Abstracts
Abstracts

Gateway Hotel and Conference Center
Iowa State University, Ames, IA

Ashraf F. Bastawros, Conference Chair
Tom Rudolphi, Award Symposia Chair
Pranav Shrotriya, Wei Hong
Bioengineering Materials, Mechanics and Structures Symposia Chairs
Hui Hu, Shankar Subramaniam, Fluid Mechanics Symposia Chairs
Valery Levitas, Michael Kessler
Mechanics of Materials and Structures Symposia Chairs
Stephen Holland, R. Bruce Thompson
Non-Destructive Evaluation of Materials Symposia Chairs
Pranav Shrotriya, Scott Beckman, Students Symposia Chairs
Contents

4 Foreword
5 Welcome from College of Engineering Dean
6 Plenary Lecture Abstracts/Presentation Awards
10 Graduate Student Abstracts/Presentation Awards
49 Undergraduate Student Abstracts
57 Abstracts by Symposium

58 Track 1: Horner Symposia
59 Symposium in honor of the contribution of Ray Ogden, the recipient of the Prager Medal (1-1)
101 Symposium in honor of the contribution of Roger Fosdick, the recipient of the Engineering Science Medal (1-3)

127 Track 2: Bioengineering Materials, Mechanics, and Structures
128 Cell Mechanics (2-2)
143 Biomechanics/Bioimaging: Inducing and Tracking Mechanical Deformations in Tissue and Living Cells for Diagnostics and Therapy (2-3)
157 Orthopaedic Bioengineering – Nano-science to Device Level (2-4)
175 Mechanics of Soft Materials (2-5)
207 Experimental Techniques for Multiphysics and Multiscale Analysis (2-6)

212 Track 3: Fluid Mechanics
213 Nonlinear Mechanics in Celebration of the 60th Birthday of K. R. Rajagopal (3-1)
230 Dynamics and Rheology of Complex Fluids (3-2)
240 Experimental Fluid Mechanics in Single and Multiphase Flows (3-3)
245 Microfluidics and Nanofluidics (3-4)
250 Fluid Issues in Renewable Energy Systems (3-5)
256 Multiphase Flow (3-8)

261 Track 4: Mechanics of Materials and Structures
262 Nanomechanics: Beyond Modulus and Hardness (4-1)
283 Theoretical and Computational Studies of Defects in Crystals and the Mechanical Properties of Solids (4-2)
294 Strain Rate Effects in Low Impedance Materials (4-3)
300 Size Scale Effects in Micro/Nano Structured Materials and Composites (4-4)
316 Phase Transformations and Mechanochemistry (4-5)
328 Multifunctional Composite Materials (4-6)
358 Multiscale Modeling of Micro/nano Structural Think Films (4-7)
365 Instabilities in Solids (4-8)
371 Failure and Fracture of Heterogeneous and Multilayer Materials (4-10)
381 Mechanics of Materials and Structures in Emerging Technologies (4-12)
406 Laser and Multi-Energy Interactions with Materials (4-13)

422 Track 6: Nondestructive Evaluation
423 Infrastructural NDE and Structural Health Monitoring (6-1)
433 Probing Inhomogeneous Media (6-2)
Foreword

The SES-organizing committee welcomes you to the 47th Annual Technical Meeting of the Society of the Engineering Science (SES 2010) hosted by Iowa State University.

This year, the SES 2010 conference has an overarching theme of multi-scale multi-physics phenomena. More importantly, this year’s conference reflects the ever-changing focus of applied mechanics into new areas such as energy storage and conversion, flexible displays and macro-electronics, and the growing area of bioengineering materials and structures. Unique to this year is the Nondestructive Evaluation of Materials track, which is a hallmark of research at Iowa State University. This year’s conference has 27 symposia with more than 350 papers and about 300 attendees. It is noteworthy that we have more than 120 graduate students attending today. The conference will have eight parallel sessions in eight rooms.

Two student paper competitions will be running in parallel. The graduate student paper competition has 23 finalists, who received either NSF or ISU travel fellowships. Their papers will be presented within regular scheduled symposia. The undergraduate paper competition has 6 entries and will be conducted on Wednesday morning. The winners will be announced by the end of the conference.

Three SES medalists will be recognized at the banquet: Raymond Ogden, recipient of the Prager Medal; Robert Ritchie, recipient of the Eringen Medal and Roger Fosdick, recipient of the Engineering Science Medal. The new SES fellow is David Steigman and the recipient of the SES Young Investigator Medal is Prof. Ioannis Chasiotis.

For many of you, this is undoubtedly your first visit to Ames and ISU, or even Iowa. If so, we extend a most hardy welcome to our beautiful campus and hope you take sometime to explore our campus and community while you are here. We wish you a great and enjoyable visit, and we hope that you will find this meeting interesting and intellectually stimulating. Finally, we would like to thank NSF for sponsoring the graduate and undergraduate travel fellowships, as well as all the symposium organizers and conference staff for all their time and effort in organizing this conference.

Ashraf Bastawros  
Conference Chair  
Department of Aerospace Engineering  
College of Engineering  
Iowa State University
Welcome From College of Engineering

October 3, 2010

Dear SES attendees,

On behalf of the College of Engineering at Iowa State University, I am pleased to welcome you to the 47th Annual Technical Meeting of the Society of Engineering Science.

The opportunity to host this meeting at Iowa State is a great honor, and the university takes pride in knowing that the diverse research on this campus is so widely recognized.

Your topical tracks during this technical meeting include areas that are not only of great interest, but also point to the strengths of our sponsoring departments—aerospace engineering, materials science and engineering, and mechanical engineering—and their associated research centers and labs. Our ongoing work encompasses micro- and nano-mechanics, nondestructive evaluation, bioengineering, and advanced materials synthesis and characterization.

The SES mission of transcending boundaries to find solutions to the critical issues that face us today resonates well with the strong tradition of interdisciplinary research at Iowa State. In particular, the College of Engineering participates extensively in research collaborations across campus, and enjoys close connections with the US Department of Energy’s Ames Laboratory, the Center for Nondestructive Evaluation, the NSF Engineering Research Center for Biorenewable Chemicals, and many others. We are an expanding college, both in terms of enrollment and research funding, and continue to attract world-class faculty who bring us international recognition.

We have much to offer and much to learn. In the SES spirit of expanding understanding and enhancing discussion, it’s exciting to consider the knowledge and ideas that will be exchanged over the next four days.

I wish you great success at this meeting and beyond.

Best regards,

Jonathan Wickert
Dean, College of Engineering
Iowa State University
Plenary Lecture Abstracts
A Causality Approach to Particle Dynamics

Roger Fosdick
Department of Aerospace Engineering and Mechanics
University of Minnesota

Abstract:

Causality in physics is an old idea which emphasizes the notion that there are 'causes' and 'responses' to those causes, and this is expressed through a fundamental equation which is supposed to describe the evolution of a physical system such as the dynamical system of a set of particles. In a most elementary example, one may identify the power input to a system as the 'cause' and the rate of change of the internal plus kinetic energy of the system as representing the 'response'. In this case, the balance of one against the other is a statement of balance of energy for the dynamical system and often this is postulated as fundamental in mechanics. We do not follow this approach here, but rather pursue a more primitive causality based approach for describing the dynamics of a system of particles. Forces intrinsic and extrinsic to the system are introduced and an evolutionary causality law, which is form-invariant under a change of frame, is proposed. We assume, as is common, that intrinsic forces are objective under a general change of frame. Extrinsic forces are assumed to be objective only under a Galilean (i.e., inertial) change of frame. This limited objectivity plays a major role in reducing the fundamental proposed 'law of causality' to what is commonly recognized as the classical balance of energy for the system. The concept of mass is not introduced as primitive in this work; the existence of 'inertial constants', each of which associates with a specific particle of the system, is a result of the theory. Motion, force, power, a law of causality and invariance are the fundamental elements of this work.

