells. In addition, we show programmable actuation of the polymeric microstructures[3] by delivering solvent through the embedded microfluidic channels. Development of this technology is very promising in the fields of drug delivery, artificial muscles and other bio-inspired devices.

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Self-Patterning Growth of Engineered Vascular Systems via Electrohydrodynamic Hele-Shaw Flows

Eric Wetzel*
Team Leader, Material Mechanics
Weapons and Materials Research Directorate, U.S. Army Research Laboratory
ewetzel@arl.army.mil

Julia L. Cutler
Graduate Student
Department of Chemical and Biological Engineering, Drexel University

Giuseppe R. Palmese
Professor and Head
Department of Chemical and Biological Engineering, Drexel University

Vascular networks enable a range of functionalities in biological systems including power and energy generation, repair, chemical and biological agent protection, thermal management, and reconfiguration. To enable analogous functionalities in man-made systems, it is necessary to develop techniques for controlled, scalable growth of vascularized structures. Existing approaches for fabricating vascularized materials include direct-write approaches [1], lithographic patterning [2], and integration of hollow, straight tubules [3]. As a complement to these approaches, we are exploring the use of self-patterning growth techniques that form multi-scale, branched structures. In particular, low viscosity, electrically conductive, scavengable fluids are injected at high voltage into a Hele-Shaw cell containing a high viscosity, dielectric pre-polymer fluid. The combination of hydrodynamic viscous fingering [4] with electrostatically driven instabilities [5] leads to the natural formation of fractal, branching structures that closely resemble biological vascular systems. The prepolymer can be cured to a structural polymer, and the scavengable fluid can be removed and replaced with vascular agent to create a functioning vascularized structure. These results suggest that this approach may provide a simple and scalable means of creating complex, multi-scale branched fluid networks in structural materials.

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Spiropyrans as Color-Generating Mechanophores

Douglas A. Davis
Chemistry, University of Illinois

Stephanie L. Potisek
Chemistry, University of Illinois

Lee D. Cremar
Chemistry, University of Illinois

Todd J. Martinez
Professor, Chemistry, University of Illinois

Jeffrey S. Moore
Professor, Chemistry, University of Illinois

The ability to detect stress and damage in polymeric materials is vital to ensuring their efficient and safe use. Current methods for detecting damage and stress involve the use of ultrasound, x-rays, or other external methods. Incorporation of a damage sensor into the polymer itself allows for the direct detection of the applied stresses and ensures that the sensor is uniformly dispersed. In order to do this, a mechanophore that would undergo an easily detected chemical reaction upon the application of mechanical stress was needed. Spiropyrans are known to be mechanochromic [1], and it was hypothesized that careful incorporation of the spiropyran into the polymer matrix would allow for the mechanochromism of the spiropyran to be utilized to detect stress. Testing of the spiropyran containing polymers showed that mechanical force could produce vivid color changes. Due to the ability to functionalize the spiropyran mechanophore with different polymerizable units, the mechanophore was incorporated into many different polymers (PMA, PMMA, PS, and polyurethane) which gave them mechanochromic, damage sensing properties. Molecular design, computational modeling, synthesis, and solution phase testing by ultrasound [2] will be discussed.

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Characterization of Mechanophore Reactivity in Bulk Polymers

Nancy Sottos
Department of Materials Science and Engineering, University of Illinois

Andrew Hamilton
Department of Theoretical and Applied Mechanics, University of Illinois

Jinglei Yang
Beckman Institute, University of Illinois

Doug Davis
Department of Chemistry, University of Illinois

Dara V. Gough
Department of Materials Science and Engineering, University of Illinois

Paul V. Braun
Department of Materials Science and Engineering, University of Illinois

Scott R. White
Department of Aerospace Engineering, University of Illinois

Jeffrey S. Moore
Department of Chemistry, University of Illinois

Damage in polymeric materials is preceded by complex spatial and temporal changes in stress state. Mechanical force activates covalent bonds in the polymer, but the typical result is chain scission and ultimately failure. We seek to utilize changes in stress state to mechanically activate, without human intervention, chemical changes that favorably alter the material properties of the polymer, prior to failure. While biology is replete with examples of active materials systems that respond to mechanical stimuli (e.g. ion channels, cellular motility, bone regeneration), a synthetic analog in solid state polymers is lacking. Here we report evidence of a productive mechanochemical response in both elastomeric and glassy polymers. Mechanophore linked polymers are prepared and subjected to a range of loading conditions. Evidence of local chemical reaction is provided by a color generating spiropyran (SP) mechanophore that undergoes an electrocyclic ring opening reaction under tensile mechanical deformation. Testing of the polymer samples was conducted in one of two ways depending on the viscoelastic nature of the polymeric solid. Elastomeric materials consisted of SPs polymerized into poly(methyl acrylate) (PMA) containing a single SP per chain. This polymer was molded into a dogbone specimen, which could then be stretched or fatigued under displacement control while monitoring the applied stress. Glassy materials consisted of SPs that were suspension copolymerized with methyl methacrylate (MMA) using benzoyl peroxide and N,N-dimethylaniline to give micron-scale beads. These poly (methyl methacrylate) (PMMA) beads were compressed with an actuator coupled to a load cell, which allowed for strain rate control while monitoring the resulting stress. In both cases a bulk color change is observed after loading past the yield point of the polymer. Color intensifies significantly with the accumulation of plastic strain as a result of the mechanochemical transduction event in these polymer systems.

New Mechanophores for Mechanochemically Active Polymers

Jeffrey Moore*
Beckman Institute, University of Illinois
jsmoore@uiuc.edu

Qilong Shen
Postdoctoral Researcher
Beckman Institute, University of Illinois

The mechanical activation of chemical reactions-mechanochemistry-is well-established.[1,2] Mechanochemical degradation of polymers is also well-known via homolytic bond scission reactions.[3] An untapped strategy with enormous potential is to channel applied mechanical forces into a "mechanophore"(MP)[4,5], a molecular unit that undergoes force-activated, productive chemistry to modify materials with enhanced properties. In an ideal mechanophore-based material, the competition between degradation and formation pathways are balanced so that mechanical properties are maintained, or even enhanced, under conditions in which failure would otherwise occur. We have designed, synthesized and tested several classes of mechanophores. These thermal-stable mechanophores can be readily incorporated into polymeric materials. The stress-activated response of these mechanically functionalized polymer molecules in solution will be presented including new colorizing mechanophores and first attempts at mechanocatalysis.

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Modeling of Photo-Mechanical Behaviors of Photo-Activated Polymers

Kevin Long
Graduate Student
Department of Mechanical Engineering, University of Colorado

Martin Dunn
Department of Mechanical Engineering, University of Colorado

H. Jerry Qi
Department of Mechanical Engineering, University of Colorado

The development of photo-functional polymers, which are capable of mechanically responding to light, promises to offer exciting, innovative, and unique material capabilities. Potential applications among others include novel sensors, actuators, switches, and valves at the micron scale to smart drug delivery and implant systems in biomedicine. Currently, several photo-responsive polymers have been developed with very different underlying photo-mechanical mechanisms. Such materials include: photo-radical mediated cleavage and reformation of the polymer backbone in cross-linked elastomers that results in local stress relaxation; photo-switching cross-links in shape memory polymers; and photo-isomerization of azobenzene groups contained in liquid crystal elastomers. Although these materials have received recent attention, only a primitive understanding of their photo-behavior exists both experimentally and theoretically, and in consequence, they are not yet accessible to applied technology.

This investigation intends to build a theoretical constitutive framework to model photo-activated polymeric materials. This framework is applied to a cross-linked elastomeric system able to undergo cleavage/reformation of the polymer backbone and photo-switching cross-links. In these systems, the presence of radical species is modeled to locally relieve stress through network rearrangement. Modeling this photo-radical-mechanical behavior constitutes a multi-physics problem with three primary constituents: the optical penetration and attenuation throughout the material; the photo-chemistry and associated radical concentration field; and the radical concentration-coupled mechanical behavior of the material. These three processes have been implemented in a finite element code. Experimental data are used to calibrate the photo-mechanical model. Finally, model prediction simulations of novel actuators are compared with experimental results.

Multiscale Modeling and Characterization of Electromagnetically Tunable Colloidal-Based Materials

Dimitris Lagoudas
Professor
Aerospace Engineering, Texas A&M University

Michael Bevan
Associate Professor
Chemical & Biomolecular Engineering, Johns Hopkins University

Gregory Huff
Assistant Professor
Electrical Engineering, Texas A&M University

Zoubeida Ounaies
Assistant Professor
Aerospace Engineering, Texas A&M University

Throughout the military there is a growing need to provide multifunctional apertures for platforms of all kinds. In modern warfare, the electromagnetic (EM) environment in combat is simply too complex to have separate apertures for all the different radio frequency (RF) functions that need to be performed (communication, radar, etc.). Size and cost usually limits the applicability of unpiloted aerial vehicles (UAVs) to brigade-level and larger military units. Small unit operations would benefit greatly if intelligence, surveillance, and reconnaissance (ISR) functionality (or a mission-critical subset thereof) could be contained in small or micro UAVs (MAVs). However, current MAV technologies are very limited in (1) payload mass and (2) aperture size for antennas. These in turn severely limit (1) payload capability, (2) onboard energy storage and (3) the lowest frequencies at which antennas can operate with reasonable bandwidth. Military platforms could meet many of these needs if they possess the capability to adaptively control the manner in which they respond—or adapt -to their EM environment.

Electronically reconfigurable surfaces (ERS), smart skins, reconfigurable antennas, and other adaptable systems that operate on the EM boundary conditions can fill many of these current and emerging needs. Novel systems using the displacement, pressure-driven flow, and electric field assisted microstructuring of electromagnetically functionalized colloidal dispersions (EFCDs) provide many unique capabilities toward this end, and have also demonstrated many facets of the strategic and dynamic control required by these complex electromagnetic systems. Miniaturized and/or distributed device technologies that can facilitate the desired EM behavior through the stimulated or autonomous control at the particle level are at the core of these adaptive surfaces and structures. The multiscale performance and control of these and other interlinked systems provide a host of opportunities and means to link the contribution of particle-sized components and novel devices to the electromagnetic behavior and adaptive EM control. If the placement of the above-mentioned variable boundary conditions is properly chosen, then the variation of their properties can have a profound impact not only on the EM fields but also on the overall system characteristics. The presentation will address the feasibility of using tunable colloids for distributed impedance control.

A Design Approach for Reconfigurable RF Surfaces and Apertures

Michael L.VanBlaricum*
Chief Scientist
Toyon Research Corporation
MikeVanB@Toyon.com

Thomas L. Larry
Chief Scientist
Toyon Research Corporation

Gregory H. Huff
Electromagnetics and Microwave Laboratory
Department of Electrical and Computer Engineering, Texas A&M University

Many current programs seek to eliminate discrete antenna apertures on vehicles by incorporating them into the surfaces or structure of the platform. There exists a growing need for the autonomous or adaptive control of electronically reconfigurable surfaces (ERS) and electromagnetic compensation mechanisms for embedded antennas. The desire is for the ERS to facilitate adaptive behavior of electromagnetic boundary conditions across these surfaces to define the communication, radar, and stealth capabilities. All of these desired capabilities require new types of adaptable material systems.

Autonomous reconfiguration and control of antennas takes on many challenges when considering the interplay of size and wavelength and the performance of the ERS and embedded antennas across the entire RF band. Several orders of magnitude must be electromagnetically accommodated. Smart materials have demonstrated many useful properties that might someday allow them to become an integral part within the design. To this end, ?black box' components can be designed around nanoscale materials and systems such as the reversible microstructuring of colloidal materials and the use of microvascular networks. These can then used across many length scales due to their small size in comparison to the range of RF wavelengths to strategically provide EM reconfiguration and/or compensation within the ERS.

Over the past decade, Toyon Research Corporation has been developing an antenna design approach to be used to design electronically reconfigurable skins, surfaces, and antennas. Network representation of electromagnetic (EM) systems is at the heart of the Toyon's ERS Design Methodology. This provides a convenient framework for design optimization as well as for the development of feedback and control techniques. It simultaneously enables systems level analysis and detailed physical modeling. In this way, physical models of new materials concepts can be incorporated and their systems impact determined. The hope is that as the materials science community develops new types of autonomous material systems, and their incorporation can be explored with this methodology to create multiscale descriptions of the coupled physical systems.

In this paper we will provide an overview of the methodology and show examples of its use. We will also discuss our interactions with the materials science community as we seek new types of autonomic materials systems that could be applied ERS systems and similar programs with which we have been involved.

Reconfigurable Dielectrics Using Fluidic/Microfluidic Technology

Richard Park*
Senior Program Manager
Advanced Concepts and Technologies Division, Northrop Grumman Electronic Systems
richard.park@ngc.com

Michael E. Cooley
Manager, Antenna Department
Advanced Concepts and Technologies Division, Northrop Grumman Electronic Systems

Leonard G. Chorosinski
Consulting Engineer
Advanced Concepts and Technologies Division, Northrop Grumman Electronic Systems

Karl F. Schoch
Senior Scientist
Advanced Concepts and Technologies Division, Northrop Grumman Electronic Systems

We will describe an approach that applies microfluidics to achieve reconfigurable electro-magnetic surfaces with potential application in a wide variety of mission and technology areas. We will discuss our results from a recent DARPA-sponsored program to develop and demonstrate this technology at the elemental level. Our approach melds a variety of diverse technologies including optics, microfluidics, and artificial dielectrics. Our concept demonstration design was based upon established reflectarray and FSS design principles.

The novelty of the design approach is in the application of microfluidics to reflectarrays and FSS's to achieve beam agility and tunability by actively reconfiguring the dielectric properties of the substrate material. Desired RF grating patterns can be created by pumping nanoliter volumes of two fluids, one conductive and one dielectric, into a single channel in a simple microfluidic system. The diffraction grating will be established based on alternating patterns of conductive and dielectric fluids, as dictated to achieve the desired diffraction effect. The pattern can be reconfigured into any combination of conductive or dielectric elements to within the resolution of the microfluidic system. Alternately, the dielectric under a fixed conductor can be varied by flowing different dielectric fluids in microfluidic channels under the conductor.

Candidate areas for application of the technology include electronic scanning antennas (ESA's), frequency selective surfaces (FSS's), reflectarray antennas. Potential system applications for this technology include radar, SIGINT, ESM, EW sensors and advanced communication antennas. Additionally, reconfigurable FSS's can be used to create tunable filtering of undesired frequency bands for electronic apertures.

Failure and Fracture of Heterogeneous and Multilayer Materials

ORGANIZERS:

Philippe H. Geubelle, *Department of Aerospace Engineering, University of Illinois at Urbana-Champaign*

Spandan Maiti, *Department of Mechancial Engineering–Engineering Mechanics, Michigan Technological University*

Thomas Siegmund, *Department of Mechancial Engineering, Purdue University*

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Predictive Peridynamic Models for Dynamic Fracture

Florin Bobaru
Associate Professor
Engineering Mechanics, University of Nebraska, Lincoln

Leonardo Alves
Engineering Mechanics, University of Nebraska, Lincoln

The dynamic fracture problem is the most fundamental in the science of fracture. Computational modeling of dynamic fracture phenomena has made considerable gains in being able to simulate some of the characteristics of the crack propagation, such as crack branching in thin brittle plates. The crack branching problem in thin brittle plates may be considered as a starting benchmark for simulation methods that attempt to predict dynamic crack propagation in homogenous or heterogeneous materials. The existing computational models, however, are not yet predictive [1], have difficulties with mesh dependency, and require somewhat arbitrary changes in the material fracture energy in order to get the cracks to propagate with speeds close to the measured ones.

The peridynamic formulation [2] of continuum mechanics is a nonlocal method that can predict with fidelity dynamic crack propagation, such as crack branching in dynamic fracture of thin brittle plates [3]. The question whether multiscale models, down to the atomic scale, are needed for capturing the experimentally measured response in dynamic crack propagation of a branched crack is answered here [4]. The peridynamic formulation shows that once the horizon becomes smaller than millimeter size, the results, in terms of crack path as well as crack propagation speed, converge.

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Spectral and Finite Element Analysis of Laser-Induced Delamination of Thin Patterned Films

Phuong Tran
Research Assistant
Department of Mechanical Science and Engineering, University of Illinois

Soma S. Kandula
Department of Aerospace Engineering, University of Illinois

Philippe H. Geubelle
Department of Aerospace Engineering, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

Motivated by recent developments of a controlled dynamic adhesion test of thin patterned films using laser-induced stress waves, we develop an explicit co-rotational finite element framework based on the von Karman non-linear beam theory to simulate the thin film delamination process. The beam element, which couples bending and stretching deformations, is linked to a rigid substrate with bilinear cohesive elements used to model the failure taking place in the vicinity of the advancing crack front. The nonlinear beam finite model is shown to have the ability to capture successfully the key features of the dynamic failure process revealed by a more complex and computationally intensive 2-D hybrid spectral/finite element scheme developed previously [1]. Special emphasis is placed in the capture of the evolution of the energy components (kinetic, strain and fracture energy) that define this problem. Additional simulation speed-up is achieved with the beam model by adaptively coarsening the mesh in front and behind the dynamically propagating crack tip. The numerical scheme is validated through comparison with laser-induced delamination experiments in terms of the final extent of the interfacial crack and the measured crack length history. Detailed studies on the effect on the debonding process of various parameters including film thickness, pre-crack length, and interfacial strength and fracture toughness are presented.

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Titanium/Aluminum Interface Morphology and Ballistic Impact Performance

Charles Randow
Mechanical Engineer
U.S. Army Research Laboratory

George Gazonas
Research Physicist
U.S. Army Research Laboratory

Laminate metal composites created by alternating layers of titanium (Ti) and aluminum (Al) have shown an improved resistance to fracture with a reduction in density. In these studies [1], hot pressing has been used to bond layers together, resulting in the creation of the intermetallic $TiAl_3$ at each Ti/Al interface. In the present work, approximately 200 layers of commercially pure Ti and 1100-Al are bonded using an ultrasonic consolidation process before hot pressing to form a CP-Ti/$TiAl_3$/Al laminate, with the goal of developing a system capable of withstanding the high strain-rate loads encountered in ballistic impact and blast applications. One of the difficulties in modeling this particular laminate is the lack of information available on the high strain-rate properties of $TiAl_3$ [2]. Based on experimental results, even the presence of relatively thin layers of $TiAl_3$ has a noticeable effect on the behavior of the laminate, emphasizing the important role of the interface characteristics. Through the use of experimental ballistic limit tests, ballistic pendulum tests, and dynamic finite element modeling of such tests, the effects of the Ti/Al interface and the laminate structure [3] on the strength of the system are investigated.

Numerical Approach to Dynamic Concrete Fracture at Meso-scale

Antonio Caballero
Research Fellow
ENAC-LSMS, École Polytechnique Fédérale de Lausanne

Jean-François Molinari
ENAC-LSMS, École Polytechnique Fédérale de Lausanne

This work presents a meso-mechanical model for the numerical analysis of 3 dimensional concrete-like specimens under dynamic axial loading. In this approach concrete is described by an arrangement of large aggregates which are surrounded by the "matrix" in which are included both, the mortar and the small aggregates. Concretes meso-structure is obtained by an automatic Voronoï tessellation process [1,2]. This geometric process allows generating virtual specimens with different random distributions of particles, different external shapes for the specimens and different ratios of aggregate volume. Eventually a continuum finite element mesh is obtained. Finite elements are 10-nodes quadratic tetahedra.

For the numerical analysis both phases, particles and matrix, are assumed to behave elastically. The non-linearity of the process is provided by the non-linear cohesive law of the interface elements [3] which are inserted dynamically through the loading process [4]. In particular, at every time step the inter-facial stress (stress on the contiguous face of two tetahedra) is evaluated. Whenever the material strength is exceeded a new interface element is inserted.

The results of this methodology provide a useful understanding of the dynamic propagation of fractures within concrete materials and of the effect that the meso-structure has on the crack patterns [5]. We discuss how microcracks percolation is affected by the strain rate.

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Failure of Sandwich Structures under Blast Loading

Serge Abrate*
Department of Mechanical Engineering and Energy Processes, Southern Illinois University
abrate@engr.siu.edu

Sandwich structures with laminated composite facings and cores made out of foam, honeycomb or balsa wood are considered for marine applications where they can be subjected to in-air or underwater explosions or transient distributed loading due to slamming. The duration of the applied pulse is typically of the order of 0.1 to 0.3 ms and the maximum pressure could be of the same order as the strength of the core material. Failure of the sandwich structure can result from the failure of the facesheets, failure or the core material or debonding of the interface. Two time scales must be considered: initially wave propagation through the thickness can cause severe damage to the core and the interface, for longer times overall bending occurs and several other failure modes must be considered. This article examines several special cases for which experimental results are available. An analysis of the problem is presented and suggestions are made for designing sandwich structures subjected to this type of loading. The stress-strain behavior of the core and its variation with density are of particular interest here along with the use of appropriate multi-axial failure criteria.

Size Effect on Strength of Bi-material Joints for Hybrid Ship Hull

Jia-Liang Le
Graduate Research Assistant
Department of Civil & Environmental Engineering, Northwestern University

Zdenek P. Bazant
McCormick School Professor and W. P. Murphy Professor
Department of Civil & Environmental Engineering, Northwestern University

Qiang Yu
Postdoctoral Researcher
Department of Civil & Environmental Engineering, Northwestern University

Ferhun C. Caner
Lecturer
School of Civil Engineering, Technical University of Catalonia

Bi-material joints of steel and advanced fiber-polymer composite are an effective structural system for hybrid ship hull. Understanding of the fracture mechanism of such a hybrid joint is essential in order to accurately predict its overall load capacity. Although significant advances have been made in fracture mechanics of the hybrid joints, scaling of fracture and the size effect on the strength of these joints has not been studied. The correct understanding of the size effect law is important for the extrapolation of small-scale laboratory tests to full-size joints, to ensure an efficient and reliable design. The objective of this paper is to investigate the size effect on strength of these joints theoretically, numerically and experimentally. The analytical formulation of the size effect is asymptotically anchored at the large size limit via linear elastic fracture mechanics (LEFM). The corner of the joint is shown to have a singular stress field with complex singularity. Within the framework of LEFM, energy criterion is used to determine the failure load corresponding to the crack initiation at the bi-material corner, from which the large-size asymptote of the size effect law can be derived. It has been shown that the large-size asymptote follows a power law, with its exponent directly related to the real part of the exponent of stress singularity at the bimaterial corner. An asymptotic approach is then used to derive the size effect law spanning all the sizes. In the numerical modeling of the joint, linear elastic continuum elements are used for composite and steel while cohesive fracturing zero-thickness interface elements are used for the steel-composite interface. Experimental analysis involves testing of geometrically similar specimens with size ratio 1:4:12. The numerical and experimental results agree well with the analytical formulation of the size effect law, which indicates that the strength of bimaterial metal-composite joints is subjected to a strong size effect.

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Zig-Zag Representative Unit Cells for Discrete Modeling of Fracturing and Size Effect in Two-Dimensional Triaxially Braided Composites

Christian G. Hoover
Graduate Research Assistant
Civil and Environmental Engineering, Northwestern University

Ferhun C. Caner
Ramon y Cajal Researcher and Lecturer
Geotechnical Engineering and Geo-Sciences, UPC

Zdenek P. Bazant
McCormick Institute Professor and W.P. Murphy Professor
Civil Engineering and Materials Science, Northwestern University

A simple, computationally effective model for the periodically repeated representative unit cell (RUC) of a two-dimensional triaxially braided composite (2DTBC) is developed. This RUC model has only several hundred degrees of freedom, compared to tens of thousands in other existing formulations. It can capture the effect of the complex meso-structural architecture of braided composites on their elastic stiffness properties. Fracturing of various orientations in the matrix and the fibers, both within and between the tows, can be simulated. Aside from the volume fractions of the polymer matrix and of the axial and braider fiber tows, the RUC model takes into account the angle between the axial tows and the braider tows, the relative amplitudes of the undulations of these tows, and their imperfections, which are features that cannot be captured by the Mori-Tanaka, self-consistent and similar homogenization methods. The RUC is verified and calibrated by the available measurements of stiffness constants of 2DTBC, and is shown capable of matching the measured axial and lateral stiffness moduli as well as the previous calculation of these constants by other methods. It is demonstrated that the model is able to represent the effect of buckling of undulated tows under compression and the fractures caused by buckling-induced out-of-plane tensile and shear stresses. This means that post-peak softening due to both tensile and compression fracturing can be reproduced. Since the RUC size implies a finite material characteristic length of the equivalent macro-scale continuum, the present model is also suitable for size effect simulations. The model is developed using the ABAQUS software, which suits applications in the automobile industry. The interaction between the axial and inclined tows is taken into account using cohesive fracturing connector elements. The tows are discretized using 8-node isoparametric elements. In the elastic range, the material laws for the fiber tows and the matrix in between the axial tows are, respectively, the transversely isotropic elasticity and the isotropic elasticity.

An Augmented Finite Element Method for Arbitrary Discontinuity and Material Heterogeneity

Qingda Yang
Professor
Mechanical and Aerospace Engineering, University of Miami

Daosheng Lin
Professor
Civil Engineering, Zhejiang University

In textile composite analyses it is critical to address the nucleation and growth of damage and failure processes (evolving discontinuities) under external loading. Modeling evolving weak (discontinuous strain) or strong discontinuities (discontinuous displacement) in textile composites using standard finite element method remains a difficult problem because of the requirement to construct a finite element mesh that conforms to the topology of a physical material boundary. In particular, in highly heterogeneous material systems such as textile composites, there exists a large number of internal material boundaries with weak or strong discontinuous nature, which makes it extremely difficult, if not impossible, to conform a finite element mesh to these discontinuities. To achieve faithful failure analysis of textile composites, new analysis tools that can adequately account for material heterogeneity and the related evolving (arbitrary) discontinuities have to be developed.

In this paper, we report a novel formulation of finite element method (FEM) that can adequately describe weak or strong discontinuity within an element. The new FEM thus allows us to build standard finite element mesh (physical mesh) without the need to consider the complex material boundaries in a textile composite. Our new formulation will then treat each physical element with internal material heterogeneity through a novel technical that utilizes multiple mathematical elements to account for material discontinuity, bi-material interface separation, and possible cohesive fracture in matrix. A distinct feature of our method is that it does not need any special enrichment treatment to describe a discontinuity (as so does in extended finite element method -XFEM) and it preserves fully the elemental locality. Hence the new FE is completely compatible with existing FEM programs. Furthermore, in our formulation, the discontinuous displacements across an internal material boundary (or a crack) can be conveniently obtained through standard nodal interpolation procedure. This greatly facilitates the integration of cohesive failure descriptions for all possible failure modes (interface debonding, matrix cracking, tow splitting/rupture, etc) at arbitrary locations. The effectiveness of this novel approach will be demonstrated through ample numerical examples.