As an extension of the particle-particle binding force structure considered in classical theory, the fundamental intrinsic force structure of this theory is composed of two kinds: (i) double-binding forces between pairs of particles, and (ii) triple-binding forces between triples of particles. The origin of the balance of linear momentum for the system and a generalized intrinsic force action-reaction principle is discussed. The emergence from the causality theory of pair- and triple-particle potential functions is noted and these potential functions are shown to be intimately related to the corresponding pair- and triple-binding forces, respectively. Additionally, the underlying invariance structure of the theory shows that the double- and triple-binding forces must be separately 'moment-balanced' and this gives rise to the balance of moment-of-momentum for the system. Finally, a constitutive theory for the intrinsic forces is introduced and it is shown that the double- and triple-binding forces are determined explicitly by the pair-particle and triple-particle potential functions.
Bone as a Structural Material: 
Origins of its Fracture Resistance and Biological Degradation

Robert O. Ritchie
Materials Sciences Division, Lawrence Berkeley National Laboratory, and 
Department of Materials Science and Engineering, University of California, Berkeley

Abstract:

The age-related deterioration in the quantity of bone and its architecture and resultant fracture properties, coupled with increased life expectancy, are responsible for increasing incidences of bone fracture in the elderly segment of the population. In order to develop effective treatments, an understanding of the mechanisms underlying the structural integrity of bone, in particular its inherent fracture resistance is essential. Here we examine the origins of the toughness of human cortical bone in terms of the contributing micro-mechanisms and their characteristic length scales in relation to its hierarchical structure. It is shown that at length-scales at or below a micrometer or so, the toughening mechanisms in bone are primarily intrinsic, and include mechanisms such as fibrillar sliding at the collagen fibril (i.e., ~100 nm) and collagen fiber (~1 μm) levels. These are essentially “plasticity” mechanisms that operate ahead of a growing crack, e.g., by forming a plastic zone to blunt the crack tip. At length-scales above a micrometer or so, the toughening mechanisms are primarily extrinsic, and are associated with crack deflection/twist and crack bridging. In terms of measured fracture toughness of bone, the latter mechanisms are particularly potent; they affect the growth rather than the initiation of cracks and as such lead to resistance-curve toughening behavior. There is also the process of microcracking, which in addition to serving as an intrinsic “plasticity” mechanism and possibly signaling the remodeling of bone, acts principally to motivate the extrinsic deflection and bridging mechanisms, which in turn results in the marked anisotropic fracture behavior. In this context, realistic short-crack measurements of the crack initiation and growth toughnesses are used to evaluate the effects of aging and certain drug treatments (e.g., steroids, bisphosphonates) in bone, and are combined with structure characterization using UV Raman spectroscopy, transmission electron microscopy, 2-D in situ fracture tests in an environmental scanning electron microscope and 3-D ex situ examination of crack paths using synchrotron x-ray computed tomography, to determine the microstructural features that underlie the toughness of bone and how this can degrade with biological factors.
Deformation invariants play an important role in the constitutive modeling of many materials, including isotropic and anisotropic elastic materials. Such materials include fibrous biological tissues, electro-sensitive and magneto-sensitive elastomers, for which one or two preferred directions can be identified within an isotropic matrix. In these examples, invariants that depend on the preferred direction(s) are constructed and included in the constitutive law along with the usual isotropic invariants. Other examples are materials that are subject to initial (or residual) stress, in which case the initial stress acts as a structure tensor from which invariants are constructed. There are many applications of constitutive laws for initially-stressed materials, ranging from modeling the properties of arteries, to shrink-fit engineering components, to non-destructive evaluation of material properties, to seismic wave propagation problems, for example. In this talk we illustrate the use of invariants in three areas of application: (1) arterial wall mechanics, (2) magnetoelasticity of elastomers, and (3) wave propagation in transversely isotropic initially stressed materials. One representative reference from each of these areas is listed below.

References
Graduate Student Abstracts/Presentation Awards

ORGANIZERS:

Pranav Shrotriya, Iowa State University
Scott Beckman, Iowa State University
Coarse-Graining Atomistic Dynamics of Dislocations: from the Atomic to the Mesoscopic

Liming Xiong and Youping Chen
Department of Mechanical and Aerospace Engineering, University of Florida, Gainesville, FL, USA

Introduction
At angstrom level, single-atom displacements account for deformations as dislocations predominate at the mesoscopic scale for metallic crystalline solids. The mesoscopic motion of dislocations, on the other hand, is the mechanism for plastic deformation at macroscale. Atomistic simulation has been the most powerful tool for understanding of the atomistic dynamics of dislocations. However, the state of art supercomputer MD can only handle about 10^9 atoms, amounting to a volume of less than a cubic micron. It is unlikely, in the near future, for MD to explain and predict complex phenomena of dislocation plasticity observed in macroscopic specimens. To model dislocation plasticity from atomic to meso- or macroscopic length scales, we are in need of multiscale methodologies.

Existing multiscale modeling methods generally fall under one of two possible catagories. One approach is hierarchical such as discrete dislocation (DD) method, in which dislocations are treated as continuum entities moving in the field determined by elasticity. Conmutative rules are used to describe the short range interactions between dislocations. The rules dictate dislocation nucleation, dislocation junction, dislocation mobility, etc. Suitable values for the parameters in these rules are fitted, in principle, from fully atomistic simulations. The second approach is concurrent such as the Quasicontinuum method, in which regions with defects are modeled by fully atomistic approach and other regions by continuum scheme. Most successful concurrent multiscale plasticity modeling methods may be the coupled atomistic and discrete dislocation (CADD) method developed by Shillor et al. Recently, as a complement to CADD, a new model that couples a region of material described by discrete dislocation to a surrounding region described by conventional crystal plasticity is presented by Wallin et al.

The New Methodology
The objective of this work is to present a new coarse-grained methodology for dynamic simulation of dislocations in L12 copper and to test its accuracy and efficiency relative to MD simulations. The new methodology combines (1) a continuum field representation of balance equations for metallic crystals with fully atomistic information built in the formulation (Chen J. Chem. Phy. 2009), and (2) a modified finite element method with rhombohedra-shaped 3D linear solid element to enable simulation of dislocations glide between elements on (111) or (111) slip systems along element boundaries. With the new formulation of balance equations, the discretized governing equations at the atomic scale are identical with the governing equations in the atomistic N-body dynamics. Using the concept of shape functions, on the other hand, atomic displacements can be constrained to reduce a majority of degrees of freedom in coarse-scale finite element simulations.

Computer Models and Simulation Results
Four computer models are simulated to compare the accuracy and efficiency of the CG method relative to MD in modeling dislocation activity. The objective of Model-1, shown in Fig. 1a-c, is to investigate dislocation-dislocation interactions. Although 1331 atoms have been embedded with each element in the CG model, it is seen that the threshold stress/strain values obtained by the CG is very close to that from MD simulation. Unlike a typical smooth stress-strain plot of bulk single crystals, the stress-strain curves from CG simulations are composed exclusively of elastic loading segments followed by discrete strain bursts, a phenomenon observed in experiment. In Fig. 2, both CG and MD simulations show that Lomer-Cottrell locks are formed due to dislocation-dislocation interactions.

Fig 1 CG Model-1: (a) Specimen (74um x 23um x 5.4um, 849,178 atoms); (b) CG model (834 FE elements); (c) Initial condition; (d) Stress-strain curves by CG and MD.

Fig 2 Atomic arrangement, dislocations and stacking faults in Model-1 under tension.
The objective of Model-2, shown in Fig. 3a-c with an asymmetric geometry, is to investigate dislocation-stacking fault interactions. In Fig. 3d, it is seen again that the stress-strain curve by CG is comparable with that by MD. In Fig. 4, we observe that when the dislocation (blue atoms) approaches the stacking faults (red atoms), its elastic field unfolds the stacking fault layers. Thereafter, we see that the stacking faults have been cut by dislocations. This is also consistent with the observation and conclusion obtained by a previously reported fully atomistic simulation (Yamakov et al. 2003). Thus, the CG method presented in this work has captured the dislocation-stacking fault interactions without the loss of detailed atomistic information.

In Fig. 5, we present the computational set-up of Model-3 for a submicron-sized specimen. Time sequences of snapshots of atomic configurations, dislocations, and stacking faults are presented in Fig. 6. With significantly less computational cost (~4 thousand finite elements for ~6 million atoms) than that of fully atomistic simulations, large amount of dislocations are nucleated and multiple stacking fault ribbons are formed simultaneously in the CG simulations. Dislocation-dislocation interactions, dislocation-stacking fault interactions, and dislocation annihilation events are captured as shown in Fig. 6.

Discussions

In summary, we have presented a new CG methodology for dynamic simulation of dislocations. The methodology combines an atomistic formulation of balance equations and a modified finite element method with rhombohedral-shaped 3D solid elements. With the majority (99.4%) of the degrees of freedom being eliminated and without additional constitutive rules for dislocation activities, the CG method is shown to be able to model complex dislocation activities including dislocation junctions, dislocation-stacking fault interactions, dislocation annihilation, etc., all comparable with MD simulations.