Fracture Analysis of an Interfacial Crack between Two Dissimilar Piezoelectric Materials

Liying Jiang*
Professor
Mechanical and Materials Engineering, The University of Western Ontario
lyjiang@eng.uwo.ca

Zhi Yan
Department of Mechanical and Materials Engineering, The University of Western Ontario

The existence of interfaces and cracks plays a significant role in the fracture behaviour of heterogeneous solids consisting of multilayer piezoelectric materials. This work provides a comprehensive theoretical investigation on an interfacial crack between two dissimilar piezoelectric materials. The interface is modelled as a layer with varying elastic, piezoelectric and dielectric material properties (i.e., functionally graded piezoelectric materials, FGPMs), which indeed represents a more realistic description for an interfacial crack. To consider the effect of dielectric medium inside the crack upon the fracture property, a dielectric crack model is used with electric boundary condition being deformation-dependent. By means of the Fourier transform and solving the singular integral equation using Chebyshev polynomials, the nonlinear response of a slit interfacial crack has been solved under an applied tensile stress and an electric loading. Numerical simulations are given to show the effect of materials gradient, the thickness of the interfacial layer, the crack position and the dielectric medium filling the crack upon the fracture behaviour.

Analysis of Constraint Effects in Fatigue Crack Growth by Use of a Dislocation Stress Activated Cohesive Zone Model

Thomas Siegmund
Professor
Mechanical Engineering, Purdue University

A novel cohesive zone model for fatigue crack growth in metals is discussed. This model accounts for plastic strains and plastic strain gradients in the proximity of a crack tip through the underlying dislocation density. The cohesive strength is overcome through enhancement of the continuum stress field provided by the action of dislocations through their stress fields. As a result, a multi-scale cohesive zone model emerges. Processes in the cohesive zone are coupled to those in surrounding strain gradient plasticity continuum. A modified boundary layer model is used to compute fatigue crack growth.

First, the basic model response is documented for a case of a homogeneous elastic-plastic solid. Constant amplitude loading and the overload case is considered. We highlight the importance of strain gradients in the development of crack closure, and demonstrate the effectiveness of the model in predicting fatigue crack growth under variable amplitude loading.

Secondly, we investigate the cases were plastic deformation is constraint. If plastic deformation is limited due to an adjacent elastic substrate fatigue crack growth rates emerge from the competition between lowered magnitudes of dislocation activity due to constraint on the plastic zone and elevated continuum level stresses due to the same constraint. If plastic deformation characteristics are heterogeneous in the solid, the relative amounts of dislocation activity and resulting stress enhancement in the cohesive zone become relevant.

Modeling Multiscale Crack Growth Due to Impact in Heterogeneous Viscoelastic Solids

Flavio Souza
Research Assistant
Department of Engineering Mechancis, University of Nebraska, Lincoln

David Allen
Dean, College of Engineering
Department of Engineering Mechanics, University of Nebraska, Lincoln

Many applications reveal that some inelastic heterogeneous solids undergo significant load and environmentally induced energy dissipation due to both bulk dissipation and the development of multiple cracks and/or voids at various length scales. In viscoelastic materials, in particular, the energy dissipated in the bulk is governed not only by the material time scale but also by the loading time scale. The problem of crack growth in viscoelastic materials is particularly complicated by the fact that there are at least two competing energy dissipation mechanisms: bulk material dissipation and fracture energy. Furthermore, especially for heterogeneous materials, cracks can coexist over a broad range of length scales simultaneously, but the energy dissipated on these differing length scales can nevertheless be of the same order of magnitude. In some applications, such as protective devices, viscoelastic materials may be preferred because of the considerable amount of energy dissipated in the bulk as well as in the fracture process. Due to the very complex nature of the problem, analytical solutions are most often precluded so that numerical solution techniques, such as the multiscale finite element algorithms, are preferred. Multiscale models have been recently used for predicting the behavior of composite materials [1, 2, 3] and some have considered growing damage [4] and inertial effects [5]. However, most of the multiscale models developed so far in the literature do not account for inertial effects, damage and viscoelasticity. In this paper, the authors focus on the application of a multiscale model to the solution of some example problems involving impact loading of viscoelastic heterogeneous materials with growing cracks at the local scale.

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Micromechanical Deformation Characterization of Soft Cellular Materials in High Strain Rate Regime

Siladitya Pal
Mechanical Engineering-Engineering Mechanics, Graduate Student
Michigan Technological University

Spandan Maiti
Mechanical Engineering-Engineering Mechanics, Assistant Professor
Michigan Technological University

Soft cellular materials exhibit progressive or uniform collapse during impact loading depending on their microstructural and material properties. It is proposed that a complex interplay among microinertia, microbuckling and microbending of the cell walls of the specimen plays an important role in determining the ultimate deformation localization and collapse behavior. An experimental evaluation of the dependency of the deformation behavior on these parameters may not be feasible due to extremely fast and complex wave propagation event occurring within the cellular specimen. We have developed a computational framework that can examine the contribution of each of these effects on the deformation history of this class of material. Our modeling effort relies on Voronoi tessellation based microstructure generation and a corotational description of the large configurational change of cell walls due to dynamic deformation. Salient findings of an in-depth parametric study for different loading, microstuctural and material parameters will be discussed in detail. It has been found that at high strain rate, shorter pulse rise times lead to higher microinertial stress enhancement due to an increase in apparent microbuckling strength. Consequently, the layer of cells at the impact end gets collapsed. A variation of cell size shows insignificant effect of microinertia and microbuckling at initial stage, but deformation localization can be observed at later stage of deformation due to increasing microbuckling and microbending effects for higher cell sizes. Moreover, variation of Young's modulus of the cell walls does not affect the initial stress enhancement, and consequently the microbuckling effect is less pronounced. Deformation localization occurs in specimens with lower modulus due to reduced buckling and bending strength of the cell walls. Cell size irregularity does not show a pronounced effect of microinertial stress enhancement whereas collapse evolves from random sites within the specimen with higher irregularities. A significant inertial stress enhancement can be found in specimens with higher bulk density leading to enhanced microbuckling resulting in localized collapse at the impact end. The research effort to be presented will be useful in characterizing and designing soft cellular materials subjected to a dynamic loading environment.

Modeling Toughening Mechanisms in Biopolymers

Siladitya Pal
Graduate Student
Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University

Spandan Maiti
Department of Mechanical Engineering and Engineering Mechanics, Michigan Technological University

Natural materials such as nacre, bone, and spider drag silk offer an enhanced toughness along with superior strength by the virtue of a heterogeneous ultrastructure at different hierarchical levels. For example, a typical nacre shell is composed of extremely brittle platelets (calcium carbonate); but these platelets are bound with a soft biopolymer adhesive (lustrin A) rendering high toughness to the resulting composite material. Such biological adhesive polymers show a characteristic "saw tooth" force-stretch behavior over a large extension and thus makes them capable of absorbing substantially higher energy prior to failure [1]. Several studies suggest that these polymer strands comprise of modular units of hidden lengths (folded fiber) and sacrificial bonds [3]. When a polymer fiber is stretched, the hidden length is exposed due to the breaking of sacrificial bonds which occurs before the failure of the actual structural backbone of the polymer. Stretching of the main structural units, failure of sacrificial bonds and further stretching of the unfolded length results in an alternate rise and fall in the force-extension response enabling the absorption of an increased amount of energy. The design of novel extremely tough materials based on these principles requires better understanding of the above toughening mechanisms. Towards this goal, a simplified modeling framework that can take into account nanoscale mechanical events occurring during the stretching of adhesive biopolymers has been developed in the present study. Current framework contains a series of 1D structural links connected by bistable modules that are designed in such a way that on application of the external stretch, an irreversible breaking of sacrificial bonds occurs and a specified length (hidden length) is exposed thus mimicking the response of the biological polymers. A cohesive damage law has been incorporated to model the energy dissipation mechanisms during bond breaking. An in-depth parametric study of the effect of hidden lengths, sacrificial bond energies and different link and module arrangements on the toughness of the structural assembly will be presented. This novel approach can be used as a tool to develop materials possessing higher strength and toughness simultaneously.

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Analyses of Correlations among Fracture Strength, Thermal Conductance, and the Presence of Grain Boundaries in a Ceramic Nanocomposite Material Using Cohesive Finite Element and Molecular Dynamics Methods

Vikas Tomar
Department of Aerospace and Mechanical Engineering, University of Notre Dame

Vikas Samvedi
Department of Aerospace and Mechanical Engineering, University of Notre Dame

An advanced nanocomposite microstructure such as that of polycrystalline Silicon Carbide (SiC)-Silicon Nitride ($Si3N_4$) nanocomposites contains multiple lengthscales with grain boundary (GB) thickness of the order of 50 nm, SiC particle sizes of the order of 200-300 nm and $Si3N_4$ grain sizes of the order of 0.8 to 1.5 μm. Spherical SiC particles are distributed inside the $Si3N_4$ matrix in the form of intergranular as well as intragranular dispersions. By properly engineering GBs and interfaces, such a nanocomposite material system can be a good candidate for material design to achieve optimum functionality. With this view, this research reports explicit atomistic nanoscale and mesoscale (both length and time) analyses of fracture resistance and thermal conductance as a function of various GB arrangement scenarios in the nanocomposite system. A cohesive finite element method (CFEM) is also presented that could match explicit atomistic mesoscale analyses.

The framework of molecular dynamics (MD) and CFEM analyses is based on the earlier work by one of the authors. MD simulations are carried out using a modified version of a scalable parallel code, DL_POLY 2.14. Termal conductance calculations are based on direct MD method. Analyses show that the fracture in the nanocomposites is strongly correlated with the rate of loading, GB distribution, location of SiC particles with respect to GBs and the $Si3N_4$ matrix. The effect of GBs becomes stronger with change in temperature (to higher temperatures) with the gap between the fracture strengths of pure intragranular and pure intergranular specimens widening with the increasing temperatures. The results also reveal that the lattice mismatch and thermal potential differences at the interfaces, and the resulting phonon interface scattering and band structure modifications in super-lattices and nanocomposites can be exploited to reduce phonon heat conduction while maintaining the electron transport. In addition, it is found that the mechanical straining plays an important role in controlling the heat conduction.

Computational Investigation of Failure in EB-PVD Thermal Barrier Coatings with Multiple Top Coat Cracks

Himanshu Bhatnagar
Mechanical Engineering, The Ohio State University

Somnath Ghosh
Professor
Mechanical Engineering, The Ohio State University

Mark E. Walter
Professor
Mechanical Engineering, The Ohio State University

A multi-layer thermal barrier coating (TBC) for nickel-based superalloys consists of a thermally insulating ceramic topcoat deposited with electron beam physical vapor deposition (EB-PVD) on an intermetallic bondcoat. As a result of the deposition processing, multiple microstructural defects appear in the topcoat. These topcoat defects can coalesce to form large-scale damage or initiate delamination at multiple sites. In addition, exposure to high temperature gases oxidizes the bondcoat, which leads to growth of a thermally grown oxide (TGO) layer between the topcoat and the bondcoat. The interface between TGO and topcoat is undulated and is most susceptible to delamination. Catastrophic interfacial delamination is preceded by propagation of new and pre-exiting cracks in the top coat until the interface.

For enhanced understanding and prediction of failure in TBCs under cyclic thermal loading, a parametric finite element model is developed using the commercial finite element code ABAQUS in conjunction with an eXtended Voronoi Cell Finite Element Model (X-VCFEM). The interaction between multiple defects and microstructural morphology is simulated by incorporating the actual topcoat microstructure in the model. The propagation of micro-cracks is explicitly modeled using a hysteretic cohesive zone. The crack trajectories are not prescribed a priori. Instead, they are determined adaptively using the maximum cohesive energy criterion at the crack tip. Numerical examples are solved and compared with experimental observations to establish the effectiveness of the model. The validated parametric model is employed to investigate the effects of geometry, material properties and morphological distribution of defects on the failure of TBCs. The morphological features considered in the study include length, orientation, and dispersion of cracks. A novel parametric relationship between various geometric and material parameters is derived to determine design specifications for safer TBCs. The model can be used for design of next generation TBCs with newer materials.

Computing Fracture Toughness of Thin Files Made Up of Single/Multilayered Polymer Composites

Harish Iyer
Graduate Student
Department of Mechanical Engineering, University of Michigan

Eugene Kheng
Graduate Student
Department of Mechanical Engineering, University of Michigan

Ellen Arruda
Department of Mechanical Engineering, University of Michigan

Tony Waas
Department of Aerospace Engineering, University of Michigan

Free standing thin films made up of single/multi layered polymer composite materials can be designed to have high fracture toughness making them suitable for a host of applications in the automotive, aerospace and defense sector. It is imperative in this quest to accurately measure the fracture toughness of these thin films so as to quantitatively compare their toughness values with other corresponding materials.

A technique known as layer-by-layer (LBL) manufacturing is highly beneficial in creating single/multi layered polymer composite materials having sandwiched structure. The exact number of layers, sequence of various polymer layers as well the thickness of the layers can be controlled accurately.

Initially, uniaxial tension tests are performed at various deformation rates in order to characterize the macroscopic mechanical response of these polymer composites and the data is used in the development of a constitutive model for the polymer composite material. The constitutive model is then used in the simulation of a boundary value problem involving the propagation of crack. Discrete cohesive zone model elements are used in the computer model, which predict the nature of crack failure. The simulation results are compared with experiments performed under the exact same boundary conditions. The key challenge is to associate the amount of work going into plastic deformation and the amount work going into the growth of crack. Through a set of fracture experiments and simulations we can then quantify the fracture toughness of the material.

A Hybrid Experimental/Numerical Approach to Characterize Interfacial Adhesion in Multilayer Thin Low-K Film Specimens

Rajesh Kitey
Postdoctoral Research Associate
Department of Aerospace Engineering, University of Illinois

Philippe H. Geubelle
Department of Aerospace Engineering, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

The interfacial strength of multilayer low dielectric (low-k) constant thin films (30 nm silicon-carbon-nitride (SiCN) and 250 nm organo-silicate glass (OSG)) deposited on silicon (Si) substrate is characterized by laser spallation technique. Four different specimen sets are fabricated by mutually switching the film stacking under two different processing conditions, with and without helium (He) pretreatment. The test specimens are prepared by depositing an inertial layer of titanium/gold (Ti/Au) film on top of the stacked films followed by bonding a fused silica (FS) disk directly to the back surface of the substrate. The top inertial layer and the back FS layer increase the interfacial stress without damaging the underlying substrate. A laser induced high amplitude rapidly rising compressive stress pulse, evolves in FS and is transmitted to the Si. The pulse reflects back from the free Au film surface as a tensile wave, subjecting film interfaces to dynamic mode-I loading. The weakest interface in the stack (first to fail) is identified by optical and profilometric analysis of the spallation zone. The strength of the failed interface is inferred from the incident stress history in combination with a computational one dimensional dynamic wave propagation study performed on the specimen in consideration.

Numerical Simulations of Wrinkling-Induced Delaminations in Multi-layered Thin-Film Systems

Kartik Srinivasan
Mechanical Engineering, Purdue University

Sanjay Goyal
Mechanical Engineering, Purdue University

Ganesh Subbarayan
Professor
Mechanical Engineering, Purdue University

Thomas Siegmund
Professor
Mechanical Engineering, Purdue University

Film wrinkling is an instability occurring in thin-film systems comprising a compliant film/substrate capped by a stiffer film. During film wrinkling, the films initially remain bonded to each other and the underlying substrate. As the compressive stress is increased, wrinkling can lead to delaminations at the interface between films or at the interface between a film and the underlying substrate. The competition between wrinkling and delaminations is a subject of recent interest. For e.g. a recent study [1] provides experimental evidence of a thin-film system which under compressive stresses undergoes film wrinkling, but upon further increase in the compressive stress, leads to delaminations at the interface. Numerical studies of wrinkling [2,3] using 1-D beam models on non-linear foundations have shown that non-linearity in the foundation traction-separation response leads to localization effects. The first goal of the present work is to provide an understanding of the mechanics of such wrinkling-induced delaminations. A secondary goal is to investigate the relation between interfacial properties and the critical load for the onset of wrinkling-induced delaminations. This could potentially provide a technique for the measurement of interfacial properties in stiff film-compliant film systems.

The stiff film is modeled using von Kármán plate theory. The combined effect of the interface and the underlying compliant film is modeled as a cohesive foundation with a non-linear traction-separation relation. The non-linearity in the traction-separation relation of the foundation can be thought to be on account of delaminations occurring at the interface resulting in a weakening of the foundation. The governing equations are solved numerically using a spectral method. The spectral method used in the present work is an extension of the technique proposed by Huang et al. [4]. A new coupling term in Fourier space captures the interaction in wrinkling amplitudes between bonded and de-bonded domains.

Various forms of foundation traction-separation responses are studied: (a) linear elastic, (b) non-linear elastic, (c) softening. For these cases, the localization behavior in dependence of the applied strain state is demonstrated. The conditions for the transition from uniform wrinkles to localized delaminations are investigated and the critical loads for this transition are related to the interfacial properties. The findings of the present work are particularly relevant to the microelectronic industry where stiff film-compliant film systems under compressive stresses occur widely during fabrication and processing.

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The Impact of Sidewall Roughness on the Macroscopic Strength of Polycrystalline Silicon

James W. Foulk III*
Sandia National Laboratories
Livermore, California
jwfoulk@sandia.gov

B.L. Boyce
Sandia National Laboratories
Alburquerque, New Mexico

E.D. Reedy Jr.
Sandia National Laboratories
Alburquerque, New Mexico

In order to design efficient, reliable microelectromechanical systems (MEMS), one must understand the statistics of failure. For brittle systems, we can better understand strength distributions through flaw distributions. Specifically, we seek to investigate the role of sidewall flaw size, shape, and spacing on the strength of polycrystalline silicon. Although the deleterious effects of sidewall roughness are well accepted and recent studies have illustrated marked improvements through reduced roughness [1], most studies have focused on the long crack toughness [2, 3] and the macroscopic strength [4] of polycrystalline silicon. Fewer efforts have conducted detailed studies of sidewall flaw distributions and their impact on the macroscopic strength.

Based on results from atomic force microscopy and transmission electron microscopy, we seek to parameterize the sidewall flaw size, shape, and spacing. Idealized, two-dimensional finite element models of MEMS tensile specimens [4] will be employed to determine the sensitivity of flaw parameters. Crack initiation and propagation will be modeled through a cohesive zone approach. Although we will initially assume the tensile specimens to be isotropic, detailed studies of long crack behavior will quantify the effects of elastic anisotropy and the competition between multiple cleavage planes. Through these initial, fundamental studies, we hope to better understand the role of defect distributions on the variation in the macroscopic strength of polycrystalline silicon.

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Constraining Effect on Brittle Fracture

C. T. Sun*
Neil A. Armstrong Distinguished Professor
School of Aeronautics and Astronautics, Purdue University
sun@purdue.edu

Bhawesh Kumar
Research Assistant
School of Aeronautics and Astronautics, Purdue University

Dependence of fracture toughness on the bondline thickness of adhesive joints is a well known fact [1-4]. However, the explanation of this dependency based on plastic zone size [1-2], interface failure, fracture zone size etc are not supported by rigorous mechanics. The main reason of the inability to explain this phenomenon lies in the fact that the adhesive material used was significantly nonlinear and inelastic and, as a result, linear elastic fracture mechanics (LEFM) which uses stress intensity factor to characterize fracture toughness becomes inadequate. Moreover, the use of the double cantilever beam (DCB) or compact tension specimen to test adhesive fracture toughness presents another type of challenge to LEFM concerning the validity of the representation by the singular stress in the fracture process zone. In the present work, PMMA (Polymethyl methacrylate), a relatively brittle material, is used for the study instead of rubber-modified epoxy. The use of PMMA minimizes the effect of plasticity and allows us to focus on the question regarding the representation of the K-field in the fracture process zone. The DCB specimen contains a cracked PMMA sheet instead of rubber modified epoxy sandwiched between two aluminum beams. The test data indicate that fracture load increases monotonically with the increase in the PMMA layer thickness. But, the apparent fracture toughness increases with the PMMA layer thickness in the range of 0.0625″-0.25″ and then decreases beyond 0.25″. To explain this unusual behavior, stress analyses using plane strain finite elements are performed. The FEA result shows that the size of the K-dominance region (in which the singular stress is dominant) is significantly affected depending on the thickness of the PMMA sheet. In fact, the K-dominance zone becomes very small when the thickness of the PMMA sheet is very small. For these cases, stress intensity factor may not be sufficient to characterize the fracture behavior of the material and the second term in the Williams crack tip stress field expansion may be needed. In this study, we include the second term in the Williams expansion to model the fracture toughness of PMMA under the influence of constraining from boundary conditions. Details of the experimental results obtained from DCB tests and the fracture model predictions will be presented.

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Deformation and Fracture of Epoxy Nanocomposites with 12 nm Silica Inclusions

Qi Chen
Graduate Student
Department of Aerospace Engineering, University of Illinois

Ioannis Chasiotis
Department of Aerospace Engineering, University of Illinois

Chenggang Chen
University of Dayton Research Institute

Ajit Roy
Senior Material Research Engineer
Wright-Patterson AFB

An experimental investigation of the effective and local mechanical and fracture behavior of epoxy with nanoscale fumed silica inclusions was carried out. Two nanofiller sizes were employed: 12 nm (primary) and 100 nm (secondary). Large particles promoted matrix stiffening at small weight fractions, which decreased at larger weight fractions and converged to that of the primary nanoparticles. The elastic modulus of the latter varied rather linearly with weight faction and increased by about 30% at 15 wt.% silica. Local strain measurements by an AFM showed major strain localization in the vicinity of 100-nm fillers, which promoted matrix softening and therefore reduction in composite stiffness. In composites with 5 wt.% secondary particles, neighboring particles located at small proximities behaved as single large particles or resulted in local matrix strain shielding and therefore no improvement in stiffness. The tensile strength of all composites was consistent irrespective of particle size and weight fraction. This was attributed to strong particle bonding and damage localization in the matrix, which caused failure initiation in the matrix. Mode I facture toughness experiments were also conducted on 12-nm silica composite samples. The critical mode I stress intensity factor increased with silica weight fraction, by as high as 35% for 15 wt.% silica composites compared to the neat epoxy. Electron microscopy fractographs showed that the nanoparticles induced micro-flake morphology to the fracture surface, which was present at all weight fractions and contributed to matrix toughening by enhancing local matrix yielding and therefore energy dissipation. Void formation at the size of nanoparticles was observed at most weight fractions, but for the largest weight fraction its extent was limited compared to matrix yielding.

Failure Surface of a Rubber-Modified Epoxy C-Fiber Composite under Multiaxial Loading

Luis Canal
Department of Material Science, Polytechnic
University of Madrid

Javier Segurado
IMDEA-Materials & Department of Material Science, Polytechnic
University of Madrid

Javier LLorca
IMDEA-Materials & Department of Material Science, Polytechnic
University of Madrid

The use of carbon fiber-reinforced polymers (CFRP) in structural applications has increased rapidly during the last thirty years as a result of their outstanding specific stiffness and strength, and of the maturation of the processing and quality control techniques. From the view point of mechanical performance, one of the main limitations of CFRP is due to the brittle nature of epoxy thermosets used as matrix, which makes the material prone to failure by interply delamination, limits the impact resistance, and leads to a brittle behavior if the lamina are subjected to transverse tensile stresses. This has led to the modification of epoxy matrices to increase the toughness through the addition of second-phase rubbery particles. The rubber particles cavitate during tensile deformation, and the relief of hydrostatic stresses leads to the shear yielding of the matrix around the cavitated particles which in turn promotes the growth of voids and the formation of discrete shear bands. These mechanisms matrices enhance significantly the strength and toughness of composite lamina in the transverse direction, in which the matrix mechanical behavior plays a dominant role. The mechanical behavior until fracture of rubber-modified epoxy unidirectionally reinforced with C fibers was studied through the finite element analysis of a representative volume element (RVE) of the lamina. The RVE was a square two-dimensional section of the lamina (perpendicular to the fibers) which contained a random and homogeneous dispersion of circular C fibers embedded in the rubber-modified epoxy matrix. The fiber volume fraction within the RVE was 50 %. Fibers were considered as linear elastic, transversally isotropic solids. The matrix behavior was followed the approximation proposed by Jeong [1-2], which takes into account the inherent pressure-sensitivity of the yield stress in the epoxy matrix, the damage induced in the matrix by the cavitation (and subsequent growth) of the rubber particles, and the particular features of deformation in glassy polymers, particularly the intrinsic softening upon yield followed by hardening. An implicit visco-plastic implementation of the model was performed to minimize the mesh dependency due to the matrix softening induced by the matrix behavior and void growth. Finally, damage by interface fracture was also included in the simulations through interface elements at the fiber/matrix interface whose behavior was controlled by the interface strength and toughness [3]. The mechanical response of the lamina under transverse tension and shear was computed for different pseudo-radial loading paths to obtain the corresponding failure surface in the s2?-t23 stress space. Two different fiber-matrix interfaces were considered (strong and weak) attending to the value of the interface strength, and the interaction among the different deformation and failure mechanisms was analyzed to understand the role played by fiber, matrix and interface properties on the composite behavior. Finally, the failure surfaces provided by the numerical simulations were compared with those provided by Hashin [4] and Puck [5] phenomenological models to assess their accuracy and range of validity.

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Microstructure Evolution in Hyperelastic Laminates and Implications for Overall Behavior and Macroscopic Stability

Oscar Lopez-Pamies
Assistant Professor|
Mechanical Engineering, State University of New York at Stony Brook

Pedro Ponte Castaneda
Professor
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

In this work, we study the evolution of the underlying microstructure in hyperelastic laminates subjected to finite deformations. To this end, we identify a set of relevant microstructural variables and derive rigorous formulae for their evolution along finite-deformation paths. Making use of these results we then establish connections between the evolution of the microstructure and the overall stress-strain relation and macroscopic stability in hyperelastic laminates. In particular, we show that the rotation of the layers may lead to a reduction in the overall stiffness of the laminates under appropriate loading conditions. Furthermore, we show that this geometric mechanism is intimately related to the possible loss of strong ellipticity of the overall behavior of these materials, which may occur even in the case when the underlying constituents are taken to be strongly elliptic.

Multiscale Damage Due to Restrained Volume Change in Cement-Based Composites

Mohammad Pour-Ghaz
Graduate Research Assistant
School of Civil Engineering, Purdue University

Gaurav Sant
Graduate Research Assistant
School of Civil Engineering, Purdue University

Ryan Henkensiefken
Graduate Research Assistant
School of Civil Engineering, Purdue University

Jae Heum Moon
Senior Researcher
Structural Materials Team, Korea Institute of Construction Materials

W. Jason Weiss
Professor and Associate Head
School of Civil Engineering, Purdue University

Cement based materials are generally thought of as homogenous at the macroscale. At the mesoscale, the heterogeneous nature of these materials can be considered with the aggregate and paste exhibiting different volume changes. This results in residual stress development in the paste. The driving forces of this volume change are dictated by the micro- and nanoscale pores. This presentation will present results from experimental and theoretical investigations of the driving forces for shrinkage at the microscale, multi-phase finite element modeling of damage developed at the mesoscale, and restrained shrinkage cracking at the macroscale. To study damage evolution acoustic emission is used to measure the fracture energy. The energy of fracture and characteristic wave form are used to differentiate between micro- and macro-cracking. The acoustic emission results indicate how microcracks form into a localized macrocrack and lead to failure.

Local Field Properties, Microstructure, and Multiscale Phenomena in Heterogeneous Media

ORGANIZERS:

Guillermo H. Goldsztein, *School of Mathematics, Georgia Institute of Technology*

Robert Lipton, *Department of Mathematics, Lousiana State University*

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Inverse Homogenization: Identification of the Structure of Composites from Effective Properties

Elena Cherkaev
Professor
Department of Mathematics, University of Utah

The talk discusses a problem of deriving information about the microgeometry of composite material from its effective properties. The approach is based on reconstruction of the spectral measure in the analytic Stieltjes representation of the effective tensor of two-component composite. This representation relates the n-point correlation functions of the microstructure to the moments of the spectral measure, which contains all information about the microgeometry. The problem of identification of the spectral function from effective measurements in an interval of frequency has a unique solution, however the problem is ill-posed. The talk discusses several stabilization techniques and Pade approximations that could be used for reconstruction of the spectral function. The reconstructed spectral function can be used to recover microstructural parameters and to compute other effective properties of the same composite.