The accuracy of the new CG simulation depends on the force fields, in addition to the size and shape of the finite elements. Future work will include more sophisticated force fields, tetrahedron-shaped elements to allow complete modeling of dislocation activities or interactions, and/or adaptive meshing to distinguish regions of higher defect concentration from coarsened regions, and parallelization of the computer code for sub-millimeter to millimeter-sized specimen.
Fracture Behavior of Mechanophore-Linked Glassy Polymers

A.N. Celestine1,4, B.A. Beiermann2,4, D.A. Davis3,4, J.S. Moore2,3,4, N.R. Sottos2,4, S.R. White1,4
1 Department of Aerospace Engineering, University of Illinois at Urbana-Champaign
2 Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign
3 Department of Chemistry, University of Illinois at Urbana-Champaign
4 Beckman Institute, University of Illinois at Urbana-Champaign

The mechanophore spiropyran (SP) has been successfully incorporated into the glassy polymer, poly (methyl methacrylate) (PMMA) giving the PMMA mechanoresponsive capabilities [1, 2]. Spiropyran is a mechanochromic molecule where rupture of the spiro carbon-oxygen bond (activation) is accompanied by a vivid color change and an increase in fluorescence. In this study we explored the fracture behavior of both linear and cross-linked SP-PMMA.

The linear SP-PMMA was prepared by Atom Transfer Radical Polymerization (ATRP) where the SP mechanophore acted as the initiator and was linked directly into the polymer chain. Samples of the linear SP-PMMA were then produced by compression molding the material at 157 °C for 15 minutes under a pressure of approximately 395 kPa. The cross-linked SP-PMMA was prepared by a free radical polymerization where the spiropyran served as one of the cross-linkers. Samples of the cross-linked SP-PMMA were made by polymerization in Argon-flushed Delrin molds. The resulting cross-link density was 1.0%. Control samples of both the linear and cross-linked PMMA were also prepared where the mechanophore (SP) was either absent, or tethered in positions in which no mechanochemical activation was expected.

Samples were then machined into rectangular test specimens for Double Cleavage Drilled Compression (DCDC) testing (Figure 1). The dimensions of each specimen were 25 mm x 8 mm x 2 mm with a hole of radius 2 mm drilled through the center. Specimens were polished and then pre-cracked by gently tapping a razor blade into the material near the upper and lower crowns on both faces [3]. Upon loading, these pre-cracks would propagate along the centerline of the sample in a stable fashion. Prior to testing, the specimens were bleached under a high intensity LED light source for 48 hours in order to fully close all SP molecules. DCDC testing was carried out under displacement control. Both the axial loading of the specimens and the data acquisition were controlled using LabVIEW. A digital CCD camera was used to collect images of the advancing crack, and monitor the crack length throughout testing.

Figure 1: Bleached DCDC test specimens (a) linear SP-PMMA (b) cross-linked SP-PMMA

All specimens exhibited stable crack growth with an average plateau stress ($\sigma_p$) of 23 MPa for the linear SP-PMMA and 18 MPa for the cross-linked SP-PMMA. The fracture toughness ($K_{lc}$) of both sample types was calculated using the beam-column model proposed by Plaisted et al [3]. This model relates $\sigma_p$ and $K_{lc}$ by an equation of the form:

$$\frac{\sigma_p \sqrt{w}}{K_{lc}} = \frac{w}{2g(w/R)}$$

where $w$ is the half-width of the sample and $R$ is the radius of the central hole. $g$ is a non-dimensional function such that:

$$g(w/R) = \frac{3 + 2\ln(w/R)}{4(w/R)} - \frac{1}{4(w/R)^2}$$
The fracture toughness for the linear SP-PMMA was found to be 0.84 MPa-$m^{1/2}$ while that of the cross-linked SP-PMMA was 0.62 MPa-$m^{1/2}$. The applied stress versus normalized crack length data is shown in Figure 2 for one linear SP-PMMA sample and one cross-linked SP-PMMA sample.

![Graph](image)

**Figure 2:** Applied stress versus normalized crack length for linear and cross-linked SP-PMMA during DCDC testing

After testing, all specimens were imaged using confocal microscopy to identify regions of activated spiropyran. Confocal microscopy uses a point laser source to achieve high-resolution interior imaging of the specimens in the regions of interest. Figure 3 is a confocal microscope image showing increased fluorescence along the crack of a cross-linked SP-PMMA specimen. This fluorescence is an indication of spiropyran activation during fracture.

![Confocal Image](image)

**Figure 3:** Confocal microscope image showing fluorescence along the crack of a cross-linked SP-PMMA specimen

Current work is focused on increasing the spiropyran activation-zone size during fracture. The effects of loading rate, cross-link density and spiropyran concentration on mechanophore activation and fracture properties are also being investigated.


Stability of periodic media under coupled electromechanical boundary conditions
Stephan Rudykh¹(a), Gal deBotton¹(b), and Kaushik Bhattacharya²(c)
¹ Department of Mechanical Engineering, Ben-Gurion University, 84105 Beer-Sheva, Israel
² Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125

Electroactive polymers (EAP) are soft dielectrics that change their shape and size in response to electric excitation. Roughly speaking, the electrostatic induced Maxwell stress results in deformation of the material. Various applications of EAP based actuators have been considered in recent years¹-⁶. Consider a planar actuator

![Deformed Configuration](image)

FIG. 1. A planar EAP actuator.

(Fig. 1) made out of dielectric elastomer. The bottom and top surfaces of the actuator are covered with thin electrodes with negligible elastic modulus¹ that enable to induce an electric field across the material. When a potential is applied the actuator expands in the plane directions to an equilibrium state with stretches \( \lambda_1, \lambda_2, \lambda_3 \).

In this study, we follow the theory of nonlinear electroelasticity⁵,⁷, where the total stress is

\[
\sigma^{(t)}_{ij} = \sigma^{(c)}_{ij} + \sigma^{(m)}_{ij},
\]

Here, \( \sigma^{(c)}_{ij} \) is the Cauchy mechanical stress, \( \sigma^{(m)}_{ij} = \epsilon_0 E E_{ij} - \frac{1}{2} \epsilon E_n E_n \delta_{ij} \) is the Maxwell stress induced by the electric field \( E \), \( \epsilon \) is a dielectric modulus, and \( \epsilon_0 \) is the vacuum permittivity. We assume that \( \epsilon \) does not depend on deformation or electric field. We adopt a quite general constitutive law for incompressible isotropic materials, in

\[
\sigma^{(c)}_k = \sum_{p=1}^{N} \mu_p \lambda_p^{2p} - q_c,
\]

where \( \lambda_p \) are the principal stretches, \( q \) is an arbitrary hydrostatic pressure, \( \mu_p \) are shear moduli, and \( \sigma_p \) are material constants. In the case \( N = 1 \) with \( \alpha_1 = 2 \), the model (2) which is commonly denoted Ogden model, reduces to the neo-Hookean one.

The main limitation of EAP originates in the need for relatively large electric fields. Fortunately, there exist some ways to enhance the actuation and reduce the need of high values of electric field.

First, the effective properties of composite EAP can be manipulated by changes in microstructure⁸. In heterogeneous EAP composite, the stiffer phase is characterized by higher dielectric constant. If we substitute the homogeneous elastomer by a laminate composite with arbitrary lamination angle \( \Theta \) (see Fig. 2) in the planar actuator, a remarkable enhancement of mechanical response to electrical excitation can be achieved. The influence of the lamination angle on the response of the plane actuator under plane strain conditions \( \lambda_2 = 1 \) is demonstrated in Fig. 3 for a neo-Hookean composites with inclusion volume fraction \( \epsilon'(k) = 0.2 \), shear modulus ratio \( t = \mu'(k) / \mu'(m) = 10 \) and dielectric constant ratio \( k = \epsilon'(k) / \epsilon'(m) = 10 \). The curves represent examples for an exact analytical solution for the equilibrium path. The value of the optimal angle of lamination can be determined for a desired actuation or electrical excitation. However, instabilities may occur during an equilibrium path which may lead to a bifurcation of the solution. Though, this phenomenon is commonly considered as a

---

¹) Electronic mail: rudykh@bgu.ac.il
²) Electronic mail: debotton@bgu.ac.il
³) Electronic mail: bhatta@caltech.edu
negative one which should be predicted and avoided, in some cases, it can be utilized for our benefits. An example of such application is the response of EAP balloons. We demonstrate that a relatively small electrostatic field can be used as a trigger for large deformations.

Consider a spherical balloon made out of a dielectric elastomer with inner \( R_i \) and outer \( R_o \) radii. The thickness of the balloon wall is \( H = R_o - R_i \). The electric field is induced by thin electrodes with negligible elastic modulus on inner and outer surfaces of the balloon wall. The balloon can be inflated with inner pressure \( P_i \), and electrically exited with electric potential \( \varphi_0 \) between the two electrodes. With the increase of the inflation pressure the balloon slowly expands until a critical pressure is reached. Further increase in the pressure leads to a sudden jump in the size of the balloon to a new stable state. This phenomenon is commonly denoted “snap-through”. Application of electric field reduces the critical pressure at which the balloon snaps. We observe that this effect cannot be recovered with the neo-Hookean material (dashed curves in Fig. 4). Similarly, electrostatic excitation which is applied in the undeformed configuration leads to expansion of the balloon up to a critical electric field. Further increase in the electric potential results in a snap-through of the balloon. When applied to a pre-inflated balloon, the critical electric field at which the instability occurs decreases. For thin-wall spheres the general solution can be simplified to

\[
P_i = \frac{2H}{R} \sum_{p=1}^{n} \mu_p \left( \lambda^{2p-3} - \lambda^{-2p-3} \right) - \epsilon_0 E_0^2 \lambda,
\]

where \( E_0 = \varphi_0 / H \) is the referential electric field.

We note that Eq. (3) provides a fair estimate for \( t \gg 0.9 \). However, for micro-actuators with a diameter of a few tenth of micrometers this approximation will lead to considerable errors.

Concerning instabilities of composite media, we provide a general condition for the onset of bifurcation in terms of homogenized electroelastostatic moduli. These moduli of the composites can be obtained analytically via homogenization procedure or numerically by technique similar to the one used for the pure mechanical case. The examples for the layered composites are demonstrated. We conclude noting that the results for onset of failure of the composites under coupled electromechanical boundary conditions recover the previous results for the pure mechanical problem.

Three Dimensional Compressible Multi-material Flows

Anil Kapahi, John Mousel, Shivkumar Sambasivan and H.S.UdayKumar
3131 Seamans Center for the Engineering Arts and Sciences, University of Iowa, Iowa city, IA

Shock Waves and Detonation waves have been topic of cutting edge research for decades. The interaction of these waves with multi-materials can result in complex wave structures in two and three dimensions. Large-scale computations are required to simulate physical phenomena involving detonation and shock waves like supernova formation, explosions and hypervelocity impact and penetration. In this paper we describe the parallel implementation of fixed Cartesian grid flow solver with moving boundaries. A higher order conservation scheme such as ENO is used for calculating the numerical fluxes and level sets are used to define the objects immersed in flow field. The Euler equations were solved using a third-order TVD based Runge-Kutta scheme for time integration and third-order convex ENO scheme for spatial discretization. A Riemann solver based Ghost fluid method (GFM) is used for interface treatment of embedded objects. This paper describes the methodology for parallelization with emphasis on strong shocks interacting with embedded interfaces (solid-fluid, solid-solid and fluid-fluid) in three-dimensional compressible flow framework. In order to accurately decouple the interface conditions and the associated impedance mismatch, a Riemann problem was constructed normal to the interface and the solution obtained from solving the Riemann problem were used to define the ghost states. In the case of embedded solid objects, a reflective boundary condition endowed with Riemann correction was employed to capture the interface conditions. The method developed was shown to be effective in solving a wide repertoire of problems involving shocks of varied magnitude interacting with the embedded object(s).

The levels set based sharp interface methods are very popular for fixed Cartesian grid problems. This treatment reduces the complexity involved in grid generation and helps in defining complicate shapes using level set functions. A simple and a unified Cartesian grid approach were developed for accurate representation of embedded solid and fluid objects in high-speed compressible multiphase flows. The methodology formulated was based on the Ghost Fluid Method (GFM) due to Fedkiw and coworkers. The pivotal theme in the GFM approach lies with the definition of band of ghost points corresponding to each phase of the interacting media. The ghost band when supplied with appropriate flow conditions, together with the respective real fluid, constitutes a single flow field. Hence higher order numerical schemes such as ENO and WENO, developed for single component flows can be directly employed with no special categorical treatment or reduction in the order of accuracy at the interface. The success of the GFM approach largely depends on the accuracy with which the ghost states are predicted.

The idea is extended to develop a distributed computing based algorithm for solving three-dimensional shock-interface interactions. The main idea of the parallel algorithm is to avoid storage of global information proportional to the size of the problem on a single processor. The algorithm is designed to execute on a distributed memory system. The inter processor communication is handled using MPI library. A domain decomposition software that creates balanced partitions is highly desirable for parallel algorithms. In the following setup, METIS a graph partitioning software is used for better load balancing. METIS uses the nodal connectivity as an input to generate partitions, which are optimally load balanced. It also minimizes the communication time by minimizing the total edge cuts. The parallel algorithm used is explained in our work with both two and three- dimension problems. We have also addressed the problems
related to handling (storage/retrieval) of global data, definition and construction of ghost layer, special treatment for moving boundaries and handling of GFM at processor boundaries. The two simulations shown below are the shock wave interaction with hundred stationary particles and the three dimensional Taylor bar impact case.

Figure 1 shows the simulation involving interface treatment of multiple particles in parallel framework. Figure 2 shows the velocity profile of Taylor bar impact case (initial velocity = 400m/s in negative Y-direction).

Figure 1. Schlieren Image of Shockwave hitting multiple particles

Figure 2. Y-direction velocity profile of Taylor bar impact
Experimental and Modeling Study to Determine the Turgor Pressure and Cell Wall Thickness of Arabidopsis

Elham Forouzesh, Ashwani Goel, Joseph A Turner
Department of Engineering Mechanics, University of Nebraska-Lincoln, W317.4 Nebraska Hall, Lincoln, NE 68588-0526, USA.

Abstract
Plant cell walls are thin, tough, complex, and dynamic structures composed mainly of a network of extended polysaccharides [1]. In higher plants the dominant structural features are cellulose microfibrils, wrapped around the cells, which are cross-linked by single-chain polysaccharides such as xyloglucans embedded in a matrix mainly composed of pectin. The cell wall is responsible for filtering large molecules that can poison the cell. It also provides the structural support for the cell against expansion. When the water enters the cell due to osmosis it results in an increase of Turgor pressure. Turgor pressure plays an important role on the physiological behavior of a plant cell; it also has a direct effect on the mechanical properties of the cell. Plant water status can be measured via water potential or relative water content. This pressure is balanced by the stresses within the cell wall that provide the necessary force required for expansion of the growing cell [2]. The cell wall stresses depend on the cell geometry, cell wall thickness, cell wall mechanical properties, and Turgor pressure. Refregier et al [3] reported that, assuming equal growth conditions, thin-walled cells grow faster than thick-walled cells. The mechanical properties of plant cell walls influence the stability of the plant and also play a major role in plant growth. Therefore, measurement of the cell wall thickness and Turgor pressure is crucial to a clear understanding of its function. The conventional method for measuring the cell wall thickness is Transmission Electron Microscopy (TEM) or Scanning Electron Microscopy (SEM) both of which methods are destructive such that no further analysis can be performed on the cell. For Turgor pressure, different destructive methods such as thermocouple psychrometers, pressure chamber [4] and non-destructive methods such as ultrasonic spectroscopy measurement [5], plant-base probe [6] and leaf thickness measurement have been suggested, but these methods are mainly used for studying the water status of a given tissue and they can not be used to study single cells. The conventional method for measuring Turgor pressure in single cells is using pressure probe. However, it is not very accurate for small cells and it is very time consuming and technically demanding. It also is a destructive test and the tested cells can not be used for further studies.

In this study a new non-destructive technique is proposed for measuring the cell wall thickness and Turgor pressure using nanoindentation. Nanoindentation has proven itself to be a powerful technique for the measurement of mechanical properties and can be used in diverse applications ranging from mineralized tissues to soft tissues. We have used this technique to quantify, in vivo, the Turgor pressure and thickness of cell wall based upon cyclic tests. Due to various unknowns in the problem, which includes shape and morphology of the plant, turgor pressure, instantaneous elastic modulus and viscoelastic material properties of the cell wall, a protocol has been developed that can be used to systematically evaluate the unknown parameters. This protocol combines the cyclic loading unloading experiments, relaxation tests, nano DMA, and a finite element model (FEM). Using the nano-DMA results and the results obtained from relaxation tests on live plant cells the cell wall was simulated. Figure 1 explains the steps for defining the turgor pressure in the cell and applying the load on the cell wall.
Tests are performed on Arabidopsis plant using nanoindentation technique within the same area on the abaxial (lower) side of leaves. Since the leaves have thinner wax layer on the bottom side, all the tests were done on the bottom part of the leaf. The leaves were mounted on a double sided tape to eliminate any movement while performing the indentations. Cyclic load was applied on the cells using a spherical indenter, R=2.5μm, and the slope at unloading were calculated versus displacement (see Fig. 2). According to the FEM simulations, the displacement where the curve changes to a plateau is half of the cell wall thickness and the value of the slope at the plateau can be fitted with FEM which gives us the turgor pressure, Figure 2.