Attainability of Hashin-Shtrikman Bounds for Multiphase Composites

Liping Liu
Engineering and Applied Science, California Institute of Technology

We address the attainability of the Hashin-Shtrikman bounds for multiphase composites, including those of conductive materials and elastic materials. It presents a new derivation of these bounds that yield a necessary and sufficient condition for optimal microstructures. A key idea is a simple characterization of the gradient Young measures associated with optimal microstructures.

Random Fluctuations of the Solutions to Equations with Highly Oscillatory Coefficients

Guillaume Bal
APAM,
Columbia University

We consider partial differential equations of elliptic or parabolic type with random highly oscillatory coefficients. In many instances, it is known that the solution converges to the deterministic solution of a homogenized equation. In this talk, we consider the correction to the homogenization procedure and look for the asymptotic law of the random fluctuations. We will present examples of elliptic equations in which the asymptotic law of the random fluctuations may be fully characterized.

In the specific example of a parabolic equation with a large spatial Gaussian random potential, we will show that the limiting equation, as the correlation length of the random potential tends to zero, very much depends on the strength of the unperturbed parabolic operator and on the spatial dimension. In large spatial dimensions, the limiting solution is a homogenized deterministic equation at least for sufficiently small times. In small spatial dimensions, the limiting equation is a stochastic partial differential equation for which we provide an existence theory.

Singular Behavior of the Overall Properties of High Contrast, Densely Packed Composite Materials

Yuliya Gorb
Department of Mathematics, Texas A&M University

Alexei Novikov
Department of Mathematics, Pennsylvania State University

Leonid Berlyand
Department of Mathematics, Pennsylvania State University

We consider high contrast media with particles close to touching. The overall or effective properties (e.g. conductivity or viscosity) of such materials exhibit blow ups as the distance between particles gets small. To derive and justify the blow up of the effective properties the discrete network approximation method is used. It is a variational approach leading to a simple algebraic problem on a graph. The differences between analyses of the scalar (conductivity) and vectorial (suspension) problems will be highlighted, and main technical tools used to handle both cases will be discussed.

Quantitative Description of the Morphology of a Randomly Distributed Particulate Composite Material

Seth E. Watts
Research Assistant
Mechanical Science and Engineering, University of Illinois

Daniel A. Tortorelli
Professor
Mechanical Science and Engineering, University of Illinois

Thomas G. Eason
Research Aerospace Engineer
Air Force Research Laboratory

The qualitative description of morphology is of interest to those working in many fields, including astronomy, geology, biology, and materials engineering. Many contributions in descriptive morphology from these fields as well as mathematics have been made over the years. For example, Minkowski functionals (MFs), which arise from the field of integral geometry, have been used as a set of morphological measures for several decades, e.g. [1]. More recently, a method for extracting more information from the MFs by weighting them by spatial moments has been described [2], [3], but this method appears to date to have been limited to the astronomical literature. This weighting technique, which results in the related tensor-valued Minkowski valuations (MVs), is discussed for characterization of the microstructure of a metal-matrix composite with a randomly-distributed particulate reinforcing phase, and is extended to generate tensors of arbitrarily high order by weighting the MFs by arbitrarily high spatial moments. Image processing techniques adapted from the fields of computer vision [4] and medical imaging [5] are used to smoothly segment micrographs of the material, and MVs are computed for sampled subsets of the resulting binary patterns. Tensor decompositions are then applied to the MVs to generate scalar measures; these measures are computed for a large number of specimens, and a statistical distribution of each measure is thereby generated. The results are used to generate a suitable set of measures which can be used to robustly characterize the material morphology.

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The Yield Strength of Composites: Analysis of a Toy Model

Guillermo Goldsztein
Department of Mathematics, Georgia Tech

We study, by means of simple analysis and examples, a toy model motivated by the computation of the yield strength of composites. Our goal is to understand the dependence of the strength of the composites on the microgeometry and the properties of the pure phases that compose the material.

A Multiscale Approach to Model Heterogeneous Materials

Qiushi Chen
Civil and Environmental Engineering, Northwestern University

Jose E. Andrade
Assistant Professor
Civil and Environmental Engineering, Northwestern University

It has already been established that fine scale heterogeneities have a great influence on mechanical behavior of materials [1]. However, the computer power needed to directly simulate field or even specimen-scale problems with microstructure resolution is prohibitive and, hence, multiscale approaches become attractive alternatives. In this work, we present a hierarchical multiscale framework to model heterogeneous materials. The core idea is to zoom into critical areas of a marcroscopic FEM mesh, impose marcroscopic information as boundary conditions to a microscopic mesh, i.e. the so called unit cell [2], where fine scale heterogeneous is taken into account and then extract material response based on unit cell computation. A novel, yet simple, method is developed to realize the multiscale computation. We formulate the multiscale approach in a finite element framework but the idea could be utilized using other methods such as discrete element methods as well. The multiscale computation is performed only in hot areas, e.g. shear band, failure path, to achieve high computational efficiency while preserving the accuracy. We present numerical simulations, using both conventional direct numerical simulation and the proposed multiscale framework to validate the efficiency and accuracy of the multiscale approach.

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Local Fields in Nonlinear Power Law Materials

Silvia Jimenez
Graduate Student
Mathematics, Louisiana State University

Robert Lipton
S.B. Barton Professor
Mathematics, Louisiana State University

We focus on strong approximations for local fields in Nonlinear Power Law Materials. The approximations are used to assess the singularity strength inside micro-structured materials. Examples are given for mixtures of different types of power law materials.

Optimal Bounds on Local Stress and Strain Fields inside Random Media

Robert Lipton
Department of Mathematics, Louisiana State University

Bacim Alali
Department of Mathematics, Louisiana State University

New optimal bounds are presented that characterize the local field behavior inside random composites. The bounds apply to the higher moments of the local fields and are given in terms of the available statistical information describing the microstructure.

It is shown that these bounds are the best possible as they are attained by by several different classes of microstructures including coated confocal ellipsoids, coated spheres, and layered microstructures.

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Materials and Mechanics Issues in Energy Conversion, Storage, and Transport

ORGANIZERS:

Pradeep Sharma, *Department of Mechanical Engineering, University of Houston*

Harley T. Johnson, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

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Using Old Materials in New Ways for Photovoltaics

John Rogers
Professor
Materials Science and Engineering, University of Illinois

Silicon, in amorphous or various crystalline forms, is used in >90% of all installed photovoltaic (PV) capacity. The high natural abundance of silicon, together with the excellent reliability and good efficiency of solar cells made with it suggest its continued use, on massive scales, for the foreseeable future. As a result, although there is significant promise for organics, nanocrystals, nanowires and other new materials for photovoltaics, many opportunities continue to exist for research into unconventional means for exploiting silicon in advanced PV systems. This paper describes modules that use large scale arrays of silicon solar micro-cells (u-cells) created from bulk wafers and integrated in diverse spatial layouts on foreign substrates by transfer printing. The resulting devices can offer useful features, including high degrees of mechanical flexibility, user-definable levels of transparency and ultra-low profile micro-optic concentrator designs. Detailed studies of the processes for creating and manipulating such u-cells, together with theoretical and experimental investigations of the electrical, mechanical and optical characteristics of several types of modules that incorporate them illuminate the key aspects. The results represent strategies that might expand the application possibilities for monocrystalline silicon PV.

Materials for the Hydrogen Economy: Embrittlement and Remediation

Petros Sofronis*
Professor
Mechanical Science & Engineering, University of Illinois
sofronis@uiuc.edu

Ian Roberston
Professor
Materials Science & Engineering, University of Illinois

Mohsen Dadfarnia
Research Assistant
Mechanical Science & Engineering, University of Illinois

Paul Novak
Research Assistant
Mechanical Science & Engineering, University of Illinois

In April of 2003, Energy Secretary Abraham summarized the new hydrogen economy by stating that consumers will have the practical option of purchasing a competitively priced hydrogen power vehicle, and be able to refuel it near their homes and places of work by 2020. However, the technology of large scale hydrogen transmission from central production facilities to refueling stations and stationary power sites is at present undeveloped. Among the problems which confront the implementation of this technology is the deleterious effect of hydrogen on structural material properties, in particular at gas pressure of 1500 psi which is the desirable transmission pressure suggested by economic studies for efficient transport.

Despite extensive study over almost a century, a complete mechanistic understanding of the hydrogen-induced degradation of engineering materials has yet to be achieved. Our current understanding leads to the recognition that there is no single mechanism causing hydrogen embrittlement. Of the many suggestions, three mechanisms appear to be viable: stress-induced hydride formation and cleavage, hydrogen-enhanced localized plasticity, and hydrogen-induced decohesion. To understand these mechanisms of embrittlement our approach integrates mechanical property testing at the micro and macroscale, microstructural analyses and TEM observations of the deformation processes at the micro- and nano-scale, thermodynamic considerations for the material cohesive properties at the atomistic scale, and finite element modeling and simulation at the micro- and macro-level. It is demonstrated that hydrogen i) enhances dislocation mobility by shielding the interactions between microstructural defects; ii) induces loss of ellipticity in the governing rate equations of the macroscopic elastoplastic material response which is manifested in the onset of severe shear localization of the plastic flow; iii) can reduce both the macroscopic stress and strain for internal void nucleation and grain boundary decohesion.

A discussion will be presented on how we can develop and verify a lifetime prediction methodology for failure of materials used in pipeline systems and welds exposed to high-pressure gaseous environments. Development and validation of such predictive capability and strategies to avoid material degradation is of paramount importance to the rapid assessment of the suitability of using the current natural-gas pipeline distribution system for hydrogen transport, as has been recommended by the National Research Council, and of the susceptibility of new alloys tailored for use in the planned hydrogen economy.

Revisiting the Origins of the Dead-Layer in Nanocapacitors and Ramifications for Energy Storage

Pradeep Sharma
University of Houston

Revisiting the Origins of the Dead-layer in Nanocapacitors and Ramifications for Energy Storage Ravi Maranganti, Mohamed Sabri Majdoub, Pradeep Sharma Department of Mechanical Engineering, University of HoustonThin films of high-permittivity ferroelectrics are considered ideal candidates for realizing high charge density nanosized capacitors for use in next generation energy storage and nanoelectronics applications. The experimentally observed capacitance of such thin film nanocapacitors is, however, an order of magnitude lower than expected. This dramatic drop in capacitance is attributed to the so-called "dead layer" which is a low-permittivity layer at the metal-dielectric interface in series with the high-permittivity dielectric. The exact nature of the dead-layer and the reasons for its origin still remain somewhat unclear. Based on insights gained from recently published ab initio work on this long-standing problem, we construct an analytical model that precisely isolates the contributions of various physical mechanisms to the intrinsic dead-layer. In particular we argue that strain-gradients automatically arise in very thin films even in absence of external strains and, due to coupling with flexoelectricity, are a dominant contributor to the dead-layer effect. Our theoretical results compare well with ours and published ab initio calculations and emphasize that inclusion of flexoelectricity is essential for qualitative reconciliation of atomistic results. Based on insights obtained from our analytical model, we suggest some remedies for mitigating the dead-layer effect.

Mechanics of Heterogeneous Media

ORGANIZERS:

Martin Ostoja-Starzewski, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Vitali F. Nesterenko, *Department of Mechanical and Aerospace Engineering, University of California, San Diego*

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Calculation of the Dependence of the Equilibrium Distribution of Configurations of Circularized DNA on Nucleotide Sequence and Salt Concentration

Bernard D. Coleman
Professor
Program in Mechanics, Rutgers University

Yoav Y. Biton
Program in Mechanics, Rutgers University

We have been developing a (Metropolis) Monte Carlo method for determining the dependence of the thermodynamical equilibrium distribution of configurations of a circularized DNA molecule on its nucleotide sequence, its topology, and the concentration of salt in the medium. The method is unique in that, as in our recent work on the mechanical equilibrium of DNA configurations [1][2], account is taken of the facts that (1) the contribution of a given base-pair step to the energy of a DNA molecule depends on which nucleotides are present in that step and (2) the presence of intrinsic and/or induced curvature implies that there can be strong electrostatic interactions between sequentially remote nucleotides. In addition the method obeys conditions sufficient for it to yield canonical distributions of generated configurations. A group at the Baylor College of Medicine [3] has succeeded in making, for specified sequences of base pairs, milligram quantities of supercoiled DNA minicircles, each having its own nucleotide sequence and linking number Lk (a topological invariant equal to the number of times either one of the two DNA strands in the molecule is inter-linked with the molecules axial curve, C. The total energy U of the molecule (in units of kT) equals the sum of its total elastic energy and its total electrostatic energy. The writhe W (which can be considered a measure of the chirality of C) equals the average, over all orientations of a plane, of the sum of the signed self-crossings in the projection of C on that plane. For several members of a set of topoisomers of a 339 base pair minicircle described in reference [3] we have calculated the minimum energy configuration for several values of the linking number and a (monovalent) salt concentration c of 0.1 M (which yields an ionic strength that is close to its value in a living cell). For the topoisomer with Lk = 29, the minimum energy values of W and U were calculated to be –1.734 and 148.7 kT, and in its minimum energy configuration the topoisomer has two points of self contact. For that topoisomer we performed a Metropolis Monte Carlo simulation to generate an ensemble of 200 million configurations for which the assumed impenetrability of the molecule is obeyed and observed that for each configuration in the ensemble there is a single couplet (n,m) of sequentially remote base pairs that are in closest proximity. Our analysis of the distribution of configurations as a function of their energy showed that, for the configurations of maximum likelihood, U = 1207.0±0.1 kT. We found that there are two domains of high probability in the n-m plane. Just one of these domains contains configurations with couplets (n,m) near the contact points present in the minimum energy configuration. Our simulation method is unique in that, when the sequence-dependence of mechanical properties is taken into account, it has sufficient precision to reveal the existence and geometric properties of such domains.

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Dynamics of Cylindrical Shell in a Coaxially Heterogeneous Solid

Bojan Guzina
Professor
Civil Engineering, University of Minnesota

Ronald Pak
Professor
Civil, Environmental and Architectural Engineering, University of Colorado

Jeramy Ashlock
Research Associate
University of Colorado

This paper aims to explore the effect of unidirectional heterogeneity of a solid “matrix on the dynamics of a coaxially embedded cylindrical shell. To this end, an exact treatment is presented for the axial vibration of a thin shell in a semi-infinite solid with i) linear, and ii) piecewise constant shear-wave and compressional-wave velocity profiles. By virtue of the relevant Greens functions established for the problem of interest, the shell-matrix interaction problem is shown to be reducible to a pair of one-dimensional integral equations. With a rigorous incorporation of the singular contact stress conditions arising at material discontinuities, a computational procedure is developed by which dynamic tractions, displacements, and complex compliance functions are evaluated to provide benchmark results.

Propagation and Localization of Acoustic and Elastic Waves in Strongly Heterogeneous Media

Muhammad Sahimi
Professor
Mork Family Department of Chemical Engineering & Materials Science, University of Southern California

Propagation of acoustic and elastic waves in strongly heterogeneous media is studied using dynamic renormalization group (RG) analysis and extensive numerical simulations. The heterogeneities are characterized by a broad distribution of the local elastic constants. We consider both Gaussian-white distributed elastic constants, as well as those with long-range correlations with a nondecaying power-law correlation function. The study is motivated in part by recent analysis of experimental data for the spatial distribution of the elastic moduli of rock at large length scales, which indicated that the distribution contains the same type of long-range correlations as what we consider in the present paper. Another motivation for studying the problem is understanding the similarities and differences between localization of classical waves, such as acoustic and elastic waves, and the classical problem of Anderson localization of electrons in heterogeneous materials and the associated metal-insulator phase transition. The problem and the results are, however, applicable to acoustic and elastic wave propagation in any disordered elastic material that contains the types of heterogeneities that we consider in the present paper. Using the Martin-Siggia-Rose method, we analyze propagation of acoustic waves in d-dimensional media, and of elastic waves in two-dimensional systems. For the acoustic waves we find that, depending on the type of disorder, the RG flows exhibit a transition to a localized or extended regime in any dimension. The results for propagation of acoustic waves in two-dimensional media are similar to what we find for the elastic waves in same type of disordered media. We also carry out extensive numerical simulations of acoustic and elastic wave propagation in one-, two- and three-dimensional disordered media. Both isotropic and anisotropic media (with anisotropy being due to stratification) are considered. The results for the isotropic media are consistent with the RG predictions. While the RG analysis, in its present form, does not make any prediction for the anisotropic media, the results of our numerical simulations indicate the possibility of the existence of a regime of superlocalization in which the waves amplitudes decay faster than exponentially.

Mechanical Damping and Softening Near the Curie Point of Barium Titanate

Roderic Lakes
Wisconsin Distinguished Professor
Department of Engineering Physics, University of Wisconsin, Madison

Liang Dong
Graduate Student
Department of Materials Science, University of Wisconsin, Madison

D. Stone
Associate Professor
Materials Science, University of Wisconsin

The classical bounds for composite properties such as modulus, damping or thermal expansion, which are derived under the assumption that both matrix and inclusion possess positive stiffness, state that these properties cannot surpass those of constituents. However, such bounds can be exceeded given the existence of negative-stiffness inclusions embedded in positive-stiffness matrix. Negative stiffness is presented as the occurrence of a reaction force in the same direction as imposed deformation, and is achieved by stored elastic energy at quasi-equilibrium. T. Jaglinski, et al. studied a composite material, of polycrystalline $BaTiO_3$ particle inclusions embedded in tin matrix which attained a stiffness (Young's modulus) almost ten times greater than that of diamond as the inclusions undergo the tetragonal-cubic phase transition. The extreme stiffness was attributed to the negative bulk modulus of this ferroelastic inclusion during the phase transition.

With the aim of directly observing the softening of bulk modulus hypothesized in the design of the above composite, we have studied pure polycrystalline $BaTiO_3$ by means of Broadband Viscoelastic Spectroscopy (BVS) as both frequency and temperature are varied. A peak in mechanical loss has been observed near the Curie point 130°C corresponding to the "tetragonal-cubic" phase transition. The height and width of the peak increase with temperature and the inverse of frequency.

Anomalous responses in mechanical loss and modulus were observed outside the transition temperature region, which may be associated with the absorption and dissipation of stored elastic energy between certain domains and their surroundings under the external oscillation stress. The observations of such anomalous responses above Curie point may indicate the existence of domain structure at cubic phase.

Softening in modulus was observed as frequency is reduced. Young's modulus softens more than shear modulus with descending frequency. Isothermal frequency scan presents a hump in mechanical loss, which may be associated with frequency dependence of the phase transition itself, in the vicinity of transformation below 1 Hz. Such a hump tends to be flat outside this temperature region.

Quasi-isothermal studies reveal a significant softening in bulk modulus (almost a factor of four) and a transient reduction in Poisson's ratio from 0.35 to a negative value –0.02 during the phase transition.

Mesomechanics of Critical and Postcritical Behavior of Polymer-Based Granular Composites

Vitali Nesterenko
Professor
Mechanical and Aerospace Engineering, University of California, San Diego

David Benson
Professor
Mechanical and Aerospace Engineering, University of California, San Diego

Eric B. Herbold
Mechanical and Aerospace Engineering, University of California, San Diego

Jing Cai
Materials Science and Engineering Program, University of California, San Diego

Ken S. Vecchio
Professor
Department of NanoEngineering, University of California, San Diego

F. Jiang
Department of NanoEngineering, University of California, San Diego

John W. Addiss
Cavendish Laboratory, University of Cambridge

Stephen M. Walley
Cavendish Laboratory, University of Cambridge

Dynamic compressive strength of cold isostatically pressed (CIP) composites of polytetrafluoroethylene (PTFE), tungsten and aluminum powders show significant differences depending on the particle size of the powder. Mixtures containing both PTFE and aluminum are known to be energetic under dynamic and/or thermal loading. The addition of tungsten particles in this study increases then density and overall strength of the sample. The compressive strength of the samples was tested experimentally in drop-weight tests and Hopkinson bar tests using samples with coarse (20 ?m) and fine (1 ?m) tungsten powders with similar constituent mass fractions for each test. It was found that the samples with higher porosity (using fine tungsten powder) were able to sustain higher loads before fracturing. Intuitively, higher porosity should be detrimental to the strength of a material. An explanation of this disparity is presented using Finite Element calculations. Multi-material Eulerian and arbitrary Lagrangian-Eulerian methods (2-D and 3-D simulations) were used for the investigation due to the complexity of the microstructure, large deformations and the ability to handle the formation of free surfaces in a natural manner. The calculations indicate that the strength disparity depends mainly on the size distribution of the aluminum and tungsten particles in the PTFE matrix and their interaction before and after cracks development. The dependence of strength on particle size can be useful in the design of compacted powder based materials and their disintegration under dynamic large strain deformation.

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Pressure Dependence of Unconsolidated Granular Media: Role of Force Chains and Local Anisotropy

James Berryman
Senior Staff Scientist
Department of Geophysics, Lawrence Berkeley National Lab

Steven R. Pride
Staff Scientist
Department of Geophysics, Lawrence Berkeley National Lab

Observations of force chains in unconsolidated granular packings have been reported in both laboratory and computational settings. Although there are obvious differences, there are some important similarities between such packings and certain amorphous systems. By melting single crystals and then rapidly quenching them (lowering their temperature), so that small single crystals form having randomly oriented symmetry axes, polycrystalline amorphous structures are formed. Such systems are sometimes called "frustrated" because the overall lower-energy, single-crystalline state has not been achieved through this rapid quenching process. For granular media, the confining pressure plays a similar (though inverse) role to that of temperature in a frustrated polycrystalline system. As pressure goes up, the grains of the system begin to lock into a state where a small region containing multiple grains may have one preferred axis of applied stress, while neighboring regions have differing preferred axes. Thus, various groupings of grains do not necessarily have their axes of symmetry aligned with each other, but rather are aligned (naturally) with the local uniaxial stresses and strains associated with the force chain concept. We use this picture together with the theory of composites for polycrystalline systems to estimate theoretically the mechanical behavior of such grain packs. We find that the overall pressure dependence of the effective elastic moduli in such a model goes as pressure to the one-half power despite the fact that each local anisotropic region in the polycrystal is varying with the Hertz-Mindlin-Walton result of pressure to the one-third power. This result is consistent with a large number of experimental data on grain packs that report a pressure to the one-half dependence when applied stresses are less than roughly 10 MPa.

Polycrystal Simulation and Analysis of Compressive Strength of Shocked AD995 Alumina

Jianbin Zhu
Graduate Research Assistant
Department of Engineering Mechanics, University of Nebraska, Lincoln

Ruqiang Feng
Department of Engineering Mechanics, University of Nebraska, Lincoln

Pure and dense polycrystalline alpha-alumina has extremely high effective shock strength, a material property important for armor structures and other impact engineering applications. However, 15-30% reduction in the Hugoniot elastic limit (HEL) and more significant reduction in the post-HEL strength have been observed for AD995, a 99.5% pure and 97% dense, low-cost alternative. To understand the difference between the inelastic deformation of shocked AD995 and that of shocked pure and dense alumina, which can be well characterized by heterogeneous crystal microplasticity on limited slip planes, we have carried out a numerical study using Voronoi polycrystal modeling in conjunction with finite element analysis. The microstructure model permits explicit modeling of the heterogeneities due to grain-to-grain topological variations, elastic and plastic anisotropies, and the presence of voids. The material model considers nonlinear anisotropic crystal elasticity, crystal plasticity and deformation twinning. First, AD995 was approximated as pure alumina with 1-4% porosities to investigate the role of pore compaction in the inelastic deformation of AD995 under uniaxial-strain shock compression. Next, the grain boundaries were treated as a glassy second phase to examine the effects of weaker grain boundaries. Simulation results will be presented to show that neither can explain the observed HEL and post-HEL response of shocked AD995. It will be further demonstrated that a much better modeling can be achieved if in addition to the presence of porosity combined deformation twinning and crystal slip are allowed to activate at a significantly lower threshold than that for crystal microplasticity in pure and dense alumina. From the polycrystal simulation results, an effective strength model describing the compressive strength behavior resulted from such a mesoscopically heterogeneous inelastic deformation was constructed for AD995. Issues related to explicit void modeling and mesh convergence will also be discussed.

Effect of Pore Clusters on the Statistics of Peak Stress and Overall Properties of Porous Material

Igor Sevostianov
Department of Mechanical and Aerospace Engineering, New Mexico State University

Volodymyr Kushch
Senior Scientist
Institute for Superhard Materials

This paper addresses the effect of pore distribution on the overall properties and local stress fields in a porous material. Thermal and elastic fields in materials with uniform microstructure are compared with those of materials containing distinguishable clusters of circular or elliptic shape. The numerical simulation combines multipole expansion of local fields with the multi-particle unit cell method. Our work demonstrates that statistics of the peak stresses follow Gumbel's rule derived for statistics of extreme values and are directly related to statistics of nearest neighbors. Based on this correspondence, an analytical expression for statistics of maximal stresses in a porous material with arbitrary microstructure is constructed in terms of porosity and statistics of minimal distances between the nearest neighbors. At the same time, the numerical analysis indicates that overall elastic constants and thermal (or electrical) conductivity are almost insensitive to the actual distribution of pores—uniform or with distinguishable pore clusters—at least in the examined interval of porosity (up to 50%).

Diffuse Ultrasonic Backscatter from Heterogeneous Solids through a Cylindrical Liquid-Solid Interface

Goutam Ghoshal
Department of Engineering Mechanics, University of Nebraska, Lincoln

Dr. Joseph A. Turner
Department of Engineering Mechanics, University of Nebraska, Lincoln

Diffuse ultrasonic backscatter techniques are useful for probing heterogeneous materials. They can be used to extract microstructural parameters and to detect flaws, which cannot be detected by conventional ultrasonic techniques. Such experiments, usually done using a modified pulse-echo technique, utilize the spatial variance of the signals as a primary measure of microstructure. Quantitative ultrasonic scattering models include components of both transducer beams as well as microstructural scattering information. Of particular interest for interpretation of many experiments is the propagation through a liquid-solid interface at normal and oblique incidence. Here, the Wigner distribution of the beam pattern of an ultrasonic transducer through a cylindrical liquid-solid interface is used in conjunction with the stochastic wave equation to model this scattering problem within a single scattering formulism. The Wigner distribution represents a distribution in space and time of the spectral energy density as a function of wave vector and frequency. A Gaussian beam is used to model the transducer beam pattern. Finally the scattered response will be derived within a single scattering formalism that is compared with experimental results. These results are anticipated to impact ultrasonic nondestructive evaluation and characterization of heterogeneous media with curved geometries.