To investigate the effect of environment on the turgor pressure, three different samples were prepared. Hypertonic samples were prepared by immersion of the leaves in 10% NaCl solution, and hypotonic samples were prepared by immersion of the leaves in pure water. The results of these two samples were compared with the healthy isotonic leaves tested in air. These results show that the proposed method can distinguish between the different pressure states of the cells as expected from environmental conditions. It is anticipated that techniques such as this will enhance the understanding of plant cell wall structure and the influence of the environment on plants.

References
Thermoresponsive Microcapsules for Autonomic Lithium-Ion Battery Shutdown

M. Baginska1, B.J. Blaiszik2,4, S.A. Odom3,4, J.S. Moore3,4, N.R. Sottos2,4, S.R. White1,4
1Department of Aerospace Engineering, University of Illinois at Urbana-Champaign
2Department of Materials Science, University of Illinois at Urbana-Champaign
3Department of Chemistry, University of Illinois at Urbana-Champaign
4Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign

Li-ion batteries are the focus of significant research due to their potential for high energy density, lack of memory effect and ability to handle hundreds of charge/discharge cycles1. Predominantly used in consumer electronics, improvements in safety of lithium-ion batteries are required before their full market penetration. Fail-safe shutdown in the event of overcharge, short circuits, or exposure to high-temperature environments could make Li-ion batteries a viable choice for defense, automotive, and aerospace applications while improving the safety of devices. The normal operational temperature for a Li-ion battery is between temperature of 40°C and 60°C. However, localized thermal hotspots (>100°C) can develop on battery electrodes. It is desirable to quench these thermal hotspots in order to prevent thermal instability of the battery. If the internal battery temperature continues to increase (>130°C), global shutdown should be initiated. The current defense against internal battery overheating, the shutdown separator2, is not ideal since localized heating can result in separator shrinking and melting, leading to physical electrode contact and potential explosions.

One approach to improved safety in Li-ion batteries is the incorporation of functional microcapsules, which can be used to trigger battery shutdown mechanisms. The proposed concept is shown schematically in Figure 1 and can be achieved by either of two approaches. In one approach, battery electrodes are functionalized with monomer-filled microcapsules, which are then triggered to rupture within a desired temperature range and deliver a thermally polymerizable core to the electrode surface, electrically isolating the electrodes and effectively shutting down the battery cell. In the second approach, the electrode is coated with capsules that undergo a phase transformation (melt) at a predetermined temperature, and coating the electrodes with a non-conductive separator.

Initial work on triggering mechanisms has been completed, including rupture experiments of several microcapsule core-shell chemistries conducted with direct observation of microcapsules on a microscope-mounted hot stage. The current triggering mechanism consists of encapsulating low-boiling point solvents which volatilize, increasing the internal pressure in the capsules until rupture occurs (Figure 2). While the low-boiling point solvent is the trigger, the rest of the core contains the thermally polymerizable monomer to shut down a battery cell undergoing thermal runaway. Initial work on thermal transition cores has also been conducted, including screening of candidate meltable polymers with melting points at approximately 100°C. Additionally, lithium-ion battery separators have been coated with thermal transition spheres and heated to investigate the shutdown potential (Figure 3).

Figure 1: Schematic representation of proposed shutdown concept for lithium-ion batteries.

Figure 2: a) Intact thermo-responsive microcapsules. b) Ruptured microcapsule after heating at 130°C/min.

Figure 3: a) PE microspheres spin-coated on battery separator. b) Microsphere coated separator post heat treatment.
Shear Activation of Mechanophore-Linked PMMA

C. M. Kingsbury1,4, D. A. Davis2,4, N. R. Sottos1,4,*, S. R. White3,4, J. S. Moore1,2,4
1 Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, 1304 W. Green St., 61801, Urbana, Illinois, USA
2Department of Chemistry, University of Illinois at Urbana-Champaign, 505 S. Mathews Ave., 61801, Urbana, Illinois, USA
3Department of Aerospace Engineering, University of Illinois at Urbana-Champaign, 104 S. Wright St., 61801, Urbana, Illinois, USA
4Beckman Institute, University of Illinois at Urbana-Champaign, 405 N. Mathews Ave., 61801, Urbana, Illinois, USA
*corresponding author: ph.: 217-333-1041, n-sottos@illinois.edu

A new strategy is employed to impart productive mechanochemical response to an elastomeric polymer [1]. Force sensitive molecules, termed mechanophores, are successfully incorporated as cross-linkers into poly-(methyl methacrylate) (PMMA) through a free radical polymerization initiated with benzoyl peroxide [2]. Evidence of local chemical reaction is provided by a color and fluorescence generating spiropyran (SP) mechanophore that undergoes an electrocyclic ring opening reaction under mechanical deformation. When spiropyran is in its closed form, it is a colorless, non-fluorescent molecule. Upon electrocyclic ring opening to the merocyanine form, it is a highly colored, fluorescent molecule. This ring opening can be driven by mechanical force, certain wavelengths of light, and heat and is also reversible. Here, we investigate the role of shear loading on bulk polymer specimens and the mechanical force required to perform this ring opening process.

Materials
Cross-linked PMMA was synthesized with a total cross-link density of 1%. Spiropyrans as either mechanically active, difunctional cross-linkers or mechanically inactive, monofunctional controls were incorporated into the polymers at 0.018 mol% with enough ethylene glycol dimethacrylate (EGDMA) or polyethylene glycol (PEG-550) to bring the total cross-link density to 1%. [2] These two molecules allow nearly identical polymers to be synthesized while allowing one polymer to have mechanically active spiropyran and the other polymer to have mechanically inactive spiropyran. Polymerization was carried out in 1 mL syringes which had been compression molded into tapered cylinders using a mold of the desired final dimensions. Nine different types of samples were prepared: PMMA cross-linked with EGDMA and either active SP, control SP, or no SP, and PMMA cross-linked with PEG-550 and either active SP, control SP, or no SP. The final sample dimensions included gauge section 2 mm in diameter and 10 mm in length.

Shear Experiment
Shear testing was performed on the mechanophore cross-linked PMMA. All 9 specimen types were tested using a torsion test fixture and a TA Instruments AR-G2 rheometer. Shear rates were held constant at 0.1 sec\(^{-1}\), 0.01 sec\(^{-1}\), and 0.001 sec\(^{-1}\) to allow the sample to undergo larger strains in torsion and to produce color change and fluorescence in the active samples. Images of samples cross-linked with EGDMA before and after testing are shown in Figure 1. Full field fluorescence imaging was employed to collect fluorescence data during mechanical testing. The cylindrical samples showed color change and fluorescence before failure and an activation stress, activation strain and activation strain energy could be found by analyzing the change in intensity of the images collected by the CCD in the full field fluorescence setup.
Results
The activation strain, activation stress and activation strain energy were higher at higher shear rates and were linearly dependent on shear rate. In an effort to lower the activation parameters, the major cross-linker (EGDMA) was replaced with PEG-550. We hypothesized that the longer length of the PEG chains compared to the spiropyran molecule would enhance load transfer to the spiropyran, thus leading to mechanical activation at a lower bulk shear stress and strain. The result of changing the major cross-linker from EGDMA to PEG was a lower activation shear strain, shear stress and strain energy for all shear rates. A summary of activation parameters is given in Table 1. Control tests were performed on PMMA with monofunctional spiropyran [2] and PMMA with no spiropyran. As expected, no color change resulted from the shear testing. (Figure 1) Experiments are in progress to understand the role of crosslink length, crosslink density, and the incorporation of other mechanophores on the shear-induced chemical reactions.

![Figure 1: Images of active and control samples cross-linked with EGDMA before and after testing at each shear rate.](image)

Table 1: Strain, stress and strain energy levels at activation for both EGDMA and PEG cross-linked polymers at each shear rate.