Transient Analysis of Hydrogels with Coupled Finite Deformation and Mass Diffusion

Hanqing Jiang
Assistant Professor
Mechanical and Aerospace Engineering, Arizona State University

Jiaping Zhang
Mechanical and Aerospace Engineering, Arizona State University

Xuanhe Zhao
School of Engineering and Applied Sciences, Harvard University

Zhigang Suo
Professor
School of Engineering and Applied Sciences, Harvard University

Hydrogel is a network of cross-linked polymeric chains that are water-insoluble. The cross-linked polymeric chains prevent the dissolving of the long polymers in the water; rather, the hydrogel swells and shrinks reversibly when the water molecules migrate in and out. In this process, the hydrogels have large volumetric change, which endows them various applications, including biomedical devices, tissue engineering, actuators, biosensors and oil industry. Recently, Hong et al. [1] formulated a theory of the coupled mass transport and large deformation. The energy in the system has two parts: elastic strain energy due to shape and volumetric change, and the work done by the chemical potential. In this presentation, the weak form was formulated and implemented in the ABAQUS finite element program via its USER-ELEMENT subroutine. Several transient problems with coupled large deformation and mass diffusion have been studied, including uniaxial creep and free swollen.

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Large Deformation Constitutive Model for Back Stress of Glassy Polycarbonate

Mehrdad Negahban
Associate Professor
Engineering Mechanics, University of Nebraska

Ashwani Kumar Goel
Research Assistant
Engineering Mechanics, University of Nebraska

Kyle Strabala
Research Assistant
Engineering Mechanics, University of Nebraska

Nathan Medeiros Barreto Oliveira
Research Assistant
Engineering Mechanics, University of Nebraska

Jonathan Hein
Research Assistant
Engineering Mechanics, University of Nebraska

Ruqiang Feng
Associate Professor
Engineering Mechanics, University of Nebraska

Polycarbonate like other glassy polymers shows a back stress, which represents conditions under which relaxation events stop and the material can carry an applied load indefinitely without a need to change the strain. In an effort to characterize the back stress response of PC, a general thermodynamically consistent model can be developed based on invariance theory that obtains the stress and back stress from derivatives of the free energy, and provides a thermodynamic force for the plastic flow. A set of experiments were performed with consecutive cycles of loading and unloading with different strain rates varying from 0.0001/s to 0.1/s in uniaxial compression and shear. In [1] and [2] we have provided a method which can be used to evaluate the back stress experimentally at different temperatures for polycarbonate in shear. A similar method was used to calculate the back stress experimentally in uniaxial compression. The method is based on evaluating the slope of the stress-strain response under conditions of similar elastic and plastic strain, but different strain rates. This experimentally evaluated back stress response in compression was used to calculate the derivatives of the free energy with respect to the invariants and modeled the back stress. The back stress calculated from compression was in close agreement with that obtained in shear experiments.

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Extremum and Variational Principles for Elastic and Inelastic Media with Fractal Geometries

Martin Ostoja-Starzewski
Department of Mechanical Science and Engineering, University of Illinois

This paper continues the recently begun extension of continuum mechanics and thermodynamics to fractal porous media which are specified by a mass (or spatial) fractal dimension D, a surface fractal dimension d, and a resolution lengthscale R [1,2,3,4]. The focus is on pre-fractal media through a theory based on dimensional regularization, in which D is also the order of fractional integrals employed to state global balance laws. In effect, the global forms of governing equations employ conventional (integer order) integrals, while the local forms are expressed through partial differential equations with derivatives of integer order but containing coefficients involving D, d and R. Here we first generalize the principles of virtual work, virtual displacements and virtual stresses, which in turn allow us to extend the minimum energy theorems of elasticity theory. Next, we generalize the extremum principles of elasto-plastic and rigid-plastic bodies. A similar procedure applies to linear viscoelasticity theory. In all the cases, the derived relations depend explicitly on D, d and R, and, upon setting D=3 and d=2, reduce to conventional forms of governing equations for continuous media with Euclidean geometries.

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On Scaling Properties of Random Semiflexible Fiber Networks

H. Hatami-Marbini
Department of Mechanical and Aeronautical Engineering, Rensselaer Polytechnic Institute

R.C. Picu
Rensselaer Polytechnic Institute

The study of semiflexible polymer networks is essential in understanding the mechanical properties of many polymeric and biological materials. The complexity of the relationship between the overall behavior of the network and the fiber properties and distribution (the microstructure) draws the attention of many investigators. This issue has been discussed in the literature primarily in connection with the mechanics of the cell, which is mainly controlled by that of the cytoskeleton. Here, we first quantify the non-affine behavior of fiber networks using a new non-affinity measure. We then study the mechanics of these materials at various length scales. Although it is currently believed that networks with high fiber density or with fibers of vanishing bending stiffness deform affinely, it is here shown that these conclusions depend on the nature of non-affinty measure. It is also seen that the degree of non-affinity decreases as the scale of observation increases. This scaling is a power law with different exponents. The large length scale scaling behavior is independent of fiber stiffness and/or density; however, the small length scale behavior is controlled by the fiber bending stiffness.

Multiscale Modeling and Characterization of Nano-structured Polymer Composites

ORGANIZER:

Jaret C. Riddick, *U.S. Army Research Laboratory*

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Elastic Constants and Coefficients of Thermal Expansion for Epoxy-Nanotube Composites from Molecular Dynamics Simulation

Sarah-Jane Frankland
National Institute of Aerospace

T. C. Clancy
National Institute of Aerospace

J. C. Riddick
Army Research Laboratory

Selective use of nano-constituents in traditional composite materials has the potential to enhance performance without adding more than negligible amounts of weight. For some time now, the addition of carbon nanotubes (CNTs) into polymeric matrices to form polymer nanocomposites has been pursued, and therefore the addition of CNTs into the resin system of a carbon fiber composite is a natural step. While processing issues are still critical, the status quo is to determine the advantages of carbon nanotube inclusion in carbon fiber composites. With NASA interest in the RS-47 pre-preg system and the possibility of including carbon nanotubes therein, studies have been undertaken to add carbon nanotubes into RS-47, and to model the mechanical, thermal and electrical behavior thereof. The exact chemistry of the RS-47 system is proprietary and remains unknown. The models of the system include detailed chemistry to incorporate appropriate atomistic effects of adding carbon nanotubes into the toughened amine-cured epoxy system, but they are idealized and intended to model the mechanical and thermal properties of the RS-47 system, not the actual chemical formulation.

In the present work, mechanical and thermal properties of an amine-cured and toughened epoxy system which includes carbon nanotubes are calculated from molecular dynamics (MD) simulation. The MD simulation calculates these properties for representative volume elements (RVE) of the material on the order of 104 atoms. In particular, elastic constants and coefficients of thermal expansion are determined for the epoxy resin, the epoxy with a nanotube, the epoxy with a functionalized nanotube, and for analogous systems with the model toughener. These systems are applicable to micromechanical models which can combine the mechanical and thermal properties from the molecular RVEs and determine the properties of the epoxy/toughener/nanotube system at the nanocomposite level. Comparison can then be made at the nanocomposite-level with available mechanical and/or thermal testing of nanocomposites made with the RS-47 system. The present work will present the elastic constants and coefficients of thermal expansion for the molecular RVEs of the amine-cured toughened epoxy system with nanotubes, and the molecular simulations methods used to determine them.

Computational Modeling of Multifunctional Materials

Thomas Clancy
Senior Research Scientist
National Institute of Aerospace

Sarah-Jane V. Frankland
Senior Research Scientist
National Institute of Aerospace

Thomas S. Gates
Senior Materials Research Engineer
Durability, Damage Tolerance, and Reliability Branch, NASA Langley Research Center

Jaret Riddick
Aerospace Engineer
Vehicle Technology Directorate, Army Research Laboratory

The influence of functionalization of carbon nanotubes on thermal conductivity is investigated with multi-scale modeling techniques. In order to improve the performance and application of polymer based aerospace materials, research efforts are being made to provide multifunctionality to these materials. One of the properties of particular interest currently is thermal conductivity. Although polymer based materials have many useful properties, the thermal conductivity is typically low. A current research approach to improving thermal conductivity is the addition of nanoparticles to the polymer matrix. In particular, the addition of carbon nanotubes to polymers is being researched in order to develop materials with improved thermal conductivity. Previous research has highlighted the effect that detailed molecular interactions at the interface of the matrix and nanoparticle can have on macroscopic properties. These interactions can be tailored by functionalization of the carbon nanotube surface. Because these interfacial details can be difficult to characterize experimentally, multiscale computational modeling techniques are in development in order to aid the experimental effort. Since nanoparticles have structural details on the nanometer length scale, it is useful to apply modeling approaches which are suitable to these dimensions. Atomistic modeling of polymer nanocomposites will be the primary focus of the material presented here. Atomistic models of polymer nanocomposites were constructed which contained a carbon nanotube embedded in an idealized epoxy system, conceptualized to model the behavior of RS-47. Several parameters associated with the chemical functionalization were varied in order to assess the effect of these parameters on properties of interest. The interfacial thermal resistance between the nanoparticle and the polymer matrix is calculated by a molecular dynamics simulation procedure. This value is used to predict thermal conductivity of polymer nanocomposites with various functionalization treatments.

Micromechanics Modeling of the Elastic, Thermal, and Electrical Properties of Carbon Nanotube-Epoxy Nanocomposites and Unidirectional Hybrid Laminates

Gary Seidel
Postdoctoral Research Associate
Department of Aerospace Engineering,
Texas A&M University

Dimitris C. Lagoudas
John and Bea Slattery Chair of Aerospace Engineering
Department of Aerospace Engineering,
Texas A&M University

Piyush R. Thakre
PhD Student
Department of Aerospace Engineering,
Texas A&M University

Sarah-Jane V. Frankland
Senior Research Scientist
National Institute of Aerospace

Thomas C. Clancy
Senior Research Scientist
National Institute of Aerospace

Jiang Zhu
Research Scientist
NanoRidge Materials Inc.

Jaret C. Riddick
Aerospace Engineer
Vehicle Technology Directorate,
U. S. Army Research Laboratory

The selective placement of nanomaterials in traditional structural composites such as carbon fiber laminates is presently being studied as means of developing multifunctional materials for aerospace applications. The resulting hybrid laminate composites are, in addition to serving in a structural role, expected to serve in non-structural function(s), e.g. thermal management and/or electrostatic discharge, without incurring a significant weight penalty. It is believed that due to the large differences in elastic, thermal, and electrical properties between the nanotubes and the epoxy matrix in which the carbon fibers are imbedded, that a small quantity of nanotubes will result in significant increases in the laminate matrix properties. As part of a collaborative effort between researchers at Texas A&M University, the National Institute of Aerospace, and NanoRidge Materials, a hybrid laminate material system consisting unidirectional IM7 carbon fibers in an RS-47 epoxy pre-preg which has been sprayed with HiPCO produced single wall carbon nanotubes has been identified as model material system for developing validated multiscale models.

In the present work, micromechanics models for the mechanical, thermal and electrical properties are developed for two distinct length scales, the submicron nanocomposite matrix length scale and the micron length scale of the hybrid laminate composite. Specifically, the elastic constants, thermal conductivity, thermal expansion coefficient, and electrical conductivity of the nanocomposite consisting of a mixture of metallic and non-metallic, randomly oriented single wall carbon nanotubes, residual iron catalyst, and a thermoplastic toughener phase dispersed in the epoxy matrix are determined. The micromechanics model is based on the use of the generalized self-consistent composite cylinders model and a multiphase averaging approach which treats each orientation of a given constituent as a separate phase. Special attention has been given to accounting for the influence of nanoscale phenomena such as interfacial thermal resistance and electron hopping, which have been identified to play a significant role on the percolation behavior of nanocomposites, and which are accounted for in the micromechanics model through the use of interphase layers in the composite cylinder assemblage. Where available, the results of lower length scale molecular dynamics (MD) simulations (discussed in detail in separate presentations) have been used as input in the micromechanics model to account for the influence of detailed intermolecular interactions, for example, providing input for the elastic constants, the coefficient of thermal expansion, and the interfacial thermal resistance for the micromechanics model some of which may also be strongly influenced by nanotube functionalization, likewise accounted for in the MD simulations. The resulting effective nanocomposite elastic, thermal and electrical properties predicted by the micromechanics model are compared with nanocomposite characterization efforts (discussed in detail in a separate presentation), and are subsequently used as the effective matrix material for the micromechanics model used to determine effective hybrid laminate properties which are also compared with characterization efforts.

Mechanical, Electrical, and Thermal Characterization of Single Wall Carbon Nanotube-Modified Unidirectional Carbon-Fiber/Epoxy Matrix Composites

Dimitris Lagoudas
John and Bea Slattery Chair of Aerospace Engineering
Department of Aerospace Engineering, Texas A & M University

Piyush Thakre
Graduate Student
Department of Aerospace Engineering, Texas A & M University

Jiang Zhu
Corporate Scientist
NanoRidge Materials

Jaret Riddick
Aerospace Engineer
Vehicle Technology Directorate, Army Research Lab

Thomas Gates
(Posthumous Submission) Senior Materials Research Engineer
Durability, Damage Tolerance and Reliability Branch, NASA Langley Research Center

Carbon-fiber/epoxy matrix composites are increasingly being used in the aerospace industry due to their excellent mechanical properties, e.g., high elastic modulus, strength and damage resistance. However, there is a growing demand for the incorporation of multifunctional properties, such as, electrical conductivity, EMI (electromagnetic interference) shielding, thermal expansion coefficient and thermal conductivity. Single wall carbon nanotubes are known to have excellent multifunctional properties, such as very high elastic modulus, high electrical and thermal conductivity. There is a potential to transfer these properties to the micro- and macro-scale by incorporating nanotubes in the epoxy matrix of carbon-fiber reinforced epoxy matrix composite laminates.

In the present work, the effect of modifying traditional carbon-fiber/epoxy matrix composites with single wall carbon nanotubes is being investigated and mechanical, electrical and thermal properties are being studied. Unidirectional IM7 carbon fiber pre-pregs are used with the RS-47 epoxy matrix system consisting of a secondary toughener phase. A spraying technique is used for the selective placement of nanotubes on the pre-preg laminae. These sprayed pre-pregs are compressed using a hot press and a specific curing cycle is developed to optimize the temperature and the time for the curing process, so as to control the fiber volume fraction of the multi-scale laminate composite. Three composite panels are produced using the hot press technique, a base composite panel without nanotubes, a second panel consisting of unfunctionalized (pristine) nanotubes and a third panel consisting of amide functionalized nanotubes.

A hybrid composite laminate system consisting of nanostructured reinforcements requires appropriate characterization at different length scales to understand the physics behind the measured material property at each length scale. The proposed work, apart from developing a processing method, focuses on characterization efforts using, for example, dynamic mechanical analysis to help optimize processing parameters and subsequently using flexure testing and double cantilever beam testing to characterize the elastic modulus and the interlaminar fracture toughness, to demonstrate the benefits of multi-scale hybrid composites for composite airframe structures.

Nonlinear Mechanics of Fiber-Reinforced Materials

ORGANIZERS:

Luis Dorfmann, *Department of Civil and Environmental Engineering, Tufts University*

Jose Merodio, *Department of Continuum Mechanics and Structures, Polytechnic University of Madrid*

Ray W. Ogden, *Department of Mathematics, University of Glasgow*

SYMPOSIUM

II

Computational Micromechanics of Fiber-Reinforced Elastomers

Joaquin Moraleda
IMDEA-Materials & Department of Material Science
Polytechnic University of Madrid

Javier Segurado
IMDEA-Materials & Department of Material Science
Polytechnic University of Madrid

Javier LLorca
IMDEA-Materials & Department of Material Science
Polytechnic University of Madrid

The finite deformation of fiber-reinforced elastomers subjected to uniaxial tension perpendicular to the fibers was studied by means of the numerical simulation of a representative volume element of the microstructure. The size and the discretization of the volume element were selected to obtain an exact response (to a few per cent) of the plane-strain deformation of a material made up of a random and isotropic dispersion of aligned circular fibers embedded in an incompressible elastomeric matrix. The matrix was modeled using both a Neo-hookean model and a Gents model with locking at a given strain. The fibers were considered as nearly-incompressible solids and modeled as Neo-Hookean materials. Materials with different volume fraction of fibers (in the range 10 to 30%) were analyzed.

The numerical results of the macroscopic stress-strain curve for the in-plane deformation of fiber-reinforced elastomers were compared with those provided by the homogenization model based on the second-order estimate with field fluctuations of López-Pamiés and Ponte Castañeda [1-2], and the constitutive model for elastomeric composites by Debotton [3]. It was found that the homogenization model [2-3] led to a better approximations to the numerical results than the other, giving a very good approximation to the "exact" numerical result in the case of Neo-Hookean matrices for the whole range of fiber volume fractions analyzed. However, in the case of Gent materials, the accuracy of the homogenization model to predict the numerical results changed with the value of the locking parameter of the matrix, Jm,, and the model tend to underestimate the locking strain for smalls values of Jm.

The effect of fiber/matrix decohesion on the overall composite response was also addressed by the numerical simulations. To this end, interface elements were inserted at the fiber-matrix interface and the interface properties were given by a cohesive crack model [4]. Interface damage was controlled by the interface strength and fracture energy, and the effect of both parameters on the macro- and microscopic response was studied. It was found that the value of the interface strength controlled the maximum strength of the composite, while the interface response was responsible for the post-peak behavior.

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Constitutive Models for Fiber-Reinforced Rubbers: Effective Response and Macroscopic Instabilities

Pedro Ponte Castaneda
Professor
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

Michalis Agoras
Mechanical Engineering and Applied Mechanics, University of Pennsylvania

Oscar Lopez-Pamies
Professor
Mechanical Engineering, S.U.N.Y. at Stony Book

A new constitutive model for the nonlinearly elastic response of fiber-reinforced elastomers will be presented. The model has been derived by means of the second-order homogenization theory, which makes use of suitably designed variational principles utilizing the idea of a linear comparison composite. In the undeformed configuration, the matrix and fiber phases are assumed to be isotropic, incompressible, hyperelastic solids, while the fibers are assumed to be perfectly aligned and distributed randomly leading to overall transversely isotropic behavior for the composite. The model takes into account the evolution of the shape, orientation, and distribution of the fibers, resulting from the finite changes in geometry at large deformations, and it can be used to predict the overall behavior of composites with phases characterized by constitutive relations that are more general than Neo-Hookean. These features of the present model are unique among the constitutive models that have been proposed thus far in the literature for this class of materials. The model recovers exact solutions that are known in the literature for composites with Neo-Hookean, as well as more general constituents under special loading conditions. In this talk, the emphasis will be on the predictions of the model for the effective response and the posible onset of macroscopic instabilities in fiber-reinforced elastomers made out of Gent and Neo-Hookean constituents for a variety of loading conditions. In spite of the (assumed) strong ellipticity of the phases, the macroscopic response may lose strong ellipticity at sufficiently large deformations for cases where such instabilities may be expected to occur from physical experience. This, in turn, suggests that the evolution of the microstructure may play a critical role in the overall behavior of the composite.

Onset of Cavitation in Compressible, Isotropic, Hyperelastic Solids

Oscar Lopez-Pamies*
Assistant Professor
Mechanical Engineering, State University of New York at Stony Brook
oscar.lopez-pamies@sunysb.edu

In this work, we derive a closed-form criterion for the onset of cavitation in compressible, isotropic, hyperelastic solids subjected to non-symmetric loading conditions. The criterion is based on the solution of a boundary value problem where

a hyperelastic solid, which is infinite in extent and contains a single vacuous inhomogeneity, is subjected to uniform displacement boundary conditions. By making use of the "linear—comparison" variational procedure of Lopez-Pamies and Ponte Castaneda (2006) [1], we solve this problem approximately and generate variational estimates for the critical stretches applied on the boundary at which the cavity suddenly starts growing. The accuracy of the proposed analytical result is assessed by comparisons with exact solutions available from the literature for radially symmetric cavitation. In addition, applications are presented for a variety of materials of practical and theoretical interest, including the harmonic, Blatz-Ko, and compressible Neo-Hookean materials.

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A Continuum Model for the Orthotropic Response of Needlepunched Nonwoven Fabrics

Simona Socrate
Department of Mechanical Engineering, Massachusetts Institute of Technology

Petch Jearanaisilawong
Department of Mechanical Engineering, Massachusetts Institute of Technology

Nonwoven fabrics are sheet structures created by bonding or interlocking a web (network) of fibers through mechanical, thermal or chemical processes. The mechanical response of nonwoven fabrics can exhibit substantial anisotropy due to preferential orientation in the arrangement of the constituent fibers and/or in the pattern of inter-fiber bonding/entanglement. The mechanisms of deformation include elastic and inelastic components, the latter being dominated by the irrecoverable evolution of the texture of the fiber network. In this work, we propose a large strain continuum model for the constitutive behavior of nonwoven fabrics that accounts for the fiber network characteristics responsible for its anisotropic behavior, and captures the effects of deformation mechanisms at the micro-scale (fiber and bonds/entanglement) level. The model comprises a nonlinear elastic component, dominated by the resistance to fiber stretch, and an inelastic component capturing mechanisms of resistance to texture evolution and compaction. For fabrics in which the anisotropy of fiber orientation is combined with random entanglement processes, we propose to capture the combined effects of fibers and junctions orientation distributions using a single tensorial representation of the network anisotropy (fabric ellipsoid). An orthotropic constitutive model for the elastic response of nonwoven fabrics is formulated based on this structural measure and deformation mechanisms of the network structure. The inelastic component of the model is then prescribed in terms of an evolution law for the fabric ellipsoid. A needlepunched web of high strength polyethylene fibers, "Dyneema Fraglight", is selected as the representative material, to be used as a test case to validate the proposed modeling approach. The model is shown to capture the macroscopic nonlinear anisotropic elastic-inelastic response of the fabric in planar deformation, as well as the underlying micromechanical deformation mechanisms, such as fiber stretch, and irrecoverable evolution of fabric texture. The proposed model can be used to predict the mechanical behavior of nonwoven fabrics and can be combined with other continuum models to aid in the design of multi-component structures. In addition, the proposed formulation can be used to model different classes of anisotropic network materials, such as biological tissues, tissue engineering scaffolds, and polymeric materials.

Nonlinear Composites with One and Two Families of Fibers

Gal deBotton
Department Mechanical Engineering, Ben-Gurion University

Gal Shmuel
Department Mechanical Engineering, Ben-Gurion University

It can be shown that for any deformation gradient F and a unit vector N there is a coordinate system where F can be represented as a product R.Fc, where R is a rotation and Fc is expressed in terms of five physically motivated TI invariants [deBotton et al, J. Mech. Phys.~Solids 54, 2006]. These invariants correspond to specific deformation modes. With the aid of this representation, it is demonstrated that under certain loading conditions there are some nonlinear materials for which the exact expression for the macroscopic behavior of a composite cylinder assemblage can be determined. The macroscopic response of the composite to shear in the transverse plane is approximated by application of a sequentially laminated technique. Next, these results are extended to the class of orthotropic composites with two families of fibers. Comparisons of the responses predicted by these effective potentials with linear comparison estimates of Lopez-Pamies and Ponte~Castaneda, phenomenological models for biological tissues, and finite element simulations reveal good agreement.

A Multiscale Model of Fabric Material under Impact

Ben Nadler
Department of Mechanical Engineering, University of Alberta

In recent years, plain woven fabric made of high strength, lightweight fiber has been utilized in a variety of engineering applications ranging from ballistic shields (e.g., soft body armor, aircraft fuselage barriers) to high-performance flexible systems (e.g., parachutes, airbags, sails and geo-textiles). In particular, fabric materials with extremely high strength-to-weight ratio, such as Kevlar® and Zylon®, are rapidly becoming mainstays in ballistic impact and penetration technologies. The mechanical properties of fabric depend crucially on the underlying microstructure, which is determined by the material properties of the constituent yarns and the geometry of the fabric weave.

In this work, a multiscale model for fabric material is introduced. The model is based on the assumption that at the continuum level fabric behaves as a finitely deformable membrane. Moreover, the fabric is assumed to be composed of two families of continuously distributed yarns constrained at all time to occupy a common evolving surface in three-dimensional space. The two families may slide relative to one another on the surface, subject to their respective equations of motion. The constitutive law at the continuum scale is derived from fine-scale considerations. On the fine-scale, the properties of the microstructure are accounted for by locally modeling the plain woven fabric as a pair of initially curved overlapping elasticae under periodic boundary conditions and subject to the constraint of non-penetration. A handshake process is developed to integrate the two levels of analysis. Making use of this process, a robust multiscale finite element-based algorithm is formulated and implemented to solve selected boundary- and initial-value problems.

Experimentally Based Constitutive Laws for Anisotropic Magnetorheological Elastomers

Nicolas Triantafyllidis
Professor
Aerospace Engineering Department, University of Michigan

Sunny Kankanala
Research and Innovation Center, Ford Motor Company

Magnetorheological elastomers (MRE's) are metal particle impregnated rubbers whose mechanical properties can be changed by the application of external magnetic fields. The recently discovered MRE materials are finding an increasing number of applications in aerospace, automotive, civil and electrical engineering fields as vibration damping devices, variable stiffness mounts and so on.

We present the continuum mechanics formulation for these solids using a direct method based on the thermodynamics approach of Coleman-Noll. A specific form of the constitutive law is subsequently proposed that accounts for the anisotropy of these solids, due to their curing in the presence of a strong magnetic field. The constitutive equation parameters are selected from three different types of experiments: uniaxial mechanical and magnetic loading in the direction of the curing field, uniaxial mechanical loading transversely to the curing field and simple shear mechanical loading in the presence of a transverse magnetic field aligned with the initial direction of the curing field. A critical comparison between theoretical predictions and experimental results concludes the presentation.

On Transverse Isotropy of Fiber-Reinforced and Electro-Sensitive Elastomers

Luis Dorfmann
Department of Civil and Environmental Engineering, Tufts University

In this talk we discuss the structure of the strain energy function of transversely isotropic materials, which are characterized by strong directional properties. These materials, characterized by a single preferred direction in the reference configuration, are unaffected by an arbitrary rotation about and/or reversal of this direction. Of particular interest are similarities in the response function of fiber-reinforced elastomers, soft biological tissues and electro-sensitive solids.

For fiber-reinforced elastomers, for example, the required symmetry reduces the strain energy function to dependence of five invariants. These are the three principal invariants of the right (equivalently left) Cauchy-Green deformation tensor and two additional invariants associated with the fiber direction.

The application of an electric field to an isotropic electro-sensitive elastomer introduces a preferred direction analogous to that arising for transversely isotropic elastic solids. The material symmetry requirements are therefore similar. The theoretical foundation, including symmetry requirements of electro-sensitive solids, is contained in recent articles by Dorfmann and Ogden [1] and Bustamante et al. [2]. Following the analysis of such materials given by Spencer [3] and Ogden [4], for example, we define an isotropic electro-sensitive material as one for which the energy function is an isotropic function of the right Cauchy-Green tensor and the tensor product of the electric field vector. The form of the energy function is then reduced to the dependence on six independent invariants. Three invariants are again associated with the Cauchy-Green deformation tensor. The forth invariant is associated with the applied electric field and the remaining two depend on both, the deformation and applied field. For transversely isotropic materials, the counterpart of the applied field is a unit vector so that the associated invariant is omitted form the list.