<table>
<thead>
<tr>
<th>Shear Rate</th>
<th>0.1 sec⁻¹</th>
<th>0.01 sec⁻¹</th>
<th>0.001 sec⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA-EGDMA-SP</td>
<td>Activation Strain: 74 ± 13 %</td>
<td>Activation Stress: 47 ± 3 MPa</td>
<td>Activation Strain Energy: 32 ± 7 MPa</td>
</tr>
<tr>
<td>PMMA-EGDMA-monofunctional SP</td>
<td></td>
<td>Activation Stress: 37 ± 1 MPa</td>
<td>Activation Strain Energy: 20 ± 2 MPa</td>
</tr>
<tr>
<td>PMMA-EGDMA</td>
<td>Activation Strain: 72 %</td>
<td>Activation Stress: 36 MPa</td>
<td>Activation Strain Energy: 26 MPa</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Shear Rate</th>
<th>0.1 sec⁻¹</th>
<th>0.01 sec⁻¹</th>
<th>0.001 sec⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA crosslinked with EGDMA and SP</td>
<td>Activation Strain: 58 ± 5 %</td>
<td>Activation Stress: 37 ± 1 MPa</td>
<td>Activation Strain Energy: 20 ± 2 MPa</td>
</tr>
<tr>
<td>PMMA crosslinked with PEG-550 and SP</td>
<td></td>
<td>Activation Stress: 28 ± 2 MPa</td>
<td>Activation Strain Energy: 12 ± 3 MPa</td>
</tr>
</tbody>
</table>


Room Temperature Healing of a Thermosetting Polymer Using the Diels-Alder Reaction

Amy M. Peterson
Drexel University, Chemical & Biological Engineering, Philadelphia, PA

A new healing system has been prepared in which a bismaleimide solution is used as a healing agent for a furan-functionalized epoxy-amine thermoset. Upon application of the healing agent to a fracture surface, the network swells and furan moieties along the crack surface form covalent bonds with maleimides via the Diels-Alder reaction. Incorporation of furan moieties in the polymer network was achieved through modification of an epoxy-amine network. Average healing efficiencies of approximately 70% were observed for the high concentration with some specimens showing >100% healing. Healing is possible multiple times.

The ability of bismaleimide solutions to function as healing agents was evaluated by direct application of the healing agent to the crack surface of modified compact tension specimens of the furan-functionalized network. As bismaleimide concentration increased from 0M (pure solvent) to 0.577M, healing efficiency for the first healing increased on average from 33% to 70%, with some specimens recovering over 100% of their initial strength when healed with the 0.577M solution. Healing was possible multiple times with bismaleimide solutions, although healing efficiency dropped off significantly after the first two heals.

Figure 1: Proposed healing mechanism. Green pentagons represent solvent molecules, red notched trapezoids represent furans, blue triangles represent maleimides, and magenta trapezoids represent Diels-Alder adducts. (a) Healing agent is injected in the crack. (b) Solvent swells the polymer network. (c) On the nanoscale, furans along the crack surface come into contact with BMIs. (d) BMIs react with furans and covalently bond across the crack surface.

Healing in this system results from a combination of covalent and physical bonding. Covalent bonds are formed through the Diels-Alder reaction of furans and maleimides. As maleimide concentration
increases in the healing agent, healing efficiency also increases. However, healing efficiency of 33% is observed when maleimides are not present in the healing agent, meaning that mechanical interlocking of crack surfaces contributes to healing. Mechanical interlocking results from swelling and subsequent deswelling of the polymer network with the solvent-based healing agent. These healing mechanisms occur on different length scales; mechanical interlocking occurs across micrometer scale cracks, while cracks must be smaller than 1.3 nm in order for the bismaleimide molecule to react across a crack. As a result, swelling and mechanical interlocking appears to enhance the amount of covalent bonding, and therefore healing efficiency. The overall healing mechanism is displayed in Figure 1. The healing system described is designed for use in fiber-reinforced composites. Three composite geometries were investigated for their ability to selfheal. In all cases, specimens were loaded to failure, healed, and loaded to failure again. An alternate healing efficiency was devised for the composite studies in order to account for the residual mechanical properties of a failed composite specimen:

\[
\frac{\alpha_{\text{healed}} - \alpha_{\text{unhealed}}}{\alpha_{\text{initial}} - \alpha_{\text{unhealed}}} \tag{1}
\]

In Equation 1, \(\alpha\) is the property measured for each geometry, i.e., maximum load or fracture toughness. Glass fiber-reinforced flexural specimens healed with a bismaleimide solution demonstrated 48% healing efficiency, while short beam shear specimens gave 37% healing efficiency. Healing efficiencies were low because failure of the composite resulted in significant irreversible failure of glass fibers. Double cantilever beam specimens were tested to focus on failure of the resin phase. However, 50% healing efficiency was obtained. Evaluation of the fracture surface revealed that only 30-35% of failure was cohesive in nature, with the remainder being adhesive (irreversible) failure. The optimal amount of healing agent is a significant consideration. Too little healing agent limits mechanical interlocking. However, more healing agent increases the time for total diffusion of solvent from the composite piece. Another challenge is optimizing the amount of bismaleimide in solution. Less bismaleimide results in fewer bonds bridging crack surfaces, but too much bismaleimide limits the number of molecules that will react across the crack, with most only reacting with one surface. Surface conditions also play a role in healing. Since covalent bonding across a crack surface is limited by the areas where the distance between surfaces is less than the size of the bismaleimide molecule, a smoother surface should result in more covalent bonding. However, another consequence of a smoother surface is less mechanical interlocking. The competing effects of surface condition on healing efficiency are under investigation. Solution-induced healing of glass-reinforced composites has been investigated. Although this study focuses on di-functional maleimide solutions as healing agents, higher functionality maleimides have been studied and their use results in improved load recovery. Systems with other furan-functionalized polymers are being investigated and have also demonstrated the ability to heal.
Collagen Fibrils: Multifunctional Nanoscale Components in Bone Structure

Majid Minary-Jolandan, and Min-Feng Yu
Department of Mechanical Science and Engineering, University of Illinois at Urban-Champaign, 61801

Collagen fibrils, as small as 50 nm in diameter, are the main organic constituents of the bone. Our experimental results using AFM-based techniques on individual collagen fibrils show that, owing to their special hierarchical structure, collagen fibrils are the origin of the two remarkable characteristics of the bone, namely the excellent toughness of the bone and its unique piezoelectric behavior.

Introduction: Collagen and Bone

Type I collagen, as the most abundant protein in mammals, is the main organic component of bone, tendon, dentine, and skin. Functioning in such diverse tissues shows the multifunctional capability of collagen fibrils. The alternating gap and overlap regions in the axial direction of a single fibril with a characteristic period of ~67 nm is believed to be an important factor enabling its multi-functionality. Inset in Fig. 1 is an atomic force microcopy (AFM) topography image of a single isolated collagen fibril with 85 nm in diameter.

Bone at the nanoscale is a composite composed of collagen fibrils and mineral nanocrystals, where mineral nanocrystals are deposited specifically in the gap region of the collagen fibrils[1]. Depicted in Fig. 1 is a high resolution surface image of cortical bone acquired using AFM. As indicated by arrows, collagen fibrils with their characteristic banding patterns are randomly oriented on the bone surface.

Bone exhibits remarkable mechanical properties, such as high toughness and strength. Strength of the bone is attributed to the hard hydroxyapatite nanocrystals (HA), with a modulus of ~100 GPa. In the case of toughness, however, there are several hypotheses; the widely accepted one is that the bone has energy dissipation mechanisms at its each seven levels of hierarchy [2]. More specifically, at the nanoscale, it has been shown that nanomechanical heterogeneity promotes energy dissipation in bone [3]. Furthermore, bone exhibits piezoelectric behavior, similar to certain crystalline materials [4]. The piezoelectric effect in bone has been proposed as the cause for the Wolff’s law, the ability of the bone to remodel itself under load [5].

In this letter, we focus on investigating mechanical (structural) and electromechanical (piezoelectric) properties at different scale levels, from sub-fibrillar microstructure of single isolated collagen fibrils up to bone samples. We show that single collagen fibrils as small as 50 nm in diameter within the bone are multifunctional nanostructures responsible for both nanomechanical heterogeneity and piezoelectricity of the bone.

FIG. 1. AFM image of cortical bone surface (scan size 5 μm) showing collagen fibrils. The inset is the topography image of a single collagen fibril with 85 nm in diameter (scan size 2 μm).

Nanomechanical Heterogeneity of Single Collagen Fibrils in Bone

We probed the nanomechanics of single collagen fibrils using two AFM-based techniques, static nanoindentation and dynamic elasticity mapping. Using near surface nanoindentation, in elastic regime below 3 nm depth, (<5% of the fibril diameter), we obtain force-deformation on more than 25 gap and overlap regions on a collagen fibril. The residual indentation footprints are shown in inset Fig. 2. Fitting the curves with the classical Hertzian contact theory between a sphere (AFM-tip) and a
cylinder (collagen fibril), we find that the overlap region is ~100% stiffer than the gap region.

![Graph showing overlap and gap regions](image)

**FIG. 2.** Nanomechanical heterogeneity within a single collagen fibril in the gap and overlap regions. The inset shows the nanoindentation footprints on a collagen fibril [6].

Dynamic nanoindentation with AFM, extracts both the elastic and viscoelastic behavior of materials with nanometer spatial resolution. In this technique, the AFM tip is modulated at a fixed frequency with small amplitude in contact with the sample surface. The resulting deformation of the sample surface is demodulated using a lock-in amplifier, and provides energy dissipation and energy storage capabilities of the sample. Depicted in Fig. 3b is a continuous map of elasticity of a single collagen fibril on a rigid surface. In agreement with the static nanoindentation, there is a nanomechanical heterogeneity along the axial direction of a collagen fibril correlating with gap and overlap regions. Fig. 3a, is a map of elasticity over the cortical bone surface showing that the mechanical heterogeneity revealed previously within isolated collagen fibrils persisted for the fibrils in the bone. *This is the smallest level of mechanical heterogeneity revealed for bone and might be related to the remarkable toughness of the bone at the nanoscale.*

**Piezoelectric Function of Collagen in Bone**

Piezoelectric measurements were conducted on single collagen fibrils using piezoresponse force microscopy (PFM), an AFM-based method that provides a map of piezoelectricity with nanometer resolution. As depicted in Fig. 3d, e, the piezoelectric map reveals that a single collagen fibril behaves as a piezoelectric material. Furthermore, there is an electromechanical heterogeneity in axial direction of the fibril, such that the overlap regions are the main piezoelectric regions of the fibril. Fig. 3c is a high resolution piezoelectric map of cortical bone surface revealing that collagen fibrils are responsible for piezoelectric effect in bone. Furthermore, the heterogeneity of piezoelectricity in bone is compatible with that of isolated collagen fibrils.

![Piezoelectric images from Fig. 3](image)

**FIG. 3.** Continuous map of elasticity on bone surface (a) and on a single collagen fibril (b) revealing persistence of nanomechanical heterogeneity of single collagen fibril for fibrils within the bone. High resolution piezoelectricity map on the bone surface (c) and on a single collagen fibril (d, e) revealing that single collagen fibrils are responsible for piezoelectricity of bone [7].

**Conclusion**

Our results revealed that collagen fibrils, as small as 50 nm in diameter, are multifunctional constituents of bone. They provide the smallest level of nanomechanical heterogeneity in bone leading to the excellent toughness of the bone. Furthermore, they are the source of piezoelectricity in bone, which is expected to be significant for bone growth and remodeling through modulating the ionic environment of the bone.

Internal Fluctuation of DNA in Nano Channels

Tianxiang Su
Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA, 19104, USA.

Prashant K. Purohit*
Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, USA.

ABSTRACT

Stretching DNA in nanochannels is an important technique for performing DNA mapping [1]. On the other hand, it also serves as a simplified model for studying single polymer behavior in concentrated polymeric solutions and melts [2]. For these reasons, mechanical behaviors of DNA inside nanochannels have been of great interest to both experimentalists and theorists in recent years. To date, scaling laws for the behaviors of confined DNA in both the de Gennes and Odijk regimes have been well developed, widely used and tested [3, 4]. However, fluctuation of the internal segments inside the DNA is still not well understood. This is important for genome mapping because it is the local fluctuation that determines the resolution of the mapping.

In this work, we study the internal longitudinal fluctuation of DNA confined in nanochannels and develop a scaling law to model the experimental data. We show that for a long DNA molecule whose contour length is much longer than its persistence length, the fluctuation versus mean value data collected from various locations along the polymer collapses onto a single curve with 0.5 power law (Fig. 1A). Without any fitting parameters, the scaling theory matches well with the experimental data. For short DNA, however, the scaling model fails and the data from different locations does not collapse onto a single curve (Fig. 1B). Following the framework in reference [5], a more detailed theory is developed. This theory models the DNA as a wormlike chain in a confined channel. The confinement effects are taken into account by quadratic potentials [6, 7]. These confinement terms together with the bending and potential energies give the Hamiltonian of the DNA chain:

\[ E = \int_0^l \frac{K}{2} \left( \frac{d\ell}{ds} \right)^2 ds + \int_0^l \left( \frac{\xi_x^2}{2} + \frac{\xi_z^2}{2} + \frac{\xi_y^2}{2} \right) ds - F \Delta x, \tag{1} \]

where \( K, L, s, \ell(s) \) are the bending modulus, contour length, arc

*Advisor of the student Tianxiang Su.
ments and turn the Hamiltonian Eq. 1 into a quadratic expression
\[ E = (1/2) \theta^T M \theta - FL, \]
where \( \theta_i \) are the angles formed by the discretized segments with respect to the longitudinal axis and \( M \) is the stiffness matrix. As shown in reference [5, 8], the partition function of the chain is determined by \( \det M \), while the angle fluctuation can be obtained by inverting the stiffness matrix \( M \):

\[ \langle \theta_i \theta_j \rangle = k_B T (M^{-1})_{ij}, \]  

(2)

where \( k_B \) is the Boltzmann constant and \( T \) is the absolute temperature. Fluctuations of the chain in both the longitudinal and transverse directions can be further evaluated from Eq. 2.

By changing the boundary conditions, regions that are most affected by the boundary effects are identified (Fig. 2). Surprisingly, not all the internal segments close to the boundaries are strongly influenced by the boundary conditions. Fluctuation of short internal segments, for example, are not significantly affected even though they are located close to the boundaries. The model for short DNA is further verified by Monte Carlo simulations (Fig. 3).

![Figure 3. Red circles: MC simulation results of (A) the longitudinal fluctuation of internal segments with one end at \( s_0 = 0 \) and (B) the angle fluctuation. Blue lines: corresponding theoretical predictions.

 \[ \text{Figure 2. Comparison of the internal fluctuation under different boundary conditions. The internal fluctuation between arc length} \ s \in [s_0, s_1] \ \text{of a short confined chain} \ (L = 100nm) \ \text{is calculated under two different boundary conditions: free ends and hinged-free ends. The difference in fluctuation is plotted with red color denoting the maximum difference regions and the blue color denoting the smallest difference regions.} \]

REFERENCES


Understanding the Influence of Strain on Quantum Transport in Graphene

Md. Zubaer Hossain
1206 W Green Street, MC-244, Urbana, IL 61801, Email: hossain2@illinois.edu

Harley T. Johnson
1206 West Green Street, MC-244, Urbana, IL 61801, Email: htj@illinois.edu

Low-dimensional systems such as graphene, graphene nanoribbons, carbon nanotubes, and quantum dots show remarkable promise for next generation electronic device applications. Nevertheless, owing to their nanoscale dimensions they are susceptible to undergo structural modifications [1-3] and respond to thermal excitations or chemical interactions with dielectric surfaces, electrode contacts, or foreign atoms [4-5]. An immediate technological concern of these nanoscale effects is the degradation or modulation of their outstanding material properties that can eventually impact their efficiency, reliability and performance in device applications. Here, using first-principles calculations it is revealed that graphene’s ballistic conductance – which is defined by $G = G_0 T(E)$, where $G_0$ is the quantum of conductance and $T(E)$ is the total transmission at energy $E$, and expressed as a sum over the transmission probabilities of the conducting eigenchannels – can be modulated by strain. In contrast to the assumption that graphene’s ballistic conductance is a constant, this research shows that strain alone can increase or decrease graphene’s ballistic conductance significantly.