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Accuracy, Robustness, and Stability of Anisotropic Hyperelastic Constitutive Models for Fiber-Reinforced Soft Biological Tissue

Joerg Helfenstein
Institute of Mechanical Systems, ETH Zurich

Mahmood Jabareen
Institute of Mechanical Systems, ETH Zurich

Edoardo Mazza
Institute of Mechanical Systems, ETH Zurich

Sanjay Govindjee
Institute of Mechanical Systems, ETH Zurich

Biological tissues exhibit complex mechanical behavior related to their inhomogeneity, anisotropy and (near) incompressibility. Many constitutive models have been proposed in the literature incorporating the anisotropic behavior by including the effects of fiber like structures, such as collagen. Due to complex geometries, the mechanics of biological systems is preferably analyzed by numerical methods, such as the finite element method. In this regard we have identified several popular constitutive models [1,2,3] that are often used and appropriate for inclusion in numerical computations using commercial FE packages such as ABAQUS [4]. The first two cited models assume an additive split of the material free energy into the matrix, fiber, and volumetric contributions; the later depends only upon the spherical part of the deformation, whereas the first two parts both depend upon the unimodular right Cauchy-Green deformation tensor. The third model, in contrast, additively splits the log-energy contributions from matrix deformation, fiber elongation, and volume strain. Thus the free energy itself is a multiplicative combination of exponential terms. It is shown that models using a strict split of the strain energy function into distortional (unimodular) and spherical parts can lead to non-physical results at large load, if proper care is not taken in the selection of individual energy terms. In particular, we show that at large loads one needs to ensure, a priori, a proper balance between the energy contributions, due to an unusual volume-fiber interaction in such models as they are normally written. Roughly speaking, the source of the pathology is the fact that in the models the fibers (proportionally) contribute more strongly to the free energy than matrix distortion or volume change; but are insensitive to volumetric changes due the "usual" unimodular assumption. Therefore under certain loading conditions, like large uni-axial loading, it is possible that the material will prefer a spherical response mode in order to reduce the material's free energy—as opposed to providing a uni-axial stretch as would be intuitively expected.In the presentation, we will show exactly how this pathology arises as well as discuss the accuracy, robustness and stability of these models in displacement and mixed formulations for the three constitutive models mentioned above. Numerical examples are used to highlight the differences of these implementations and provide a basis for a critical discussion of the different model formulations.

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Multiscale Large-Deformation Mechanics of Collagenous Tissues: Elasticity and Fracture

Markus J. Buehler
Esther and Harold E. Edgerton Assistant Professor
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Alfonso Gautieri
Graduate Student
Laboratory for Atomistic and Molecular Mechanics, Department of Civil and Environmental Engineering,
Massachusetts Institute of Technology

Here we focus on recent advances in understanding the deformation and fracture behavior of collagen, Nature's most abundant protein material and the basis for many biological composites including bone, dentin or cornea. We show that it is due to the basis of the collagen structure that leads to its high strength and ability to sustain large deformation, as relevant to its physiological role in tissues such as bone and muscle [1-4]. Experiment has shown that collagen isolated from different sources of tissues universally displays a design that consists of TC molecules with lengths of approximately 300 nanometers. Using a combination of theoretical analyses and multi-scale modeling, we have discovered that the characteristic structure and characteristic dimensions of the collagen nanostructure is the key to the ability to take advantage of the nanoscale properties of individual TC molecules at larger scales, leading to a tough material at the micro- and mesoscale. This is achieved by arranging TC molecules into a staggered assembly at a specific optimal molecular length scale. During bone formation, nanoscale mineral particles precipitate at highly specific locations in the collagen structure. These mineralized collagen fibrils are highly conserved, nanostructural primary building blocks of bone [5]. By direct molecular simulation of the bone's nanostructure, we show that it is due to the characteristic nanostructure of mineralized collagen fibrils that leads to its high strength and ability to sustain large deformation, as relevant to its physiological role, creating a strong and tough material. We present a thorough analysis of the molecular mechanisms of protein and mineral phases in deformation, and report discovery of a new fibrillar toughening mechanism that has major implications on the fracture mechanics of bone. Our studies of collagen and bone illustrate how hierarchical multi-scale modeling linking quantum chemistry with continuum fracture mechanics approaches can be used to develop predictive models of hierarchical protein materials. We conclude with a discussion of the significance of hierarchical multi-scale structures for the material properties and illustrate how these structures enable one to overcome some of the limitations of conventional materials design, combining disparate material properties such as strength and robustness [6].

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Planar Radial Extension Testing for Material Identification in Fiber-Reinforced Soft Tissues

Madhavan Raghavan*
Department of Biomedical Engineering, University of Iowa
ml-raghavan@uiowa.edu

Natural and biologically derived planar soft tissues such as arterial wall or tissue-engineered skin tend to be reinforced by microstructural fibers rendering them anisotropic. A-priori knowledge of gross tissue fiber orientations is necessary for performing traditional tests such as planar biaxial extension testing (pulling simultaneously in orthogonal directions) so that the test axes maybe aligned with the fiber axes prior to testing. However, unlike in man-made anisotropic materials, the fiber alignments of these tissues may not be known a priori—especially when the tissues become pathological such as in the case of aneurysms. In this work, planar radial extension testing (PRET) is proposed to simultaneously delineate the underlying directionalities and their property values. The method is demonstrated using both physical testing in a prototype PRET device and through numerical simulations. A force controlled PRET involves applying the same force all around the circumference of the circular specimen and studying the deformed shape. If the specimen becomes elliptical, then the minor axis of the ellipse is its stiffest direction. A numerical simulation of PRET of a circular aortic specimen was performed using a UMAT subroutine (material model: Orthotropic Fung type exponential strain energy density function) in ABAQUS. Under uniform radial loading, the circular specimen deformed into an ellipse. It was found that when a 30 mm diameter circular specimen is pulled via 16 pins around its perimeter, the edge effects dissipates rapidly allowing for a homogeneous stress/strain field within a circular area at the center half (15 mm diameter) suggesting a suitable spot for placement of markers for strain measurements. A PRET system was fabricated using a 40-inch diameter circular block mounted on a table top as the base. A series of 16, 2" diameter pulleys were fixed along the periphery of this base, each 22.5° apart (360°/16). Sixteen suture wires with connector pins to grip the specimen at one end and plastic containers for holding weights at the other end ran over the pulleys. A porcine aortic specimen was tested by gradually increasing the radial force to 2.5N. The specimen changed into a perceptible elliptical shape allowing for the identification of its stiffest direction. Nielsen et al. [1] has reported earlier on a computer-controlled device for radial extension testing of heterogeneous and homogeneous elastic membranes. The methods proposed here allow for an easy and simple way to assess anisotropic soft tissues.

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The Effect of Fiber Dispersion in Fiber-Reinforced Elastic Membranes

Ray Ogden
Professor
Mathematics, University of Glasgow

In a recent paper [1] it has been shown that dispersion in the orientation of collagen fibers can have a very significant effect on the mechanics of soft biological tissue, in particular arterial tissue, as compared with the situation described without dispersion based on the model in [2]. The dispersion examined in [1] has a three-dimensional transversely isotropic nature. In fiber-reinforced membrane structures, in the biomechanics context and elsewhere, it is more appropriate to consider a two-dimensional dispersion of fiber orientations. The purpose of the present work is to set up the theoretical framework for analyzing the effect of fiber dispersion in elastic membranes and to apply the theory to representative examples that illustrate how the dispersion influences the overall mechanical response. Examples include the uniaxial extension of a thin sheet and the extension and inflation of a membrane tube.

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Measurement of the Nanostructural Features in Polymer Nanocomposites

Monon Mahboob
Graduate Research Associate
Mechanical Engineering, The Ohio State University

Stephen E. Bechtel
Professor
Mechanical Engieering, The Ohio State University

Mesoscale performance properties of nanocomposites are dictated by the nanoscale structure developed in the composite during processing. We present a procedure that directly measures the relevant nanostructural features of carbon nanofibers in carbon nanofiber/polymer composites developed in processing. The significant contribution of the research in this paper is the ability to produce quantitative 3-dimensional measurements of the evolution of nanostructure in time and space. Mesoscale performance properties of nanocomposites combine contributions of a sufficient nanostructure volume. To model the development of the mesoscale performance properties one must relate the development of the nanostructure during processing, and relate nanostructure and mesoscale properties. Such a model therefore relates processing to nanostructure development, and relates nanostructure to performance properties. The technique demonstrated in this paper to directly quantify nanostructure from physical measurements enables these two components (relation of processing to nanostructure development and nanostructure to performance properties) to be decoupled, with powerful effect. With nanostructure known from direct measurements the model predictions of nanoscale structure development through processing can be validated and/or refined. Further, with the nanostructure known from measurement, one can isolate and test a model's prediction of mesoscale performance properties as a function of nanostructure. In this study fiber projection dimensions measured in TEM sections provide the complete three dimensional orientation of each fiber. We have benchmarked the method through numerically generated 3D nanostructures. The method is then successfully applied to observe the effect of extensional rheology on fiber orientation.

On Simple Deformations of Fiber-Reinforced Materials According to a Second Gradient Hyper-elasticity Theory

Kostas P. Soldatos*
Theoretical Mechanics, University of Nottingham
kostas.soldatos@nottingham.ac.uk

The continuum theory of finite deformations of elastic materials reinforced by inextensible cords was initiated by Adkins and Rivlin [1], and was further developed by Adkins; they assumed that the cords are embedded in an isotropic material and occupy no volume. The result of their assumptions is that the material becomes a constrained isotropic material and the theory is appropriate for materials in which fibres are sparsely distributed. Following a slightly different approach, Spencer [2] developed a theory in which the fibres are characterized by a unit vector field which defines the fibre direction, it is convected with the material and is treated as a constitutive variable with appropriate invariance properties. These assumptions led to a theory of constrained materials which are locally transversely isotropic; the theory is therefore more appropriate for materials in which fibres are densely distributed.

In [1, 2], as well as in relevant subsequent publications, there is an assumption, either explicit or implicit, that fibres have negligible thickness and they are perfectly flexible. This assumption is a valid approximation in many cases of interest, but is not invariably applicable; the theory cannot account for size effects, such as those due to fibre diameter or fibre spacing. To incorporate fibre bending stiffness effects, Spencer and Soldatos [3] developed recently a second gradient hyper-elasticity theory based on the constitutive assumption that the elastic strain energy depends not only on the deformation and the fibre vectors, but also on the space derivatives of the deformed fibre vector, subject to appropriate invariance requirements. The theory requires the inclusion of couple-stress and non-symmetric stress and, in its most general form, it leads to complicated constitutive equations. Nevertheless, plausible ways of simplifying the obtained equations are also provided in [3], when (i) only gradients related to the curvature of the deformed fibre vector are retained, (ii) in cases involving in addition plane strain deformations, and (iii) in the elucidating case of the linearised (small deformations) theory.

Unlike [1] and [2], the new developments described in [3] are principally based on the assumption that the fibres are extensible and the material is completely unconstrained. However, in appropriate cases, some simplification can still be achieved by introducing the kinematic constraints of inextensibility and/or incompressibility. This presentation deals with the implications that these constraints of material incompressibility and fibres inextensibility have on some simple, large deformations patterns of fibre-reinforced materials, when modelling is based on the theory developed in [3]. Particular attention is paid to large deformations of an elastic circular cylinder reinforced by a family of helices distributed symmetrically throughout the cylinder and the problem of plane strain bending of a rectangular block with a family of straight fibres running parallel to one of its sides.

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Simulation Model for Anisotropic Fibrous Materials

Anna Ask
Graduate Student
Division of Solid Mechanics, Lund Universtity

Matti Ristinmaa
Division of Solid Mechanics, Lund University

Inelastic constitutive models are often needed in order to simulate actual material behavior. Here, a plasticity-based constitutive model for fibrous materials allowing for finite strains is developed. The anisotropic behavior of fibrous materials is modeled by assigning vectors to the material directions and constructing structural tensors to represent planes of material symmetry. Since finite strains are modeled the kinematic description of the deformation of the continuum is based on the multiplicative split of the deformation gradient. A similar approach is used for the substructure, which is represented by the material directions. The deformation of the substructure is assumed to be described by a separate mapping which is also subject to a multiplicative split. For the elastic part of the deformation it is assumed that the continuum and substructure deform together in some sense while the model allows for separate plastic evolution. A consistent spatial formulation based on the logarithmic strain and associated plasticity for the continuum is derived and implemented. Since a spatial formulation is used it is not necessary to make a choice of the intermediate configuration when introducing the multiplicative split.

The orthotropic fibrous structure of industrially manufactured paper material is due to the paper-making process where the fibres tend to align in the direction of motion in the machine. The elastic modulus and yield strength in the paper plane are typically of an order two greater than in the out-of-plane direction. The present model uses a yield function where the anisotropy enters through yield planes related to loading in different directions. The yield plane gradients are described in terms of the material directions. Focus is placed on the in-plane behavior. In order to validate the model finite element simulations are performed for a paper material known as corrugated board which is used to make cardboard boxes. The model is first calibrated against experimental data. Simulations in two and three dimensions are then performed for a part of the manufacturing process. Comparisons with experimental evidences suggest that the model does seem to capture the true behavior rather well.

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Ellipticity and Non-dissipative Solutions in Fiber-Reinforced Nonlinearly Elastic Materials

Jose Merodio
Professor
Continuum Mechanics, Universidad Politecnica de Madrid

Stationary kinks are examined in the context of a base neo-Hookean response augmented with unidirectional reinforcing that is characterized by a single additional constitutive parameter for the additional fiber reinforcing stiffness. In particular, the problem of rectilinear shear of a slab of transversely isotropic incompressible non-linearly elastic material is studied. The analysis focuses on the ellipticiy and non-dissipative status of the discontinuos soluitions.

Micromechanics-Based Failure Surfaces for Debonding of Reinforced Composites

Jay Patel
Graduate Student
Aerospace Engineering, University of Illinois

Helen Inglis
Graduate Student
Mechanical Science & Engineering, University of Illinois

Philippe Geubelle
Professor
Aerospace Engineering, University of Illinois

Henry Tan
School of Mechanical, Aerospace & Civil Engineering, University of Manchester

One of the primary damage modes for composites is failure of the interface between the matrix and the inclusions. Micromechanics models, which seek to provide analytical or semi-analytical solutions for the constitutive response of such reinforced materials, must take particle debonding into account to give physical results. We present a 2D Mori-Tanaka model incorporating nonlinear interface debonding, which captures the damaged constitutive response under any in-plane loading condition. This model provides a powerful tool for understanding the competing effects of material and interface properties, inclusion size and volume fraction on the physics of debonding. Further, compiling the constitutive response for loading paths spanning the principal stress plane allows us to generate failure surfaces. These failure surfaces, analogous to yield surfaces in plasticity, could help engineers in the design of composite structures.

SYMPOSIUM

JJ

Science and Engineering of Self-Healing and Remediation

ORGANIZERS:

B.L. Lee, *Air Force Office of Scientific Research*

David M. Stepp, *Army Research Office*

Douglas Kiserow, *Army Research Office*

Self Healing over All Material Classes: A Dutch Approach

Sybrand van der Zwaag
Department of Aerospace Engineering, Technical University, Delft

Triggered by the inspiring example of encapsulated self healing polymers developed at the University of Illinois (USA), the Delft Centre for Materials at the TU Delft developed a university funded program on self healing materials, covering metals, polymers, civil materials and composites. This program has led to a national Dutch research program on self healing materials, in total leading to no less than 44 postdoctoral positions at various Dutch universities and involving more than 40 companies. Our research not only focusses on the experimental development of self healing materials but also on model based material development.

In this presentation an overview of the Dutch research directions in this challenging field and some recent results will be presented.

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“Self-Healing” Biological Molecules for Use in Engineering Materials

M. Austin Creasy
Graduate Research Assistant
Department of Mechanical Engineering, Virginia Tech

Donald J. Leo
Department of Mechanical Engineering, Virginia Tech

Biological systems demonstrate autonomous healing of damage and are an inspiration for developing “self-healing” materials [1]. Our recent experimental study has demonstrated that a bilayer lipid membrane (BLM) has the ability to “self-heal” after mechanical failure. Recent work has looked at combining biological and synthetic material to make a new class of material that will exploit some of the unique properties associated with the biological materials [2-3]. One proposal for a new material is to use a planar BLM to seal the pores of a porous synthetic material [2]. The BLM is made from phospholipid molecules which are the fundamental building blocks of cell membranes in living organisms and these molecules have a unique property that they spontaneously self assembly into organized structures in an aqueous medium. The BLM forms an impervious barrier to ions and fluid between two volumes and strength of the barrier is dependent on the pressure and electrical field. A previous study to characterize the strength of the BLM showed that the failure pressure is inversely proportional to the aperture size [2]. This paper expands on this subject by characterizing the ability of a BLM to spontaneously reform or “self-heal” after the BLM has failed. The BLM for this study is form from 1-Stearoyl-2-Oleoyl-sn-Glycero-3-Phosphocholine (SOPC) lipids and suspended in the pores of a sub-micron thick silicon nitride membrane. The BLM is pressurized till failure and allowed to self-heal and the entire process is monitored by chrono-amperometry measurement (70 mV DC using Ag/AgCl electrodes). A failure event is characterized by an increase in the measure current from 0.1 nA to 650 nA. Without further pressurization, the lipids self-assemble into a BLM and the current returns to its pre-failure values. It is observed that the failure and self-healing events can be repeated on the BLM multiple times.

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Sub-micron Capsules for Small Size-Scale Self-Healing

Aaron C. Jackson
Graduate Assistant
Materials Science and Engineering, University of Illinois

Benjamin J. Blaiszik
Graduate Assistant
Mechanical Science and Engineering, University of Illinois

Nancy R. Sottos
Professor
Materials Science and Engineering, University of Illinois

Scott R. White
Professor
Department of Aerospace Engineering, University of Illinois

Paul V. Braun
Professor
Materials Science and Engineering, University of Illinois

Current autonomic self-healing technology has the ability to improve the life time of bulk polymers where cracks on the order of tens of micrometers may be present. However, applications such as microelectronics, composites, and thin films may fail when cracks are only hundreds of nanometers in size. As a result, techniques for encapsulating healing agents, dicyclopentadiene (DCPD) and Grubbs catalyst, have been developed to meet these small size-scale requirements. Previously, DCPD has been encapsulated in polyureaformaldahyde using a mixer blade but capsule diameters are limited to larger than 10 m. Grubbs has been encapsulated in wax but minimum diameter sizes are around 50 m and the particles are difficult to work with. For DCPD capsules, sonication and hydrophobes can be used to reduce the diameter to below 1 m. For Grubbs catalyst, polystyrene can be used as the encapsulant making the Grubbs particles more stable in epoxy and easier to work with in general. In addition, silica protection schemes have resulted in important improvements over polymer capsules and particles. Silica-protected capsules and catalyst have the advantage of improved dispersion in epoxy and a better diffusion barrier for enhanced stability. In addition, the silica protection provides a substrate for functionality that could improve the interface between capsules and their surrounding environment.

Two-Part Self-Healing in Epoxy Matrix Composites Utilizing Epoxy Chemistry

David McIlroy
Graduate Assistant
Department of Materials Science and Engineering, University of Illinois

Benjamin J. Blaiszik
Graduate Assistant
Department of Mechanical Science and Engineering, University of Illinois

Mary M. Caruso
Graduate Assistant
Department of Chemistry, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

Scott R.White
Department of Aerospace Engineering, University of Illinois

Paul V.Braun
Department of Materials Science and Engineering, University of Illinois

Jeffrey S. Moore
Department of Chemistry, University of Illinois

Self-healing in an epoxy thermoset matrix is accomplished by use of a novel encapsulation strategy and two-part chemistry identical to that used to create the cured matrix. An aminofunctional curing agent, DEH-52 (Dow Chemical), is encapsulated by interfacial polymerization of toluene diisocyanate (TDI) and diethylenetriamine (DETA), and a solution of Epon 828 (Miller-Stephenson) in hexyl acetate is encapsulated by the urea-formaldehyde system previously described[1]. Healing efficiency is assessed by recovery of fracture toughness. Healing is observed in samples containing microcapsules of DEH-52 and solvent-borne epoxy injected into the crack plane (self-activated test) and in samples containing microcapsules of both DEH-52 and epoxy (in situ test). Here we demonstrate significant healing efficiency with this system. This new two-part self-healing chemistry will extend service life of advanced composites, and presents a substantial cost advantage over previously reported self-healing systems[2].

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Solvent-Based Self-Healing of Polymers

Mary M. Caruso
Graduate Student
Department of Chemistry, University of Illinois

Benjamin J. Blaiszik
Graduate Student
Department of Mechanical Science and Engineering, University of Illinois

Scott R. White
Department of Aerospace Engineering, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

Jeffrey Moore
University of Illinois

A robust catalyst-free self-healing system has been developed using microencapsulated organic solvents. Healing efficiencies of ca. 100% were acheived by embedding microcapsules with urea-formaldehyde shell walls in an epoxy matrix that contained a mixture of unreacted epoxy monomer and solvent. Chlorobenzene, phenylacetate, and ethyl phenylacetate with varying amounts of epoxy monomer were microencapsulated by an in-situ polymerization procedure. The healing event was triggered by a crack propagating through the epoxy matrix to rupture the microcapsules, releasing solvent into the crack plane, and restoring structural continuity to the material. Solvent capsules have also been incorporated into thermoplastic matrices and demonstrated self-healing capability at room temperature.

Microencapsulation of Isocyanates for Self-Healing Polymers

Nancy Sottos
Department of Materials Science and Engineering, University of Illinois

Jinglei Yang
Beckman Institute, University of Illinois

Michael Keller
Beckman Institute, University of Illinois

Scott White
Department of Aerospace Engineering, University of Illinois

Microcapsules containing reactive diisocyanate were synthesized based on interfacial polymerization of polyurethane (PU) prepolymer for development of future self-healing polyurethane coating materials. The isocyanate has potential for healing in humid or wet environments without catalyst. The preparation of PU prepolymer and microencapsulation of isophorone diisocyanate (IPDI) are presented. Microcapsules of 40-400 m in diameter were synthesized by changing agitation rate in the range of 500-1500 rpm. A power relation exists between average diameter of capsules and agitation rate. Smooth outer surface morphology and variable shell wall thickness were investigated by optical and scanning electron microscopy. Shell wall thickness is linearly increased with increasing capsule diameter. High yields (~70%) of a free flowing powder of spherical microcapsules were produced with a liquid core content of 70 wt% as determined by TGA analysis. After manufacturing, microcapsules showed long shelf life of 6 months with only 10 wt% loss of IPDI. Brittle behavior of microcapsules was illustrated by direct compression test, and the normalized strength of capsules presented a power relation with capsule diameter.

Torsion Fatigue Response of Self-Healing Poly(dimethylsiloxane) Elastomers

Michael Keller
Assistant Professor
Mechanical Engineering, University of Tulsa

Scott White
Professor
Aerospace Engineering, University of Illinois

Nancy Sottos
Professor
Materials Science and Engineering, University of Illinois

Incorporating self-healing functionality in a polysiloxane elastomer successfully retards the growth of fatigue cracks under torsional fatigue loading. The self-healing material consists of two microcapsule types embedded in an elastomeric matrix, similar to the material developed by White et al. [1]. One microcapsule species contains a vinyl-terminated poly(dimethylsiloxane) resin and dissolved platinum catalyst compounds. The second capsule species contains a polymerization initiator (methylhydrosiloxane). Quasi-static testing of this composite material demonstrated the capability to routinely recover 70-100% of the original tear strength [2]. Addition of microcapsules also improved the tear strength when compared to the neat elastomer. The ability to heal a dynamically propagating crack is assessed via a torsion fatigue protocol for two different elastomeric matrices. Significant recovery of torsional stiffness occurs after approximately 5 hours, the time required to achieve a measurable degree of cure of the healing agents. Total fatigue crack growth in a self-healing specimen is reduced by 24% in comparison to relevant controls. The retardation of growing fatigue cracks is attributed, in part, to a sliding-crack-closure mechanism [3], where polymerized healing agent shields the crack tip from the applied far-field stress.

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Peripherally Decorated Binary Microcapsules Containing Two Liquids: A Novel Capsule Architecture for Self-Healing Design

Steven Mookhoek
Department of Aerospace Engineering, Delft University of Technology

Benjamin Blaiszik
Department of Mechanical Science and Engineering, University of Illinois

Nancy Sottos
Department of Materials Science and Engineering, University of Illinois

Sybrand van der Zwaag
Department of Aerospace Engineering, Delft University of Technology

Microencapsulation provides the capability to store and protect functional liquids from the external environment and to handle them as solids. Many review articles and books have been published on the subject [1-3], addressing numerous techniques to create a wide variety of liquid filled microarchitectures. Microcapsules having a liquid core can be found in a wide variety of products ranging from carbon copy paper to drug delivery systems, and food additives.

Recently, the use of microcapsules as liquid storage containers inside structural materials has received great interest with the development of self-healing polymer systems. [4] In these systems, microcapsules act as a storage medium for liquid monomers inside a polymer matrix and release their reactive contents upon fracture of the surrounding material. In order to design new microcapsules containing reactive liquid media for self-healing materials, we investigated the possibility of creating capsules releasing two reactive liquids upon capsule failure.

In this work, we used 1.4 m dibutylphthalate (DBP) filled urea-formaldehyde (UF) microcapsules as solid emulsion stabilizers [5] to create 140 m binary microcapsules containing two encapsulated liquid phases within a single structure. These binary microcapsules with dicyclopentadiene (DCPD) as the core phase were made by encapsulating the dispersed DCPD liquid (stabilized with the UF(DBP) microcapsules in water) via an isocyanate-alcohol interfacial polymerization reaction. We confirmed the novel capsule architecture by fluorescent optical microscopy and scanning electron microscopy (SEM). Our experiments show that the the morphology of the resulting microcapsule has a central liquid core decorated at its periphery with a layer of smaller microcapsules containing the secondary liquid. The presence of both the encapsulated liquids within a single capsule structure was demonstrated by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). DSC data analysis indicated a DBP volume fraction of 8.8 %. This value is in good agreement with the calculated theoretical fraction on the basis of the observed architecture and dimensions.

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Enhancing Liquid-Based Self-Healing Composites via Anisotropic Capsule Geometry

Steven Mookhoek
Department of Aerospace Engineering, Delft University of Technology

Hartmut Fischer
Department of Materials Performance, TNO Science and Industry

Sybrand van der Zwaag
Department of Aerospace Engineering, Delft University of Technology

Liquid encapsulation was one of the first approaches to generate self-healing in polymer systems. In the early approach spherical capsules, containing reactive resin or monomer, were embedded as attributes in a matrix material [1]. When fracture or crack formation occurs the embedded containers break and liquid will flow out into the crack-plane where it undergoes a chemical reaction to crosslink and bridge the crack faces. This will redistribute local stresses at the crack-tip and therefore stop the propagation of damage. A disadvantage in this concept relates to the damage sensing efficiency of the system. It seems that a random distribution of spherical capsules in a matrix material has a relatively low sensing capability. The isotropic geometry of the capsules together with their random distribution namely results in a low probability of a propagating crack hitting a capsule. Furthermore, the amount of liquid resin released from the spherical capsule is relatively small. When changing the geometry of the containers from spherical to anisotropic structures, e.g. fibres, the fracture probability increases. Hence, liquid epoxy filled hollow fibres have been used successfully for self-healing composites [2,3], following large scale damage. Two major drawbacks of using hollow fibres, i.e. a one compartment container, are bleeding (the release of excess reactive agents) and clotting (the propagation of the repairing reaction into the stored agent still in the hollow fibre. In order to design more efficient and reliable liquid containers for Self-Healing systems we theoretically examined the self-healing liquid release as function of capsule size, geometry and concenration. The research that we present here, shows the design and application of a numeric statistical model to determine the healing efficiency of liquid based self-healing systems as function of these parameters. By changing the capsule geometry from classical spherical objects into anisotropic cylindrical objects our model shows that, for an equal capsule size, capsule concentration and distribution, a large increase in theoretical efficiency is found, close to a factor of 1.7. When we also adjust other variables such as: capsule concentration, capsule aspect ratio and capsule order parameter we are able to optimize the healing efficiency of liquid-based systems based on capsule size and geometry. Currently we are validating our model by examining capsule-composite fracture surfaces and are developing actual anisotropic capsules through an earlier demonstrated method. [4]

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Self-Healing Adhesives

Scott White
Professor
Aerospace Engineering, University of Illinois

Henghua Jin
Mechanical Science and Engineering, University of Illinois

Gina Miller
Aerospace Engineering, University of Illinois

Nancy R. Sottos
Professor
Materials Science and Engineering, University of Illinois

Thin epoxy adhesive films are widely used in the aerospace industry for composite laminate repairs of metal structures. A self-healing epoxy adhesive film has the potential to increase the service life of both the laminate repair and the parent structure. In this study, two self-healing epoxy adhesive systems are developed based on film matrices of an unsupported commercially available adhesive FM®73 and EPON" 828/DETA (diethylenetriamine). A two-part self-healing system of dicyclopentadiene (DCPD) loaded microcapsules and Grubbs' catalyst particles is considered. Recovery of mode I fracture toughness is assessed using width tapered double cantilever beam (WTDCB) test specimens. Healing efficiencies ranging from 25-75% are measured for control and in situ specimens. Scanning electron micrographs of fracture surfaces reveal that high healing efficiencies are obtained for adhesives that fail in a cohesive manner.

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Multiscale Cohesive Failure Modeling of Self-Healing Adhesives

Mohan Kulkarni
Department of Aerospace Engineering, University of Illinois

Philippe H. Geubelle
Professor
Department of Aerospace Engineering, University of Illinois

Karel Matous
Computational Science and Engineering, University of Illinois

Scott R. White
Professor
Department of Aerospace Engineering, University of Illinois

Adhesive joints are often considered as the weak link in bonded structures. To improve the mechanical performance of heterogeneous adhesives, the thermoset polymer-based adhesives have been combined with several reinforcements such as rubber particles, glass fibers, carbon nanotubes, nanoparticles. Beyond the improvement of mechanical properties, the second-phase constituents can also introduce multi-functionality in adhesives. For example, Miller [1] embedded micro-capsules filled with a healing agent and a living catalyst in an epoxy-matrix to extend the fatigue life of adhesives by incorporating the self-healing capability.

A multi-scale cohesive scheme [2] with the ability to relate the failure processes occurring at the micro-scale to the macro-scale homogenized cohesive constitutive behavior of heterogeneous adhesives has been developed. In this work, we use this multi-scale scheme to model failure phenomena within self-healing adhesives. The discrete cracking in quasi-brittle epoxy matrix is modeled using a cohesive segments method based on generalized finite element method [3]. This method allows a discontinuity to pass through a finite element thereby making the crack path independent of the mesh structure. The micro-capsules containing the healing agent are replaced by a micro-sphere of equivalent constitutive properties.

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Self-Sealing Fiber-Reinforced Composites

Jericho Moll
Materials Science and Engineering, University of Illinois

Nancy Sottos
Professor
Materials Science and Engineering, University of Illinois

Scott White
Professor
Aerospace Engineering, University of Illinois

Fiber reinforced composite tanks provide a promising method of storage for liquid oxygen and nitrogen for aerospace applications [1]. The inherent thermal fatigue of these vessels leads to the formation of microcracks, which allow gas phase leakage across the tank walls. Self-healing functionality provides a potential solution to this problem. The integration of an encapsulated dicyclopentadiene (DCPD) monomer and wax protected Grubbs' catalyst into an epoxy matrix has shown the ability to self-heal micron scale crack damage in polymeric materials [2, 3]. As a crack propagates through the polymer, microcapsules rupture and release the monomer, which comes into contact with the embedded catalyst and polymerizes in the crack plane. The incorporation of this healing chemistry into a fiber reinforced epoxy composite provides the necessary functionality for autonomic sealing of crack damage subject to modest pressures. In this work, sealing is assessed through the use of a pressure cell apparatus to detect nitrogen flow through the thickness direction of a damaged composite. A controlled amount of microcracking is introduced through cyclic indentation of one surface of the composite. The resulting damage zone is proportional to the indentation load. Using several sizes of DCPD microcapsules and wax encapsulated Grubbs catalyst, we demonstrate efficient self-sealing of a plain weave E-glass epoxy composite. For larger capsule sizes, 100% of the self-healing composite panels fully sealed with no leaking, compared to 0% of the control panels with no healing ability.

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Self-Healing of Impact Damage in Structural Composites

Amit Patel
Department of Materials Science and Engineering, University of Illinois

Scott R. White
Department of Aerospace Engineering, University of Illinois

Eric D. Wetzel
Multifunctional Materials Branch, Army Research Laboratory

Nancy R. Sottos
Department of Materials Science and Engineering, University of Illinois

Fiber-reinforced composite laminates with polymeric matrices are extensively used in many structural applications. Despite successful implementation, their susceptibility to damage due to transverse impact loads remains a major limitation. Low-velocity or ballistic impact events can create significant matrix damage that is often hidden and difficult to repair. In this study, fiber-reinforced composites with self-healing, polymeric matrices are under investigation for the repair of impact-induced damage. The self-healing system based on dicyclopentadiene and 1st generation Grubbs' catalyst, as described by White et al. [1] and Rule et al. [2], is incorporated in a woven S2 glass reinforced epoxy composite using a hand lay-up technique. Low-velocity impact tests reveal that self-healing materials are able to repair large portions of delaminations. Fluorescent labeling of matrix damage combined with image processing shows that total crack length per imaged cross-section is reduced by 51% upon self-healing. Closer inspection of damage with SEM and optical microscopy also shows clear evidence of damage repair. In addition, self-healing panels tested by a compression-after-impact protocol exhibit significant recovery of maximum tangent stiffness and load at maximum tangent stiffness.

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Interfacial Self-Healing for Advanced Composites

Benjamin J. Blaiszik
Department of Mechanical Science and Enginering, University of Illinois

Brett A. Beiermann
Department of Materials Science and Engineering, University of Illinois

Scott R. White
Department of Aerospace Engineering and Beckman Institute for Advanced Science, University of Illinois

Nancy R. Sottos
Department of Materials Science and Engineering and Beckman Institute for Advanced Science, University of Illinois

A method was developed for sequestration of healing agent filled microcapsules and catalyst to the fiber-matrix interface region in single fiber composites. Interfacial self-healing was assessed through a combination of microbond and pullout tests for model steel wire-PDMS specimens and single glass fiber-epoxy specimens. A custom-made testing frame was built, and mounted under an optical microscope to provide simultaneous load-displacement and optical observation of the crack front propagation during debonding and subsequent healing events. We investigate the effects of healing agent capsule and catalyst concentrations on recovery of interfacial strength and fracture energy. Since microcracking and interfacial failure is one of the key failure mechanisms in composite materials, healing this damage at such an early stage may allow for a substantial increase in expected lifetime by preventing catastrophic growth of smaller flaws.

Autonomous Restoration of Polymer Barrier Coatings

Natalia Sitnikova
Aerospace Engineering, Delft University of Technology

Steven D. Mookhoek
Aerospace Engineering, Delft University of Technology

Hartmut R. Fischer
Materials Performance, TNO Science & Industry

Sybrand van der Zwaag
Aerospace Engineering, Delft University of Technology

Development of self-healing coatings which are sensitive to the changes in the local environment could open a way for the manufacturing of new generation of high-tech functional materials. Such protective coatings can be composed of active components for appropriate response of the surface properties to outer impacts.

In this work we discuss a possibility to develop more sustainable barrier coating which could repair its surface properties if protective properties are lost by damage. A protective coating that consists of polymer blend has been explored. The work concentrates on systematic study of the surface and bulk properties of polymer films during isothermal annealing at different temperatures. An increasing of the ambient temperature plays a role of external trigger mechanism that activates phase separation within the system and initiates a migration of more mobile component with a lower surface free energy towards the surface. Subsequent hardening of this component may lead to the reformation of the protective surface. These particular self-restoring coatings may be used in the gas scrubber as barrier liners preventing corrosion of steel constructions in highly aggressive environment.

In Situ Self-Healing via Microvascular Networks

Andrew Hamilton
Research Assistant
Mechanical Science and Engineering, University of Illinois

Nancy Sottos
Professor
Materials Science and Engineering, University of Illinois

Scott White
Professor
Aerospace Engineering, University of Illinois

Healing in biological systems is accomplished by a pervasive vascular network that supplies the necessary biochemical components. Recent advances in soft lithographic and direct-write assembly methods have enabled the creation of materials with complex embedded microvascular networks that emulate many of the key responses of biological vascular systems. Toohey et al. [1] have applied this concept to heal crack damage in a brittle coating on a ductile substrate. Healing agent is delivered to cracks in the coating via a three-dimensional microvascular network embedded in the substrate, which remains undamaged. In the current work, we explore the interaction of cracks with the microvascular network and the ability to repeatedly heal the damaged network in situ. A testing protocol based on the double cleavage drilled compression (DCDC) fracture specimen geometry [2] is adopted to induce stable crack growth through a microvascular network of channels containing the sequestered components of a two-part epoxy system. When released into the crack plane, the two components mix and cure, forming a bond between the crack faces. We demonstrate recovery of up to 55% of the virgin fracture toughness and as many as 15 healing cycles in a thermosetting epoxy matrix material.

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Self-Healing Materials with Interpenetrating Microvascular Networks

Christopher Hansen
Predoctoral Fellow
Department of Materials Science and Engineering, University of Illinois

Kathleen Toohey
Post-doctoral Research Associate
Department of Bioengineering, University of Illinois

Willie Wu
Graduate Research Assistant
Department of Materials Science and Engineering, University of Illinois

Jennifer Lewis*
Department of Materials Science and Engineering, University of Illinois
jalewis@uiuc.edu

Recent work on self-healing materials has focused on a shift from one-time healing to the possibility of repeated healing, which can be achieved with embedded microvascular networks [1]. Prior work focused on a coating/microvascular substrate architecture in which the coating contains catalyst particles and the microchannels housed a healing agent. Here, for the first time, we create a coating/microvascular substrate architecture that consists of an interpenetrating network of microchannels that deliver a two-part epoxy system for surface crack healing. This interpenetrating network design is produced by direct-write assembly [2] of two fugitive organic inks, with differing temperature-sensitive rheological properties. Upon crack formation during mechanical testing, each constituent of the two-part epoxy system flows into the crack plane via capillary action, where they mix and undergo curing resulting in restoration of coating's fracture toughness. Through this new design, we demonstrate repeated healing of these polymeric structures.

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Biomimicry of Plantae Vascules in the Development of Self-Healing Composite Structures

Richard Trask
Aerospace Engineering, University of Bristol

Ian Bond
Aerospace Engineering, University of Bristol

This paper presents the first investigation into the concept of creating a Plantae inspired vascular network within a fibre reinforced polymer composite laminate which provides an ongoing self-healing functionality but does not incur a mass penalty. Through the application of a loss-wax technique, parallel hollow channels, similar to 'ray cells' in ring porous hardwoods, were successfully introduced within a carbon fibre reinforced epoxy polymer composite laminate. Their influence on the surrounding composite fibre architecture (i.e. introduction of fibre waviness and resin rich pockets) was characterised and assessed both experimentally using a compression-after-impact test methodology, and analytically by applying finite element analysis. It has been shown that impact damage can interact with the network thereby releasing any healing potential stored within these vascules. Furthermore, the non-linear response of damaged specimens when subjected to a compressive load, coupled with microscopic investigation, suggests that internal damage propagates towards and into the open channel network prior to catastrophic failure. Following this new understanding, better bioinspired composite materials can be designed which harness the inherent damage tolerant capabilities to 'direct' a propagating crack into a predetermined healing feature.

Vascular Networks for Self-Healing in Composite Sandwich Panels

Ian Bond*
Aerospace Engineering, University of Bristol
I.P.Bond@bristol.ac.uk

Hugo Williams
Aerospace Engineering, University of Bristol

Richard Trask
Aerospace Engineering, University of Bristol

Composite sandwich construction offers a competitive design option for advanced structures subject to bending or compression loading. However, low-velocity impact damage can have a detrimental effect on the performance of these structures, with the primary damage mode being a cohesive disbond in the core just under the impacted face with consequent loss of skin stability. Residual strengths well below 50% of the undamaged value have been reported in flexure-after-impact of beam specimens [1]. The loss of skin support has also been shown to reduce the compressive strength of sandwich panels by over 25% [2]. An alternative, bioinspired, approach from 'traditional' damage tolerant designs is to provide an ability to self-heal [3] via a vascular network [4]. This approach has been shown to recover failure mode and load in sandwich beams subject to flexure-after-impact [5]. In the latter case, a simple vascular network was introduced into the foam core of a composite sandwich structure. Rupture of the channels by impact damage allowed the healing agent to infiltrate the damage and cure. This work discusses a compression-after-impact test configuration, improved manufacturing technique and a tailored network layout.

Vascular sandwich cores were manufactured by bonding silicone tubing in channels between two sheets of Rohacell closed-cell foam. Riser holes were formed through the foam and tubing at strategic points to connect the silicone supply channels to the skin-core bond region. Pre-impregnated [0,90]S unidirectional E-glass/epoxy laminates were co-cured onto the vascular core. Samples were sectioned into specimens (60x90mm) and the edges ground flat and perpendicular. Each specimen contained five supply vessels feeding a total of 18 risers. Impact damage (3J) was introduced using an Instron Dynatup 9250HV drop tower. Self-healing specimens were simultaneously infiltrated with both an epoxy resin and the corresponding hardener in adjacent supply tubes prior to impact and allowed to heal for 48 hours after impact. Edgewise compression tests were performed under displacement control according to ASTM C364.

The impact, although leaving virtually no visible damage, reduces the failure load to 70% of the undamaged load. The self-healed specimens recover 82% of the undamaged load but destructive sectioning showed the presence of uncured healing agent in the damaged area. When the damage was infiltrated with a pre-mixed resin, the undamaged strength was fully recovered. These data and observations suggest that the reason for the incomplete recovery in the self-healed specimens in the failure of the resin system to fully cure, most likely because of inadequate mixing between resin and hardener. Work continues to overcome this challenge and assess the effect of the network on the basic panel properties.

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Preparation and Properties of a Remendable Coating Concept Based on the Retro-Diels Alder Reaction

Marielle Wouters
Innovative Materials, TNO Science and Industry

Hartmut Fischer
TNO Science and Industry

Niki Stroeks
TNO Science and Industry

Eric Craenmehr
TNO Science and Industry

Key properties of organic coatings, like for instance mechanical strength, solvent resistance and barrier properties are greatly influenced by the polymeric structure in the coating layer. In general, a 3-dimensional polymeric network gives the best properties and therefore most performance coatings have a 3-dimensional network structure. But upon damage these systems are not easily repaired.

Through molecular design in combination with different synthetic routes, a series of new building blocks containing Diels-Alder reaction products for coatings were prepared that are capable to repair a damaged layer by the formation of a covalent bond upon cooling of the coating formulation in a heating-cooling cycle. These cycles and hence repair actions can be repeated many times without noticeable detoriation of the general coating properties. By the incorporation of various functionalities like mechanical properties, optical appearance and processing properties the properties of the final coatings can be tuned. This can lead to completely formulated industrial useable coating formulations.

The self-healing concept was shown by various techniques, and it was proven that the processing window for the different formulations can be tuned. The thermally remendable crosslinked materials show an interesting potential for coatings in various applications, other areas of applications are also possible but are beyond the scope of this contribution.

Self-Healing Composites

Sia Nemat-Nasser
Distinguished Professor
CEAM/Mechanical and Aerospace Engineering, University of California, San Diego

A material that can heal its micro-cracks is of great utility where access for manual repair is limited or impossible, as in a biological implant or a material that is launched into orbit in the solar system. Structures made of such a material may have significantly prolonged service life in addition to improved safety if failure mechanisms such as cracking can be repaired in-situ. We focus on a novel self-healing polymer which is strong, tough, and forms a high degree of thermally reversible, covalent cross-links. Mechanical failure of this polymer occurs preferentially along these cross-links, and due to the reversible nature of this bond it may be repaired by application of moderate pressure and heat. We have produced this polymer and have shown its healing ability experimentally, using compression-induced stable cracking of relatively long and slender samples of rectangular cross section containing a central hole, with cracks made to grow in the compression direction axially along the length of the specimens. These cracks are then healed and the test is repeated. In this manner the fracture strength of the healed sample is experimentally measured and the results are compared with model estimates. We have observed that healing at reasonable temperatures, 85 to 95°C, after repeated fracture-healing cycles, for as little as 30 minutes results in full fracture toughness recovery. We have also processed small samples of carbon and glass reinforced composites using this polymer, and have shown quantitatively that microcracks created in the composite through thermal cycling can be healed. It thus appears that this class of polymers offers an excellent opportunity for creating self-healing composites with the potential for a variety of important applications.

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Fabrication of a Self-Healing Composite Using a Thermally Mendable Polymer and Carbon Fabrics

Jong Se Park
PhD Candidate
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles
jongsepark@ucla.edu

H. Thomas Hahn
Department of Mechanical and Aerospace Engineering, University of California, Los Angeles

Since a self-healing composite with a thermally mendable polymer has multiple cycles of healing capability, it has a big advantage compare to other one-time healing methods. Also their healing processes do not need any extraneous catalysts or micro-particles and thus will not bring to the system any other compounds that may compromise the performance of the materials. Chen et al. [1] reported a group of polymers, mendomers, which exhibit a remendable property upon heating using the reversible Diels-Alder reaction. This polymer can be healed by resistive heating using graphite fiber networks [2-3]. In addition, matrix damages can be located by monitoring changes in electrical resistance using the same networks [4].

In spite of all advantages, a real mendomer/graphite composite hasn't fabricated yet because of the difficulties in the synthesis and mass production of mendomers. Different from other thermosetting polymers, mendomers are solid state powders at room temperature, which make the fabrication process harder. To show the possibility of a mendomer as a matrix of a composite, a two-layer 10×10 cm composite panel with a mendomer and carbon fabrics was fabricated. Medomer powders were distributed on carbon fabrics and cured inside an autoclave with the curing cycle decided by thermal characterizations using digital scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Microcracks are induced by 3-point flexural tests on a mendomer matrix surface of coupon samples followed by electrical resistive heating using graphite fiber networks. The healing behavior is observed under an optical microscope as a function of time at the healing temperature. The self-healing composite exhibits a reasonable healing ability evidenced by the shrinkage or disappearance of microcracks on the surface observed by a scanning electron microscope (SEM). Also healing efficiency of the self-healing composite which is defined by a ratio of failure strains before and after healing is calculated from 3-point flexural tests with a long distance microscope and composite coupons.

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Development of a Healable Carbon Fiber Composite Using a Reversibly Cross-Linked Polymer

Anthony Starr
President
R&D, SensorMetrix

Timothy Perram
R&D Engineer
SensorMetrix

Thomas Darlington
Sr. Vice President
nanoComposix

Steven Oldenburg
President
nanoComposix

Richard Baldwin
Sr. Scientist
nanoComposix

Thomas Hahn
Professor
Mechanical & Aerospace Engineering, University of California, Los Angeles

A new class of polymers has been developed with the ability to repair internal cracking[1]. This was accomplished this by synthesizing a polymer based on a thermally reversible Diels-Alder (DA) and retro-DA cycloaddition. The monomer linkages, or cross-links, are formed by DA cycloaddition and exhibit the retro-DA reaction and hence enable a form of healing to occur. The mechanical properties of the polymer are comparable to those of commercial epoxies used in FRPs. It is desired to incorporate this new polymer as the matrix phase in a CFRP to create a healable carbon fiber composite. Progress on production of the required constituent monomers, infusion and polymerization into carbon fiber performs, and preliminary data demonstrating healing of CFRP samples is reported.

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Modeling of Matrix Damage Healing in Fiber-Reinforced Composite Materials Containing Embedded Shape Memory Wires

Ton Bor*
Departments of Mechanical Engineering and Production Technology, University of Twente
T.C.Bor@utwente.nl

M.S.R. Parlapalli
Departments of Mechanical Engineering and Production Technology, University of Twente

L. Warnet
Departments of Mechanical Engineering and Production Technology, University of Twente

R. Akkerman
Departments of Mechanical Engineering and Production Technology, University of Twente

A. de Boer
Department of Mechanical Engineering and Applied Mechanics, University of Twente

The geometrical and thermal conditions for (self) healing of matrix damage in continuous fiber reinforced composite materials containing embedded shape memory wires are investigated. Upon (local) heating the contracting action of pre-strained shape memory wires supports the healing / welding of a damaged region in a thermoplastic matrix. Several types of shape memory wire distributions are considered. A damaged region includes matrix cracks and delaminations. The healing model takes into account the constitutive behaviour of the fibers, the thermoplastic matrix and the shape memory wires as a function of stress, temperature and time. The progress of the healing of the damaged regions is based on a reptation model that uses the local temperature and pressure exerted onto the crack / delamination sides by the contracted shape memory wires. The effect of manufacturing related residual stresses is included.

Nanoscale Characterization of Self Healing in Iron-Based Model Alloys

Shangming He
R3, Faculty of Applied Sciences, Delft University of Technology

N.H. van Dijk
Assistant Professor
R3, Faculty of Applied Sciences, Delft University of Technology

H. Schut
Assistant Professor
R3, Faculty of Applied Sciences, Delft University of Technology

S. van der Zwaag
Professor
R3, Faculty of Applied Sciences, Delft University of Technology

Steels are among the most widely used construction materials as their mechanical properties can be tailored to obtain the required combination of strength and formability. However, in highly demanding applications the lifetime until failure of steels is limited due to the accumulation of damage. This damage causes the formation of ultrafine cracks that subsequently grow and finally lead to fracture of the components. The primary goal of our research is to achieve self healing of ultrafine cracks in iron-based B and Cu containing alloys by the formation of nanoscale precipitates at the crack surface to significantly enhance the creep lifetime. In order to investigate the self-healing behaviour in these model alloys on a fundamental level we are using radiation techniques (positron annihilation spectroscopy, small-angle neutron and X-ray scattering) in combination with thermo-mechanical testing.

New Self-Healing Polymers Based on DA/rDA Reactions

Bui Tien Dung*
Fundamentals of Advanced Materials, Technical University Delft
t.d.bui@tudelft.nl

Theo Dingemans
Fundamentals of Advanced Materials, Technical University Delft

Self-healing polymers based on monomers and pre-polymers bearing reactive functional groups with thermally reversible functionalities have been synthesized and characterized. Thermally reversible reactions, particularly the Diels-Alder/retro Diels-Alder reaction, for linear copolymers (AB)n, containing low Tg "soft-block" segment oligomers or polymer segments, were designed and synthesized. Our reactive monomers and oligomers were functionalized with furfuryl alcohol or furfurylamine "dienes" and maleimides acting as the "dienophile". The thermo-reversible linear copolymers were prepared either in solution or melt at temperatures between 700C and 900C by combining stoichiometric quantities of the maleimide-functionalized moiety and the furan-functionalized moiety. The structure of the polymers was confirmed using 1H-NMR spectroscopy. The thermal behavior (Tg and Tm) and reversible polymerization characteristics were evaluated by DSC and DMTA. The molar mass of our products was investigated with GPC using CHCl3 as the eluent. We will report on the synthesis and thermal polymerization/de-polymerization behavior of our new polymers.

Shape Memory Alloys—Mechanisms, Multifunctionalities, and Applications

SYMPOSIUM
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ORGANIZERS:

Ibrahim Karaman, *Department of Aerospace Engineering, Texas A&M University*

Dimitris C. Lagoudas, *Department of Aerospace Engineering, Texas A&M University*

Huseyin Sehitoglu, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Shape Memory Alloy Composites: Modeling and Experiments

E. Patoor
4, rue Augustin Fresnel, LPMM/ENSAM

Shape memory alloys (SMA) are widely used to develop smart composites. Experimental characterisation and modelling the behaviour of such materials are key issues. This presentation deals with new results obtains within the MAFESMA project. This project belongs to the European Science Foundation Eurococores programme Smart Structural Systems Technologies (S3T).

Two different cases are considered, the shape memory alloys can be used as fibre to give new functionalities to the composite or it can be the matrix itself. In this last case the nature of the precipitate within this SMA matrix is important. Micromechanical modelling is used to capture the influence of the behaviour of these precipitates (elastic or elasto-plastic) on the overall composite response.

Different topics will also be addressed in this presentation like interfacial debonding and two-way memory effect observed in elastomer/superelastic NiTi composite.

Porous Shape-Memory Alloys

David Dunand
James and Margie Krebs Professor, Co-Director of the Central Laboratory for Materials and Mechanical Properties (CLaMMP)
Department of Materials Science and Engineering, Northwestern University

NiTi foams are of interest for biomedical implants (because of their biocompatibility, low stiffness and bone infiltration of the porosity), actuators (because of light weight and high surface area increasing heat transfer) or energy-absorbing devices (where the collapse of the pores adds to the naturally high damping properties of NiTi).

This talk provides an overview of our work in the area of porous NiTi with either shape-memory or superelastic properties. We first review processing techniques based on powder metallurgy using prealloyed NiTi powders, with argon expansion or salt space-holder to form closed or open porosity. We then describe the microstructure and architecture of these foams, based on 2D cross-sections or 3D tomographic reconstructions. We finally report on the foam thermo-mechanical properties observed in compression, as well as synchrotron X-Ray diffraction results of phase fraction as a function of stress in superelastic foams.

Multiscale Characterization of Shape Memory Alloys Using Digital Image Correlation

Keith Gall
Research Assistant
Department of Mechanical Engineering, Northwestern University

L. Catherine Brinson
Professor and Chair
Department of Mechanical Engineering, Northwestern University

Shape Memory Alloys (SMA's) refer to a class of materials whose ability to recover large inelastic deformation has enabled a variety of unique mechanical designs ranging from biomedical devices to aerospace components. To accommodate the large macroscopic strains associated with the Shape-Memory (recovery upon heating) and Psuedo-elastic (recovery upon removal of applied stress) response, these materials rely on a reversible, phase transformation within the material's crystallographic structure [1]. The onset of this phase transformation is dependent on the elemental composition, processing technique (microstructure/ grain size/ precipitates), thermal conditions, and applied stresses. To date, much of the research aimed at characterizing the thermo-mechanical performance of these materials is based on empirical macroscopic data or micromechanics based macroscopic models. However, recent advances in personal computing and digital imaging have given rise to a technique that provides a closer connection between the material microstructure and the observed macroscopic behavior. Popularized by the experimental mechanics community, Digital Image Correlation uses digital images captured during material deformation and applies search and track algorithms to generate displacement and strain field maps of the material's surface [2]. In particular, the study presented here uses high resolution imaging (1392x1040 pixels) at both 5x optical magnification and at low magnification, to provide a details of localized strain behavior during the stress induced phase transformation in polycrystalline (200 micron grain) Nickel-Titanium SMA samples.

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In Situ Strain Field Measurements during Intermartensitic Transformations

Christos Efstathiou
Department of Mechanical Science and Engineering, University of Illinois

Huseyin Sehitoglu
Department of Mechanical Science and Engineering, University of Illinois

Jay Carroll
Department of Mechanical Science and Engineering, University of Illinois

John Lambros
Department of Aerospace Engineering, University of Illinois

Hans J. Maier
Department of Mechanical Engineering, University of Paderborn

Using insitu digital image correlation to obtain full-field measurements, we studied the intermartensitic transformations in single crystal NiFeGa. Full-field strain measurements identified the coexistence of modulated martensite phases during the first plateau of the multistage stress-strain curve at room temperature. At a higher temperature, the measurements indicated the bypassing of one of the modulated phases. Strain as high as 13% was measured as a result of the transformation to the intermediate monoclinic modulated and final tetragonal phase. Based on the full-field strain measurements, the phase fractions during the nucleation and the progression of the transformation were obtained. The evolution of the local strain and the phase fractions proved critical in explaining strain softening, hysteresis and other phenomena observed in the stress-strain curves. These results, obtained from DIC, would prove difficult and in some instances impossible to obtain using other conventional techniques. The DIC technique has far-reaching implications for phase identification, strain measurements, and heterogeneous deformation in new materials displaying complex mechanical response.

Transformation Memory Effect of Titanium-Based Shape Memory Alloys

Ji Ma
Department of Mechanical Engineering, Texas A&M University

Ibrahim Karaman
Department of Mechanical Engineering, Texas A&M University

During superelastic loading of certain shape memory alloys (SMAs) under ambient conditions, a transformation memory effect can be observed. When incrementally larger strain is applied in successive load-unload cycles, the stress-strain path of and any two successive cycles do not coincide except at one point—the precise stress and strain values at which the cycle with the lower strain was unloaded. This point is referred to as a "memory" point, and is maintained as long as the specimen is not heated above a certain temperature. When the material is strained in such an incremental fashion, with the exception of the very first cycle, all subsequent cycles exhibit a two-stage loading behavior, where the slope of the loading curve would suddenly increase in the middle of the transformation stage to meet the memory point before decreasing back to the expected slope for the phase transformation process. This behavior has been described previously in a NiTi shape memory alloy by Euken and Duerig [1], and has now been observed in the present TiNb SMAs. Not only is this phenomenon interesting scientifically in understanding the nature of martensitic transformation, but it also holds practical significance in that the precise memory of a point, which correspondences to a certain stress and strain value, can be used in precise control of mechanical systems.

We have concluded that the existence of memory points is caused by preferential nucleation and propagation of martensite in certain sections of the austenite phase. Namely, for any given mode of deformation, the material "knows" which section of the material to transform in order to achieve a certain strain level, and will repeat the transformation in the same section if strain is not increased to a higher level. If a higher strain is applied, the old sections will transform first until the memory point is reached, at which point new sections of the austenite must transform. In fact, any given section can be stabilized relative to other sections by repeated cycling to a corresponding strain level. We suggest this to be a universal mechanism in SMAs, but its activation requires the presence of certain microstructural features. The origin of this behavior is most likely diffusion-based, and a consequence of the point defect structures. In this talk, we will demonstrate the aforementioned concept in both TiNb and NiTi SMAs and its time and temperature dependence. We will also present a model to describe this behavior.

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Actuation and Transformation Characteristics of Pd-based High Temperature Shape Memory Alloys

Parikshith Kumar
Graduate Student
Materials Science and Engineering, Texas A&M University

Dimitris C. Lagoudas
Professor
Aerospace Engineering, Texas A&M University

High Temperature Shape Memory Alloys (HTSMAs) are a new class of SMAs capable of operating at temperatures higher that 100°C [1]. These alloys are formed by addition of palladium, platinum, hafnium, zirconium or gold to binary NiTi [2, 3]. Early work on TiPdNi compositions, have studied the transformation behavior of these alloys by studying the SME and pseudoelastic behavior [3]. Results from early studies on HTSMAs as well are recent investigations of the actuation characteristics (i.e. the ability to do work through the SME) have shown that the maximum actuation strain observed in these HTSMAs is approximately 3.0%. To improve the actuation behavior, it is crucial to understand the effect of different processing methodologies on the microstructure.

The focus of the current work is to study the actuation characteristics and the cyclic actuation behavior of a TiPdNi HTSMAs. For this purpose alloy ingots were processed by a vacuum arc melting and were subsequently hot rolled. Preliminary DSC study was performed to obtain the transformation temperatures of the alloy. Compression and tension specimens were fabricated and a high temperature setup for testing was assembled on a MTS. The actuation behavior under different constant load levels, for different applied levels of pre-strain was studied. The transformation and actuation behavior observed was different in tension and in compression. In tension, during the first thermal cycle under a constant applied load, the SMA expanded upon heating from martensite to austenite. Cooling from austenite to martensite resulted in a further expansion of the SMA. The total actuation strain generated as a result of this unique two stage expansion during the first thermal cycle was approximately 7.0% [4]. Subsequent thermal cycling under the constant load resulted in contraction upon heating and expansion upon cooling with an actuation strain of approximately 4.0%. The strain generated due to the expansion, during the first thermal cycle, under load, was recoverable during the first thermal cycle in the absence of stress. Diffraction patterns and optical micrographs were obtained during different stages of the transformation. The results from the microstructural investigation revealed that the two stage expansion and contraction observed during the first thermal cycle under a constant load and in the absence of load respectively, was as a result of favorably oriented martensite variants formed during the processing stage.

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Representative Bulk Thermomechanical Properties from Micron-Diameter NiTiPd Specimens

Raj Vaidyanathan
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

M. Fox
Graduate Student
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

M. Manjeri
Graduate Student
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

G. Bigelow
NASA Glenn Research Center

S. Padula
NASA Glenn Research Center

R. Noebe
NASA Glenn Research Center

R. Vaidyanathan
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

The roles of composition and thermomechanical processing on shape memory alloy behavior can never be emphasized enough. Experimentally assessing the effects of varying composition and thermomechanical processing parameters can be cost intensive, especially when expensive and high purity elemental additions are involved (e.g., Pd or Pt for increasing phase transformation temperatures). Thus to save development costs, there is value in establishing a methodology that facilitates the fabrication, processing and testing of smaller specimens, rather than larger specimens from commercial billets. Such a methodology can include arc-melting of button melts (e.g., 10-30 g), followed by their subsequent thermomechancial processing and testing. With the objective of establishing such a methodology, this work compares thermomechanical test results from bulk samples with that of micron-diameter wires. Thermomechanical tests were carried out at NASA GRC on a Ni29.5Ti50.5Pd20 alloy using cylindrical dog-bone specimens (gauge section approx. 16 mm in length and approx. 4 mm in diameter). Previous work has established that Ni29.5Ti50.5Pd20 specimens of the aforementioned dimensions are representative of bulk behavior and not influenced by geometry or size-scale effects. From directly comparable untested specimens, wires were obtained by wire electrical discharge machining. The wires were subsequently electropolished to remove the heat-affected zone resulting in specimens with gauge lengths of 20 mm and rectangular cross sections of approx. 130 x 125 microns. Stress-strain curves and load-bias tests were then performed on these wires using a dynamic mechanical analyzer. In general, there was excellent agreement between data from the bulk and micron-diameter samples, with identical qualitative trends being observed. The quantitative differences in the magnitude of the transformation strains and the hysteresis were attributed to differences in the variant distribution owing to geometrical constraints in the smaller samples. However, the smaller samples did appear to contain a starting variant distribution representative of the larger samples, as evidenced by similar stresses required for elastic deformation and the onset of detwinning in both samples. This work has thus established that carefully prepared micron-diameter samples can be used to obtain representative bulk thermomechanical properties and is useful for fabricating and optimizing composition and thermomechanical processing parameters first in prototype button melts prior to large scale commercial production.

Effects of Severe Plastic Deformation and Quaternary Additions on the Dimensional Stability of NiTiPd High Shape Memory Alloys

Kadri C. Atli
Mechanical Engineering, Texas A&M University

Ibrahim Karaman
Professor
Mechanical Engineering, Texas A&M University

Mohammed Haouaoui
Mechanical Engineering, Texas A&M University

Parikshith K. Kumar
Aerospace Engineering, Texas A&M University

Dimitris C. Lagoudas
Professor
Aerospace Engineering, Texas A&M University

Ronald D. Noebe
MS 49-3, NASA Glenn Research Center

Glen S. Bigelow
MS 49-3, NASA Glenn Research Center

The growing demand for shape memory alloys (SMA) with high transformation temperatures has driven the development of new alloy systems that can operate at elevated temperatures. The use of ternary additions to conventional NiTi has been successfully implemented to achieve increased transformation temperatures above 100°C. Within this framework, NiTiPd alloys have attracted considerable attention as high temperature shape memory alloys (HTSMA), since their transformation temperatures can be as high as 500°C while they also exhibit significant strain recovery under both constrained and unconstrained conditions. However, as the deformation temperature is increased, dislocation processes and thermally driven mechanisms become more dominant and the amount of recoverable strain drops significantly.

The objective of this study is to thermo-mechanically strengthen NiTiPd25 alloys in order to obtain enhanced shape-memory characteristics, in particular dimensional stability under repeated thermal cycles. This is accomplished using severe plastic deformation via equal channel angular extrusion (ECAE) and solid solution hardening with quaternary additions of Sc and Ta. ECAE has already been implemented to enhance the shape memory behavior of a NiTiHf HTSMA by increasing the critical shear stress (CSS) levels for dislocation slip [1]. Au, Pt and Hf additions to NiTiPd have been found to increase the relative strengths of martensite and austenite phases [2]. For both ECAE processed NiTiPd and NiTiPd-X, differential scanning calorimetry (DSC) analysis is conducted for multiple cycles to characterize cyclic stability of transformation temperatures. Isothermal monotonic tensile tests are performed to assess the CSS for slip of both martensite and austenite phases. Finally, thermal cycling experiments at various constant stress levels are utilized to characterize transformation temperatures, dimensional stability and work output. The effects of Sc and Ta additions and the selected processing parameters on the dimensional stability of the NiTiPd alloys will be discussed in the light of the results of these experiments and microstructural findings from electron microscopy.

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Plasticity in TiPdNi High Temperature Shape Memory Alloys

Parikshith Kumar
Graduate Student
Department of Materials Science and Engineering, Texas A & M University

Kadri C. Atli
Graduate Student
Department of Materials Science and Engineering, Texas A & M University

Dimitris C. Lagoudas
Department of Aerospace Engineering, Texas A & M University

Ibrahim Karaman
Department of Mechanical Engineering, Texas A & M University

Glen Bigelow
National Aeronautics and Space Administration

Ronald Noebe
National Aeronautics and Space Administration

High Temperature Shape Memory Alloys (HTSMAs) are a class of Shape Memory Alloys (SMAs) that can operate at temperatures higher than 100°C [1, 2]. HTSMAs have been investigated for their use as actuators in the aerospace, automotive and oil industries [3]. As a consequence, recent efforts have focused on improving the work characteristics as well as the formability of these alloys [4]. However, the need to understand the relationship between the transformation behavior and the associated development of plastic strains in these alloys is necessary for actuator design. Additionally, the high operating temperatures of HTSMAs can lead to viscoplastic behavior in addition to rate independent plastic strain generation. Quantifying the development of the strains due to plasticity and viscoplasticity, and understanding their relationship with the generated transformation strain is important to develop accurate models to capture the material behavior.

This effort focuses on characterizing the plasticity that occurs in Ti50Pd25Ni25 HTSMA and the influence of the martensite-to-austenite transformation on its evolution. For this purpose an ingot of the alloy was fabricated by vacuum induction melting, cast and hot extruded into a bar. Tensile specimens were fabricated from the extruded bar by electrical discharge machining. A high temperature test setup was assembled for thermomechanical testing. Constant load, thermal cycling tests were conducted on the specimens to establish a preliminary phase diagram indicating the transformation regions. To study the influence of transformation on plasticity, specimens were loaded along pre-determined paths in the phase diagram and the yield stress is determined as a function of thermomechanical cycle history. The microstructural mechanisms (i.e. formation of retained martensite, dislocation accumulation), which occur during the phase transformation, and which ultimately influences the yield stress, will be investigated using x-ray diffraction and transmission electron microscopy. Based on the experimental results and microstructural observations, internal variables will be chosen and evolution equations are postulated for incorporation into a phenomenological thermodynamic constitutive model for SMAs.

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Constitutive Modeling and Simulation of Shape Memory Polymers

Joga Rao
Associate Professor
Mechanical Engineering, New Jersey Institute of Technology

Gautam Barot
Postdoctoral Research Associate
Computational Science and Engineering, University of Illinois

Mahesh Khanolkar
Graduate Student
Mechanical Engineering, New Jersey Institute of Technology

Shape Memory Polymer's (SMP's) belong to a large family of active or smart materials which are defined by their capacity to store a deformed (temporary) shape and recover an original (parent) shape. Shape memory materials have the ability to change size and shape in response to changes in temperature, moisture, pH, or electric and magnetic fields.

Here we present a general framework to model both crystallizable SMP's (CSMP's) and glassy SMP's (GSMP's) and use the developed models to solve boundary value problems of interest. CSMP's utilize crystallization to form the stiff temporary phase while GSMP's utilize glass transition for the same purpose. First we present the framework that has been developed to model the thermo-mechanical behavior of CSMP's. The model involves a typical shape memory cycle which entails formulating and then solving mathematical equations for the original amorphous (rubbery) phase, the semi-crystalline phase and the transition process where the material is a mixture of both the phases. Modeling of the phase transition process is done using a framework that was developed recently for studying crystallization in polymers and is based on the theory of multiple natural configurations. Predictions of the model are verified against experimental data available in literature and the agreement between theory and experiments are good. The model is able to accurately capture the drop in stress observed on cooling and the return to the original shape on heating. To solve complex boundary value problems in realistic geometries a user material subroutine (UMAT) has been developed for use in conjunction with the commercial finite element software ABAQUS. A few representative solutions with practical import will be presented.The same framework has also been adopted to develop constitutive models for GSMP's. The predictions of the model have been compared with experimental data and the agreements are very good.

Thermo-mechanical Behavior of Thermally Induced Shape Memory Polymers

Francisco Castro
Graduate Student
Department of Mechancial Engineering, University of Colorado

H. Jerry Qi
Department of Mechanical Engineering, University of Colorado

Robin Shandas
Department of Mechanical Engineering, University of Colorado

Shape memory polymers can offer a large shape change as the environment changes. For thermally induced shape memory polymers, an SMP can be pre-deformed from an initial shape to a deformed shape by applying an external mechanical load at temperature Td. A subsequently lowering down the temperature to Ts will freeze this deformed shape after the external mechanical load is removed. The shape memory effect is then activated by increasing the temperature to Tr, where the initial shape is recovered. In general, Td and Tr are in the vicinity of the glassy transition temperature Tg, whilst Td is above Tg and Ts is below Tg. In such a shape-frozen and shape-recovery cycle, the sample needs to go through its Tg twice. For polymers, as the temperature traverses the Tg, the mechanical behaviors of the polymer will change from a rubbery behavior to a glassy behavior which is a direct result of the transition in the polymer structure, a process that is strongly dependent on time.

In this paper, the effects of thermal rate to the thermal-mechanical recovery of shape memory polymers are investigated. Thermal rates essentially have two effects: the first one is concerned with the thermal conductivity of the polymer; the second one is concerned with the glassy transition. Both effects are investigated. Possible modeling scheme for capturing these effects are also proposed.

Inter-martensite Strain Evolution in NiMnGa Single Crystals

Reginald F. Hamilton
Department of Mechanical Science and Engineering, University of Illinois

Huseyin Sehitoglu
Department of Mechanical Science and Engineering, University of Illinois

Kubilay Aslantas
Department of Mechanical Education, University of Afyon, Kocatepe

Christos Efstathiou
Department of Mechanical Science and Engineering, University of Illinois

Hans J Maier
Lehrstuhl f Werkstoffkunde, University of Paderborn

Stress-induced martensitic transformations are clarified in classes of NiMnGa alloys which undergo the stress-free, thermal-induced inter-martensite transformation austenite (A) pre-martensite (PM) martensite [1]. In our work [2], we implement a comprehensive experimental approach, including analysis of the strain-temperature and stress-strain response, which discloses stress-induced inter-martensite transitions. The evolution of the transitions is elucidated utilizing in-situ digital image correlation (DIC) measurements of meso-scale strain fields. Due to the intermediate transition, the thermal hysteresis in the strain-temperature response is tiny (< 10 °C). Meso-scale DIC measurements quantify inter-martensite strain levels, which are indistinguishable from macro-scale stress-strain and strain-temperature responses.

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Magnetic Field-Induced Phase Transformation in NiMnCoIn Metamagnetic Shape Memory Alloys

Burak Basaran*
Research Assistant
Department Of Mechanical Engineering, Texas A&M University
bbasaran@tamu.edu

Ibrahim Karaman
Department Of Mechanical Engineering, Texas A&M University

Haluk E. Karaca
Department Of Mechanical Engineering, University of Kentucky

Yuriy I. Chumlyakov
Professor
Syberian Physical Technical Institute, Tomsk State University

Magnetic Shape Memory Alloys (MSMAs) has recently been evolved as a new class of functional materials that are capable of magnetic field-induced actuation, magneto-thermo-mechanical sensing, magnetic refrigeration, and harvesting of waste mechanical energy. In the present work, magnetic field-induced martensitic phase transformation (FIPT) in Ni45Mn36.5Co5In13.5 MSMA single crystals is characterized as a new actuation mechanism with potential to result in ultrahigh actuation work outputs. The effects of applied magnetic field on the phase transformation temperatures, lattice parameters, magnetization, and superelastic response are systematically investigated and the selected results will be presented. The magnetic work output of NiMnCoIn alloys is determined to be more than 1 MJm?3 per Tesla which is one order of magnitude higher than the magnetic work output of the most well-known MSMAs, i.e. NiMnGa alloys. In addition, the work output of NiMnCoIn alloys is orientation independent, potentially surpassing the need for single crystals, and not limited by a critical magnetic field, thus by a maximum work output, as opposed to NiMnGa MSMAs. Experimental and theoretical transformation strains and magnetostress levels are also determined as a function of crystal orientation. It will be shown that [111] orientation can demonstrate a magnetostress level of 140 MPa/Tesla with 1.2% axial strain under compression. These field-induced stress and actuation strain levels are significantly higher than those from existing piezoelectric and magnetostrictive actuators. A thermodynamical framework will introduced to comprehend magnetic energy contributions during martensitic phase transformation.

Neutron Diffraction Measurements during Thermal-Mechanical Testing of Shape Memory NiTi

Raj Vaidyanathan
Associate Professor
AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

S. Qiu
Graduate Student
AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

V. Krishnan
Postdoctoral Associate
AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

S. Padula
NASA Glenn Research Center

R. Noebe
NASA Glenn Research Center

D. Brown
Los Alamos National Laboratory

B. Clausen
Los Alamos National Laboratory

A NiTi (55 wt.% Ni) shape memory alloy is currently being considered as a solid state actuator for use with noise mitigating variable geometry chevrons and other aeronautic applications. However, fundamental mechanisms related to the phase transformation against external thermal and mechanical loading are still not fully understood. For example, the role of retained or stabilized martensite and the internal strain evolution in influencing actuator behavior has not been established. Here, we report on in situ neutron diffraction measurements performed on NiTi during selected combinations of heating, cooling and mechanical loading. Compared to x-rays from a conventional source, neutrons can penetrate much deeper, making surface stress effects negligible and hence neutron diffraction measurements representative of bulk behavior in polycrystalline samples. Rietveld refinement and single peak fitting were used to analyze neutron spectra and quantify the micromechanical and microstructural changes, i.e., texture, strain and phase volume fraction. The lattice strain evolution during heating and cooling in an unloaded sample was used to determine coefficient of thermal expansion (CTE) tensors for both the monoclinic and cubic phases. The tensors thus determined from the neutron diffraction data were subsequently used to obtain average CTE values that compared well with macroscopic dilatometric measurements previously reported in the literature. The texture and phase fraction evolution was also quantified during heating and cooling in the unloaded sample (i.e., free-recovery experiment). The results from the free-recovery experiment were compared with measurements made during heating and cooling of a sample subjected to a constant load. This comparison helped assess the effect of external loads on the internal strain, texture and phase volume fraction evolution. Lastly, results from the load-bias experiment were also compared with results from an isothermal experiment wherein samples were subjected to monotonic loading. For the same externally applied stress, martensite that forms during cooling under load had stronger texture and generated more strain than martensite that was monotonically and isothermally stressed. Furthermore, the volume fraction and texture of the retained or stabilized martensite and the associated internal strains were quantified in the aforementioned load-bias experiments. In conclusion, the ability to quantitatively follow the micromechanical and microstructural changes during the phase transformation under external load and heating/cooling has provided valuable information for future engineering of these alloys, especially with ternary and quaternary elemental additions.

Analysis of Plastically Deformed Shape Memory Alloys Exhibiting Tension-Compression Asymmetry

Dimitris C. Lagoudas
Professor
Aerospace Engineering, Texas A&M University

Darren J. Hartl
PhD Student
Aerospace Engineering, Texas A&M University

Santo A. Padula
Materials Research Engineer
Materials and Structures Division, NASA Glenn Research Center

The need to accurately account for the response of Shape Memory Alloys (SMAs) under complex loading paths has become increasingly important. Such paths are general in a stress-temperature space and may induce irreversible deformation (plasticity) and require consideration of tension-compression asymmetry. Past work on plastic strain generation in SMAs has focused on two distinct phenomena. Transformation-induced plasticity (TRIP) accounts for irrecoverable strain generated due to cyclic transformation [1]. The second phenomena is associated with slip mechanisms that initiate at sufficiently high stresses (i.e., yield surfaces in stress space). Such models have been derived and implemented in 1-D [2] and 3-D [3]. However, available models address only permanent plastic yield which occurs outside of active transformation regions. With regards to tension-compression asymmetry, several investigations have been performed, though none in the context of a 3-D model which accounts for plasticity as well [4].

This work involves experimental investigation, model development, and numerical analysis pertaining to rate-independent inelasticity in SMAs while considering tension-compression asymmetry. The experimental characterization effort is reviewed. The material behavior is examined during the yielding of pure phases and during the simultaneous occurrence of plastic slip and martensitic transformation. Motivated by these experiments, an SMA model which captures the formation and evolution of plastic strains is proposed. The 3-D model is derived using continuum thermodynamics where appropriate elastic domains and hardening functions have been chosen. Multiple "yield" surfaces are used to capture the transformation and plastic yield simultaneously. Implementation in an FEA framework is performed using return mapping algorithms [5] specially derived to consider simultaneous transformation/yielding. The analysis results from various boundary value problems with complex boundary conditions and stress states are presented, including investigation of stress concentrations and SMA indentation.

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Effects of Constrained Aging on the Shape Memory and Pseudoelasticity Response of Ni-Rich NiTi Shape Memory Alloys

Fatmata Barrie
Research Assistant
Department of Mechanical Engineering, Texas A&M University

Kadri Can Atli
Research Assistant
Department of Mechanical Engineering, Texas A&M University

Ibrahim Karaman
Department of Mechanical Engineering, Texas A&M University

Yuri Chumlyakov
Siberian Physical Technical Institute, Tomsk State University

Precipitation through aging heat treatments has been shown to notably affect the pseudoelasticity and transformation behavior of Ni-rich NiTi shape memory alloys (SMAs) in the past. Selected aging treatments can result in two-way shape memory effect, surpassing the need for time-consuming and costly thermo-mechanical training in practical applications. In addition, aging treatments at low temperatures (< 500°C) tend to produce multiple stage phase transformations including the martensitic R-phase in addition to the customary monoclinic B19' martensite (M). Although the R-phase only appears at low stresses and produces small transformation strains, it has a significantly smaller temperature hysteresis than the B19' martensite. Aging NiTi under mechanical constraints affects the number of precipitate variants giving a way to manipulate the internal stress fields due to precipitates. This in turn helps controlling the two way shape memory effect and the shape that the sample would remember, possibly providing flexibility in the use of these SMAs in practical applications.

To better understand the effects of different constraining conditions during aging on the two way shape memory effect, shape memory characteristics and R-phase formation, Ti-50.6 at.% Ni single crystals oriented along the [112] direction were aged under no stress, and 150 MPa uniaxial compression and uniaxial tension conditions for 1.5 hours at 400°C, for the purpose of selecting different precipitate variants during aging. The samples then underwent isobaric thermal cycling under incrementally increasing stress levels and isothermal pseudoelastic tensile experiments. Transformation strains up to 10% were observed. During the isobaric thermal cycling experiments, the R-phase was present up to stress levels of 400 MPa. Notable irrecoverable strain levels were observed upon cease of the R-phase above 400 MPa. These observations support the fact that the R-phase is an intermediate phase between B2 austenite and B19' martensite enhancing the compatibility. Thermal hysteresis decreased slightly with increasing stress levels for the sample aged under no stress, however for the sample aged under compression, the thermal hysteresis decreases only up to a certain stress level. During the pseudoelasticity experiments, a two stage stress-strain response having two distinct plateau regions was detected where the second plateau region was attributed to extensive deformation twinning in martensite. The R-phase and B19' martensite transformation strains and temperatures were compared as there were differences due to the different aging histories. Selected results from this extensive work will be presented in this talk.

Deformation in NiTiFe Shape Memory Alloys

Raj Vaidyanathan
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

R.M. Manjeri
Departments of AMPAC and Mechanical, Materials and Aerospace Engineering, University of Central Florida

The use of binary NiTi shape memory alloys in certain actuator applications is limited by specific requirements associated with hysteresis, fatigue and temperature of operation, among others. Addition of Fe to NiTi introduces an intermediate trigonal R-phase and lowers the monoclinic B19 martensitic transformation temperature. There has been practical interest in the R-phase transformation in NiTiFe alloys as it offers a useful temperature window for actuator operation due to reduced hysteresis at low temperature coupled with a favorable fatigue response. In addition there is theoretical interest—not much is known about the thermal-mechanical deformation characteristics of the R-phase in the NiTiFe system, information that is required to facilitate their use in low temperature switches, seals, valves, etc. This study focuses on examining competing mechanisms, i.e., detwinning and stress-induced transformation, that govern inelastic deformation in the R-phase. Additionally, stress-induced transformations in the parent B2 austenite phase were also investigated. A Ni46.8Ti50Fe3.2 alloy billet was fabricated by vacuum induction melting followed by vacuum arc remelting. Samples from the billet were cold worked by 30%, annealed at 600°C for 30 minutes and electrical discharge machined for subsequent testing. The resulting wires (rectangular cross section of approximately 130 x 125 microns and a gauge length of 20 mm) were electropolished and subjected to mechanical tests in a dynamic mechanical analyzer. Previous work that adopted the aforementioned testing methodology has established that results from these wires are comparable to more conventional bulk specimens. Regions in stress-temperature space are identified based on detwinning in the R-phase followed by a stress-induced transformation to B19' martensite and regions where the onset of the stress induced transformation occurs without any prior detwinning. The decreasing propensity for the R-phase to detwin with decreasing temperature is also investigated and quantified. The stress-temperature equivalence of the R to B19 and the B2 to R reversible stress-induced phase transformations were studied within the framework of the Clausius-Clapeyron relation. The temperature range in which the reversible B2 to R stress-induced phase transformation occurs is very narrow suggesting that the martensite desist temperature of the R-phase is very close to the austenite finish temperature. By quantifying stresses and strains and identifying temperature ranges associated with various deformation mechanisms in NiTiFe alloys, this work has implications for using these NiTiFe alloys in applications that require low-temperature, low-hysteresis actuators with superior fatigue behavior.

The Mechanical Response of Shape Memory Alloys under a Rapid Heating Pulse

Doron Shilo
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Shahaf Wallach
Department of Mechanical Engineering, Technion, Israel Institute of Technology

Shape Memory Alloy (SMA) actuators are very promising due to their large strains but are considered to be very slow due to their cooling rate. In this presentation we explore the capabilities of a fast one-directional actuation mode based on one-occasional rapid Joule heating of SMA elements. For this purpose a unique experimental system has been developed which applies a high-voltage electric pulse to a detwined NiTi wire and measures the resulted displacement due to the martensite to austenite phase transformation. The electric pulse is tuned to produce a temperature jump of 40-100 degrees within a risetime of few microseconds. One end of the wire is clamped while the displacement of the other end is monitored both by a laser vibrometer and by an optical encoder that measure the displacement of a grating device. The response of the SMA under different dead-weight loads allows studying the kinetics of temperature induced austenitic transformation. In particular, dynamic stress-strain curves are extracted and the nucleation time is investigated. A comparison with several previous studies of stress induced martensitic transformation will be presented. The results demonstrate the great potential of SMA for applications that require high speeds and large displacements one-occasional actuation.

Constitutive Behavior of Polymers and Polymer Nanocomposites

SYMPOSIUM
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ORGANIZER:

Harley T. Johnson, *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign*

Effect of Particle Clustering on the Viscoelastic Properties of Polymer Nanocomposites

Rui Qiao
Research Assistant
Mechanical Engineering, Northwestern University

Cate Brinson
Professor
Mechanical Engineering, Northwestern University

A numerical approach is developed and implemented to analyze the effect of nanoparticle agglomeration on the glass transition temperature of polymer nanocomposites. In this method, a representative volume element is created, including nanoparticle dispersions with different degrees of clustering and their associated interphase domain. The viscoelastic properties are studied using a statistical approach to account for variation in results due to the random nature of the microstructure. Results show that a monotonic increase in nanofiller clustering not only results in the loss of interphase volume but also obstructs the formation of a percolating interphase network in the nanocomposite. The combined impacts lead to a remarkable decrease of glass transition enhancement for clustering nanofillers compared to well-dispersed configurations. Our simulation results provide quantitative support for experimental observations that clustering negatively impacts the effects of the nanofiller.

High Thermal Conductivity Nanocomposite Encapsulants for Submarine Weapon Arrays

Vijaya B. Chalivendra
Department of Mechanical Engineering, University of Massachusetts, Dartmouth

John V. Costa
Research Assistant
Department of Mechanical Engineering, University of Massachusetts, Dartmouth

Thomas Ramotowski
Scientist
Sensors, & Sonar Systems, Naval Undersea Warfare Center

Current polymer encapsulants, with their thermal insulating properties are an obstacle to deployment of "next-generation" high power/high duty cycle acoustic sources that will necessarily generate considerable amounts of heat in operation. Past attempts to create highly conductive polymer composites used ceramic micropowders such as boron nitride (BN) with high filler loadings (>25%) that impaired crucial properties such as sonic clarity, strength and fracture toughness.

In our project we take advantage of the nano-effect to develop polyurethane nanocomposites with significantly lower BN loadings (<5.0%) to achieve the needed 10 times increase in thermal conductivity from 0.2W/mK to 2.0W/mK. BN particles combine the ideal qualities of being dielectric with high thermal conductivity and a non-abrasive nature allowing ease of machining and processing. Proper nanoparticle dispersion is the key factor to determining the percolation threshold for the maximized phonon transfer rate at lowest possible loadings. A combination of shear mixing, ultrasonification and particle functionalization will be used to properly deagglomerate and disperse the particles in the polyurethane matrix. TEM and SEM will be used to verify dispersion with accurate static and dynamic mechanical characterization being performed on test equipment calibrated for machine compliance. In addition to measurements of thermal conductivity and sonic transparency, we also intend to do quasi-static and dynamic characterization where we expect to see some improvement over the matrix material alone.

The study is currently in progress and results will be ready for presentation at the October 2008 conference.

Mechanical Fields of a Multiphase Cylindrical/Spherical Inhomogeneity System

H. Hatami-Marbini
Rensselaer Polytechnic Institute

H. M. Shodja
Department of Civil Engineering, Sharif University of Technology

The thermo-mechanical behavior of composite materials depends on the stress field in and around a single phase inhomogeneity. Using the Boussinesq displacement potentials, mechanical field of cylindrical and spherical multi-phase inhomogeneity systems with perfect or imperfect interfaces is investigated. An imperfect bond is often present in the system because of chemical interaction between inhomogeneity and matrix. It may also be introduced deliberately to control the properties during manufacturing process. Here we present the exact closed-form thermo-elastic solutions of the inhomogeneity system consisting of homogeneous phases. In other cases where the constituent phases of the inhomogeneity system are made of a number of different functionally graded (FG) and homogeneous materials, a systematic numerical methodology are utilized to find the mechanical fields. The thickness of each phase is arbitrary and each interface may have a perfect or imperfect boundary condition, as desired.

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Presenting Author Contact List

A.H. England
england@84burnside.freeserve.co.uk

A.P.S. Selvadurai
patrick.selvadurai@mcgill.ca

Aaron C. Jackson
ajacks22@illinois.edu

Adrian Lew
lewa@stanford.edu

Alaa Ahmed
aaa52@cam.ac.uk

Alan M. Rosenwinkel
alanmr@seas.upenn.edu

Alan Wineman
lardan@umich.edu

Alejandro M. Aragon
aaragon2@illinois.edu

Alexander Vakakis
avakakis@illinois.edu

Aman Haque
mah37@psu.edu

Amir H.G. Isfahani
ghalayan@illinois.edu

Amit Kaushik
akaushik@umich.edu

Amit Patel
ajpatel4@illinois.edu

Amy Wagoner Johnson
ajwj@illinois.edu

Andrew Hamilton
ahamilt3@illinois.edu

Angela A. Triplett
alt25@uakron.edu

Anil K. Kodali
kodali@illinois.edu

Anja Schlömerkemper
schloem@mis.mpg.de

Anna Ask
anna.ask@solid.lth.se

Anne Staples
astaples@lcp.nrl.navy.mil

Anthony Starr
astarr@sensormetrix.com

Antonio Caballero
antonio.caballero@epfl.ch

Antonio Valdevit
avaldevit@aol.com

Arif Masud
amasud@illinois.edu

Asha Nurse
asha_nurse@brown.edu

Ashraf Bastawros
bastaw@iastate.edu

Ashwani Kumar Goel
ashwanikg@rediffmail.com

Badel Mbanga
mbanga@lci.kent.edu

Bart Prorok
prorok@auburn.edu

Ben Nadler
bnadler@ualberta.ca

Benjamin J. Blaiszik
blaiszik@illinois.edu

Benjamin J. Polly
pollyben@yahoo.com

Bernard D. Coleman
bcoleman@jove.rutgers.edu

Bhawesh Kumar
kumar5@purdue.edu

Bin Chen
binchen@mcmaster.ca

Birbal Singh
Birbal.Singh@Lakeheadu.ca

Bojan Guzina
guzina@wave.ce.umn.edu

Brendan Harley
bharley@illinois.edu

Brian Berg
bergb@bsci.com

Brian Kozola
bkozola2@illinois.edu

Bui Tien Dung
t.d.bui@tudelft.nl

Carl Boehlert
boehlert@egr.msu.edu

Carlos Alberto Figueroa
cafa@stanford.edu

Catherine Cozad
ccozad@memphis.edu

Cathy Chu
cchu4@illinois.edu

Cecile Smeesters
Cecile.Smeesters@USherbrooke.ca

Charles Randow
charles.randow@arl.army.mil

Charles Thodeti
charles.thodeti@childrens.harvard.edu

Christian G. Hoover
c-hoover@northwestern.edu

Christian Schwartz
cschwartz@tamu.edu

Christopher Hansen
chansen3@illinois.edu

Christopher Kovalchick
ckovalchick@caltech.edu

Christos Efstathiou
efstathi@illinois.edu

Chwee Teck Lim
ctlim@nus.edu.sg

Concetta Tripepi
concetta.tripepi@unirc.it

Corey O'Hern
corey.ohern@yale.edu

Cristian Ciobanu
cciobanu@mines.edu

Cynthia Reinhart-King
cak57@cornell.edu

D. Michael McFarland
dmmcf@illinois.edu

Dae-Jin Kim
dkim46@illinois.edu

Dagmar Sternad
dxs48@psu.edu

Daniel Ferris
ferrisdp@umich.edu

Daniel Isabey
daniel.isabey@inserm.fr

Daniel Z. Turner
dzturne1@illinois.edu

David Bortz
dmbortz@colorado.edu

David Clements
david.clements@adelaide.edu.au

David Dunand
dunand@northwestern.edu

David Harris
david.harris@manchester.ac.uk

David Kinderlehrer
davidk@cmu.edu

David McIlroy
mcilroy2@illinois.edu

David Saintillan
dstn@illinois.edu

Denis Torres
dotorres@purdue.edu

Dimitrios C. Karampinos
karampin@illinois.edu

Dimitrios Eftaxiopoulos
eftaxiop@central.ntua.gr

Dimitris C. Lagoudas
lagoudas@tamu.edu

Dominique Schryvers
nick.schryvers@ua.ac.be

Doron Shilo
shilo@tx.technion.ac.il

Douglas A. Davis
dadavis2@illinois.edu

Douglas Bammann
bammann@me.msstate.edu

E. Patoor
patoor@lpmm.univ-metz.fr

Earl H. Dowell
dowell@mail.ee.duke.edu

Elena Cherkaev
elena@math.utah.edu

Elham Hamed
ehamed2@illinois.edu

Elisa Budyn
ebudyn@uic.edu

Elizabeth Hsiao-Wecksler
ethw@illinois.edu

Ellad Tadmor
tadmor@aem.umn.edu

Eric N. Brown
en_brown@lanl.gov

Eric O. Potma
epotma@uci.edu

Eric Weeks
weeks@physics.emory.edu

Eric Wetzel
ewetzel@arl.army.mil

Erik Herbert
erik.herbert@agilant.com

Evan Ma
ema@jhu.edu

Farhan Chowdhury
fchowdh3@illinois.edu

Flavio Souza
fsouza2@unl.edu

Florin Bobaru
fbobaru2@unl.edu

Frances Pounder
fkeith2@illinois.edu

Francisco Castro
francisco.castro@colorado.edu

Franziska Schmidt
Franziska.Schmidt@entpe.fr

Gabriel Popescu
gpopescu@illinois.edu

Gal deBotton
debotton@bgumail.bgu.ac.il

Gang Bao
gang.bao@bme.gatech.edu

Gareth McKinley
gareth@mit.edu

Gary Seidel
gary.seidel@gmail.com

Gautam Barot
gautam.barot@gmail.com

Gearoid Mac Sithigh
macsithi@mst.edu

George A. Gazonas
gazonas@arl.army.mil

George Lykotrafitis
gelyko@mit.edu

George Voyiadjis
voyiadjis@eng.lsu.edu

German Drazer
drazer@jhu.edu

Ghadir Haikal
haikal@illinois.edu

Goutam Ghoshal
gghoshal@bigred.unl.edu

Graeme Milton
milton@math.utah.edu

Gregory McKenna
greg.mckenna@ttu.edu

Gregory Odegard
gmodegar@mtu.edu

Guillaume Bal
gb2030@columbia.edu

Guillaume R. Ragetly
ragetly2@illinois.edu

Guillermo Goldsztein
ggold@math.gatech.edu

Guruswami Ravichandran
ravi@caltech.edu

Guy M. Genin
gmg@me.wustl.edu

H. Hatami-Marbini
hatamh@rpi.edu

H. Jerry Qi
qih@colorado.edu

Hady Joumaa
hjoumaa2@illinois.edu

Haizhen Pan
hpan@seas.upenn.edu

Hanqing Jiang
hanqing.jiang@asu.edu

Haoxiang Luo
haoxiang.luo@vanderbilt.edu

Harish Iyer
hiyer@umich.edu

Harley Johnson
htj@illinois.edu

Harry Dankowicz
danko@illinois.edu

Harry H. Hilton
h-hilton@illinois.edu

Hashem Mourad
hmourad@lanl.gov

Henghua Jin
jin6@illinois.edu

Henry Fu
Henry_Fu@brown.edu

Himanshu Bhatnagar
bhatnagar.12@osu.edu

H.J. Kwon
hkwon@caltech.edu

Hong Zhao
hongzhao@illinois.edu

Hongjin Qiu
h-qiu@northwestern.edu

Horacio Espinosa
espinosa@northwestern.edu

Huck Beng Chew
Huck_Beng_Chew@brown.edu

Huseyin Sehitoglu
huseyin@illinois.edu

Hyung-Do Kim
hyungdo@mit.edu

Ichiro Takeuchi
takeuchi@umd.edu

Igor Sevostianov
igor@nmsu.edu

Ileana Carpen
icarpen@tntech.edu

Irene Chang
iytchang@mit.edu

Irene Fonseca
fonseca@andrew.cmu.edu

Irina Hussainova
irhus@staff.ttu.ee

Isaac Chenchiah
Isaac.Chenchiah@bristol.ac.uk

J. Patrick Wilber
jw50@uakron.edu

JaeHyuk Kwack
jkwack2@illinois.edu

Jae-Sung Moon
icmoon@illinois.edu

Jagannathan Rajagopalan
jrajago2@illinois.edu

James Berryman
JGBerryman@LBL.GOV

James Norman
jjnorman@stanford.edu

James W. Foulk III
jwfoulk@sandia.gov

Jane Liu
jliu@tntech.edu

Janelle Totten
janelle.totten@materialise.com

Jason G. Vogeler
jasongv88@hotmail.com

Javier Segurado
jsegurado@mater.upm.es

Jay Carroll
jcarrol2@illinois.edu

Jay Patel
patel3@illinois.edu

Jay Walton
jwalton@math.tamu.edu

Jeff Morris
morris@ccny.cuny.edu

Jennifer Lewis
jalewis@illinois.edu

Jennifer Serres
serres.3@wright.edu

Jeongsik Kim
cafe4068@tamu.edu

Jericho Moll
jmoll2@illinois.edu

Jerome Crest
jcrest@mit.edu

Jessica Sanders
jds37@duke.edu

Jessica Sparks
jsparks@wfubmc.edu

Ji Ma
jm@tamu.edu

Jia Lu
jia-lu@uiowa.edu

Jia-Liang Le
jialiang-le@northwestern.edu

Jinglei Yang
jlyang@illinois.edu

Jinjin Ma
jinjinma@umich.edu

Jo Ann Cameron
joanncam@life.illinois.edu

Joachim P. Spatz
spatz@mf.mpg.de

Joby John
jzj109@psu.edu

Joe Goddard
jgoddard@ucsd.edu

Joel Bernier
bernier2@llnl.gov

Joerg Helfenstein
joerg.helfenstein@imes.mavt.ethz.ch

John Clayton
jclayton@arl.army.mil

John L. Bassani
bassani@seas.upenn.edu

John Lambros
lambros@illinois.edu

John Rogers
jrogers@illinois.edu

John Schmidt
jschmid7@illinois.edu

John Selby
jcselby@illinois.edu

John V. Costa
u_j4costa@umassd.edu

John Willis
J.R.Willis@damtp.cam.ac.uk

Jonathan B. Dingwell
jdingwell@mail.utexas.edu

Jooeun Ahn
aje@mit.edu

Jorgen Bergstrom
jbergstrom@veryst.com

José Manoel Balthazar
jmbaltha@rc.unesp.br

Jose Merodio
jose.merodio@upm.es

Joseph P. Cusumano
jpc3@psu.edu

Jun Li
junli3@illinois.edu

Kadri C. Atli
catli@tamu.edu

Kamakshi Singh
singh.257@osu.edu

Kara Muckley
muckley.2@wright.edu

Karl-Heinz Lang
karl-heinz.lang@iwk1.uni-karlsruhe.de

Karthik Srinivasan
krsriniv@illinois.edu

Katerina D. Papoulia
papoulia@uwaterloo.ca

Kathleen Toohey
ktoohey@illinois.edu

Kaushik Bhattacharya
bhatta@caltech.edu

Kaushik Das
kdas@vt.edu

Kaushik Dayal
kaushik@cmu.edu

Kei Masani
k.masani@utoronto.ca

Keith Gall
k-gall@northwestern.edu

Kevin Long
kevin.long@colorado.edu

Kostas Soldatos
kostas.soldatos@nottingham.ac.uk

Krishna Garikipati
krishna@umich.edu

Kristin Bernick
kbernick@mit.edu

Kristofer Westbrook
westbrkk@gmail.com

Krystyn Van Vliet
krystyn@mit.edu

Kumar Vemaganti
Kumar.Vemaganti@uc.edu

L.B. Freund
freund@brown.edu

Lawrence Friedman
lfriedman@psu.edu

Lei Fang
luf110@psu.edu

Leila Ladani
ladani@engineering.usu.edu

Leonard G. Chorosinski
len.chorosinski@ngc.com

Leonid Manevitch
lmanev@chph.ras.ru

Lesley Hamming
lmeade@northwestern.edu

Leslie Lamberson
les@caltech.edu

Liang Feng
lfeng4@illinois.edu

Liming Xiong
lmxiong@ufl.edu

Liping Liu
liulp@caltech.edu

Liying Jiang
lyjiang@eng.uwo.ca

Lorna Gibson
ljgibson@mit.edu

Louis DiBerardino III
diberard@illinois.edu

Luis Dorfmann
luis.dorfmann@tufts.edu

M. Austin Creasy
mcreasy@vt.edu

M. Fox
aerofox13@gmail.com

M.S.R. Parlapalli
M.S.R.Parlapalli@ctw.utwente.nl

Maciej Rysz
mwrysz@engineering.uiowa.edu

Madhavan Raghavan
ml-raghavan@uiowa.edu

Maen Alkhader
alkhmae@iit.edu

Majid Minary-Jolandan
mminary2@illinois.edu

Marcus Slavenas
slavenas@illinois.edu

Marielle Wouters
marielle.wouters@tno.nl

Marisol Koslowski
marisol@purdue.edu

Markus J. Buehler
mbuehler@MIT.EDU

Martin Ostoja-Starzewski
martinos@illinois.edu

Martin Tanaka
mtanaka@wfubmc.edu

Mary M. Caruso
mcaruso2@illinois.edu

Massimo Ruzzene
ruzzene@gatech.edu

Matthew Barham
mbarjam@yahoo.com

Matthew D. Alley
mdalley@purdue.edu

Matthew Leach
mmleach@umich.edu

Matthew Thorpe
mthorp3@illinois.edu

Medhat Hussainov
medhat.hussainov@ttu.ee

Mehrdad Massoudi
massoudi@netl.doe.gov

Michael Czabaj
mwc35@cornell.edu

Michael F. Insana
mfi@illinois.edu

Michael Graham
graham@engr.wisc.edu

Michael J. Prayson
mjprayson@mvh.org

Michael Keller
mwkeller@utulsa.edu

Michael L. VanBlaricum
mikevanb@toyon.com

Michael Ortiz
ortiz@aero.caltech.edu

Michael Sacks
msacks@pitt.edu

Michael Solomon
mjsolo@umich.edu

Michael Walsh
m.walsh@lancaster.ac.uk

Millard F. Beatty
mbeatty2@unl.edu

Ming Dao
mingdao@mit.edu

Mitchell Luskin
luskin@umn.edu

Mohammad Naraghi
naraghi2@illinois.edu

Mohammad Pour-Ghaz
pourghaz@purdue.edu

Mohan Kulkarni
mkulkar2@illinois.edu

Mohsen Dadfarnia
dadfarni@illinois.edu

Monchai Duangpanya
dmonchai@yahoo.com

Muhammad Sahimi
moe@usc.edu

Nadine Aubry
aubry@andrew.cmu.edu

Nancy Sottos
n-sottos@illinois.edu.

Natalia Sitnikova
n.l.sitnikova@tudelft.nl

Natarajan Chennimalai Kumar
chennima@illinois.edu

Nathaniel Huebsch
nhuebsch@fas.harvard.edu

Nicholas Fang
nicfang@illinois.edu

Nicolas Triantafyllidis
nick@umich.edu

Nikhil Karanjgaokar
nkaranj2@illinois.edu

Nilesh Billade
nileshsbillade@yahoo.com

Nimal Rajapakse
rajapakse@mech.ubc.ca

Oscar Lopez-Pamies
oscar.lopez-pamies@sunysb.edu

Parikshith Kumar
parik@tamu.edu

Patrick O'Hara
pohara@illinois.edu

Paul DeVita
devitap@ecu.edu

Paulo Arratia
parratia@seas.upenn.edu

Pedro Ponte Castaneda
ponte@seas.upenn.edu

Petros Sofronis
sofronis@illinois.edu

Philip Kao
philkao@gmail.com

Philip Yuya
pyuya1@bigred.unl.edu

Phuong Tran
tran3@illinois.edu

Pilwon Hur
phur2@illinois.edu

Piyush Thakre
piyushthakre@tamu.edu

Pradeep Sharma
psharma@uh.edu

Pranav Agarwal
agar0108@umn.edu

Prashant Purohit
purohit@seas.upenn.edu

Qi Chen
qichen2@illinois.edu

Qian Xue
qianxue@gwu.edu

Qilong Shen
qlshen@illinois.edu

Qingda Yang
qdyang@miami.edu

Qiushi Chen
qchen@northwestern.edu

Quentin Z.Q. Yue
yueqzq@hkucc.hku.hk

Qunyang Li
Qunyang.Li@alumni.brown.edu

R.M. Manjeri
maddy@mail.ucf.edu

Rachel C. Paietta
rpaietta@nd.edu

Rafal Ablamowicz
rablamowicz@tntech.edu

Raffaella De Vita
devita@vt.edu

Raffaella Rizzoni
rzzrfl@unife.it

Raghavender Cheerkapally
cheerkrr@email.uc.edu

Raguraman Kannan
rkanna2@uic.edu

Raj Kumar Narisetti
rajknarisetti@gatech.edu

Rajesh Kitey
kitey@illinois.edu

Rajiv Kalia
rkalia@usc.edu

Ramji Kamakoti
ramjik@gmail.com

Ramon Calderer
rcalder4@illinoise.du

Rashid K. Abu Al-Rub
rabualrub@civil.tamu.edu

Ray Ogden
rwo@maths.gla.ac.uk

Rebecca Dupaix
dupaix.1@osu.edu

Rebecca Yapp
ryapp2@illinois.edu

Reginald F. Hamilton
rhamilto@illinois.edu

Rezwanur Rahman
djrezwan@yahoo.com

Richard James
james@umn.edu

Richard Lehoucq
rblehou@sandia.gov

Richard Springman
springma@seas.upenn.edu

Richard Trask
R.S.Trask@bristol.ac.uk

Richard W. Neu
rick.neu@me.gatech.edu

Robert Gracie
rgracie@northwestern.edu

Robert Lipton
lipton@math.lsu.edu

Robin Selinger
robin@lci.kent.edu

Roderic Lakes
lakes@engr.wisc.edu

Romain Bellet
bellet@lma.cnrs-mrs.fr

Ronald Miller
rmiller@mae.carleton.ca

Ross Schumer
rossaf44@yahoo.com

Rouholla Alizadegan
alizadeg@illinois.edu

Rui Qiao
r-qiao@northwestern.edu

Ruqiang Feng
rfeng1@unl.edu

Ryan Elliott
elliott@aem.umn.edu

Ryan Finnan
finnanr@hotmail.com

S. Qiu
sqiu@mail.ucf.edu

Sara Matrangola
smatrang@vt.edu

Sara Olesiak
sarasoup@gmail.com

Sara Wilson
sewilson@ku.edu

Sarah-Jane Frankland
sjvf@nianet.org

Sascha Hilgenfeldt
sascha@illinois.edu

Scott J. Spector
sspector@math.siu.edu

Sean Andersson
sanderss@bu.edu

Seetha Raghavan
seetharaghavan@alumni.purdue.edu

Serge Abrate
abrate@engr.siu.edu

Seth E. Watts
watts2@illinois.edu

Shangming He
S.He@tudelft.nl

Shawn Gargac
gargac.2@wright.edu

Shirish Ingawale
ingawale.2@wright.edu

Shivakumar Ranganathan
srangan3@illinois.edu

Shorya Awtar
awtar@umich.edu

Shreehari Elangovan
selangov@mtu.edu

Shuman Xia
Shuman_Xia@brown.edu

Sia Nemat-Nasser
sia@ucsd.edu

Siladitya Pal
spal@mtu.edu

Silvia Jimenez
sjimenez@math.lsu.edu

Simona Socrate
ssocrate@mit.edu

Sivakumar Yagnamurthy
syagnam2@illinois.edu

Soumit Salman Rahman
soumit.s.rahman@gmail.com

Srinivasa Salapaka
salapaka@illinois.edu

Stephen Cowin
scowin@earthlink.net

Stephen E. Bechtel
bechtel.3@osu.edu

Steven Mookhoek
s.d.mookhoek@tudelft.nl

Steven Shaw
shawsw@msu.edu

Suncica Canic
canic@math.uh.edu

Sungsoo Na
sungna@illinois.edu

Susan Enders
senders@mac.com

Taehyo Park
cepark@hanyang.ac.kr

Tanil Ozkan
tozkan2@illinois.edu

Tawhid Ezaz
tezaz2@illinois.edu

Thao Nguyen
vicky.nguyen@jhu.edu

Themistoklis Sapsis
sapsis@mit.edu

Thibault Prevost
prevost@mit.edu

Thomas Berfield
tom.berfield@louisville.edu

Thomas Clancy
tclancy@nianet.org

Thomas Siegmund
siegmund@purdue.edu

Tian Tang
tian.tang@ualberta.ca

Tim Healey
tjh10@cornell.edu

Ting Zhu
ting.zhu@me.gatech.edu

Toby Heyn
heyn@wisc.edu

Todd Williams
oakhill@lanl.gov

Traian Dumitrica
td@me.umn.edu

Troy Brachey
tnbrachey21@tntech.edu

Upadrasta Ramamurty
ramu@materials.iisc.ernet.in

Valery Levitas
valery.levitas@ttu.edu

Vikas Tomar
vikas.tomar@nd.edu

Vikram Gavini
vikramg@umich.edu

Vitali Nesterenko
vnesterenko@ucsd.edu

Warren Ruder
wruder@cmu.edu

Wei Hong
whong@seas.harvard.edu

Weinong Chen
wchen@purdue.edu

William S. Klug
klug@ucla.edu

Willie Wu
williewu@illinois.edu

Xin Tang
xintang2@illinois.edu

Xiupeng Wei
xiupeng-wei@uiowa.edu

Xu Nie
xnie@purdue.edu

Xuefeng Zhao
xuefeng-zhao@uiowa.edu

Xuxin Tu
x-tu@northwestern.edu

Yashashree Kulkarni
ykulkarni@ucsd.edu

YongKeun Park
ykpark@mit.edu

Young Lee
yslee4@illinois.edu

Youping Chen
ypchen2@ufl.edu

Yucun Lou
louyucun@seas.upenn.edu

Yu-Lin Shen
shenyl@unm.edu

Yuliya Gorb
gorb@math.tamu.edu

Yuly Starosvetsky
staryuli@tx.technion.ac.il

Zdenek P. Bazant
z-bazant@northwestern.edu

Zhigang Suo
suo@seas.harvard.edu

Zhonghua Xu
zxu@iastate.edu

Conference Center Floor Plan