Strain is unavoidable in graphene – either suspended or supported on a dielectric substrate, such as SiO$_2$. In suspended graphene, strain is biaxial type and one-atom thick graphene is under tension along the transport direction. On the other hand, supported graphene can have hydrostatic strain arising from wellknown structural corrugations. It is therefore crucial to identify the role of strain on transport properties in graphene. In a recent experiment [4], it is shown that local strain in graphene on a SiO$_2$ substrate can modify graphene’s conductance near the Fermi energy. The modification is attributed to a coupling of strain and phonon-mediated inelastic tunneling effects. However, conductance on the dielectric substrate is not ballistic and isolating the influence of strain is not possible. In this study, strain effects on ballistic conductance, an experimentally attainable transport property for suspended graphene [7], is studied using a combination of density functional theory and the Landauer-Buttiker formalism, and the results are presented in an article published recently [Appl. Phys. Lett. 96, 143118 (2010)]. The lattice constants for strained graphene are computed using the simple elasticity relation: $a(\varepsilon) = (1+\varepsilon)a_0$, where $\varepsilon$ is a strain tensor, $a(\varepsilon)$ and $a_0$ are strained and unstrained lattice vectors. The strained lattice parameter perpendicular to the transport direction is obtained through computing Poisson’s ratio using DFT calculations. The geometry of the supercell for transport calculations is shown in Fig 1.

It is found that, unlike in a CNT [8], regardless of the applied strain graphene’s conductance at the Fermi energy is 0.21$G_0$. Furthermore, for conducting electrons with energies higher or lower than the Fermi energy of the system tensile hydrostatic strain is found to increase conductance but compressive hydrostatic strain decreases conductance, as shown in Figs 2 and 3. For an 8% compressive hydrostatic strain conductance increases by as large as 30%. Surprisingly, for biaxial strain, if the energy of the conducting electrons is higher than the Fermi energy, conductance remain approximately unchanged, whereas conductance by electrons less than the Fermi energy decreases (increases) with compressive (tensile) strain along the transport direction. With technological advances, approaching ballistic values of electron conductance and harnessing the maximum possible
conductance in graphene have now become possible. Thus the findings of this work would advance efforts in further enhancing superior transport characteristics in graphene.
Thermodynamic Based Higher-Order Gradient Plasticity Captures Size and Interfacial Effects at the Micron and Submicron Length Scales

Masoud K. Darabia and Rashid K. Abu Al-Rubb
Zachry Department of Civil Engineering, Texas A&M University
College Station, TX 77843, USA
amasouddrb@neo.tamu.edu, brabualrub@civil.tamu.edu

Abstract
A thermodynamic based higher-order gradient plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces is presented. The elastic strain tensor, the effective plastic strain, and its gradient are assumed as the state variables. It is shown that interfacial effects have a profound impact on the scale-dependent yield strength and strain hardening of micro/nanosystems even under uniform stressing. All of the thermodynamic conjugate forces are decomposed into energetic components related to the Helmholtz free energy and dissipative components related to the rate of energy dissipation. Moreover, a procedure based on maximum energy dissipation principle is proposed for deriving the dissipative components directly from the rate of energy dissipation. A systematic way for derivation of different local/nonlocal plasticity/viscoplasticity yield surfaces is also proposed. Finally, the model capabilities in capturing size and interfacial hardening effects in metal matrix composites, interfacial effects on the yield strength of thin metal films on substrates, and nonuniform size-dependent deformation of micropillars under uniform stressing are illustrated through several examples.

Introduction
It is well-known by now that the classical (local) plasticity theories cannot be used successfully in either eliminating the meshdependency when simulating the strain localization problems or predicting the experimentally observed size-effect (i.e. smaller is stronger) at the micron and submicron length scales. Therefore, in the last decade there has been a significant interest by the mechanics community in formulating higher-order gradient plasticity theories based on principle of virtual work/power and/or the laws of thermodynamics. Most of these theories have been shown to completely or partially solve the problem of strain localization and/or size-dependent problems at the micron and submicron length scales. However, very few of these theories correctly estimate the rate of energy dissipation. The correct estimation of rate of energy dissipation requires the decomposition of thermodynamic conjugate forces into energetic and dissipative components as it is shown in the pioneering works of Shizawa and Zbib [1] and Gurtin [2]. Also, a lower-order gradient plasticity theory could not predict any boundary layer effect, which makes them unsuitable for modeling interfacial effects in thin films, particle-matrix interfacial effects in nanocomposites, and nonuniform and scale-dependent response of micropillars under uniform stressing. Hence, this work is an attempt to enhance the gradient-dependent plasticity theories by including the interfacial effects and make them more thermodynamically consistent by decomposing all thermodynamic conjugate forces into energetic and dissipative components and subsequently deriving the dissipative components directly from the definition of the rate of energy dissipation.
Nonlocal Thermodynamic Framework

We start with the principle of virtual power. Hence, the internal and external expenditures of power are assumed to have the following forms:

\[ P_{int} = \int_{\Omega} \left( \sigma : \delta \varepsilon + q \delta t + q \delta p \right) dV \]
\[ P_{ext} = \int_{\Gamma} \left( \sigma : \delta \varepsilon + R \delta t + Q \delta p \right) dA \]

where \( u \), \( t \), \( p \), and \( q \) are the displacement vector, traction vector, effective plastic strain, and microtraction force conjugate to \( p \) at free surfaces and interfaces. The internal expenditure of power is assumed to arise from a macroscopic surface traction \( t \) and the microtraction force \( q \). Moreover, \( R \) and \( Q \) are the drag stress and the nonlocal drag stress, respectively. Using the principle of virtual power (i.e., \( P_{ext} = P_{int} \)) and after some mathematical manipulations the following equations are obtained:

\[ \sigma : \delta \varepsilon + (R - Q) = 0 \quad \text{(over } \Omega) \]
\[ q = Q \quad \text{(over } \partial \Omega) \]

where \( N \) is the unit second-order tensor showing the direction of plastic strain. Eq. (2) is the nonlocal microforce balance, whereas Eq. (2)_2 defines the microtraction condition which is a higher-order internal boundary condition. Motivated by the fact that additionally to the bulk free energy, an interfacial energy \( \phi \) (free energy per unit area) exists in the plastic boundary layer at interfaces, the following decomposition of the Helmholtz free energy is postulated [3]:

\[ \Psi = \Psi^\prime (\varepsilon^\prime) + \Psi^\prime (p, p_s) + \frac{1}{\ell^s} \phi (p, p_s) \]

where \( \ell^s \) is the microstructural length-scale parameter related to the interface which is different from the bulk length-scale. We obtain the following equation for rate of energy dissipation by using the nonlocal Clausius-Duhem inequality:

\[ \Pi = \left( R - \frac{\partial \Psi}{\partial p} \right) p + \left( Q_s - \frac{\partial \Psi}{\partial p_s} \right) p_s + \frac{1}{\ell^s} \frac{\partial \phi}{\partial p_s} p_s^{(m)} - \frac{1}{\ell^s} \frac{\partial \phi}{\partial p_s} p_s^{(m)} \geq 0 \]
where \( \dot{\sigma}^{(i)} \) is the effective plastic strain at interfaces. Eq. (4) clearly shows that: (a) the hardening functions at bulk and interface are different; and (b) the hardening function at the interface depends on the interfacial length-scale. Hence, we re-write Eq. (4) for bulk and interface separately, such that:

\[
\Pi = (R - R^i) \dot{p} + (Q - Q^i) \dot{p}_s = R^i \dot{p} + Q^i \dot{p}_s \geq 0 ;
\]

\[
\Pi^{(i)} = (R^{(i)} - R^{(i)}) \dot{p}^{(i)} + (Q^{(i)} - Q^{(i)}) \dot{p}^{(i)}_s = R^{(i)} \dot{p}^{(i)} + Q^{(i)} \dot{p}^{(i)}_s \geq 0
\]

where \( R^i \) and \( R^{(i)} \) are energetic components of drag stress at bulk and interface, respectively, and \( Q^i \) and \( Q^{(i)} \) are energetic components of nonlocal drag stress vector, respectively. The superscript “(i)” indicates the dissipative component. The energetic terms depend on Helmholtz free energy and defined as follows:

\[
\dot{R} = \rho \frac{\partial \dot{V}}{\partial \dot{p}} \; , \; \dot{Q} = \rho \frac{\partial \dot{V}}{\partial \dot{p}_s} \; ; \; \dot{R}^{(i)} = \rho \frac{\partial \dot{V}^{(i)}}{\partial \dot{p}} + \frac{\partial \dot{V}}{\partial \dot{p}_s} \; \chi \; , \; \dot{Q}^{(i)} = \rho \frac{\partial \dot{V}^{(i)}}{\partial \dot{p}_s} \; \chi \; ; \; \notag
\]

(7)

Here, we show the procedure for determining the dissipative components in bulk materials. We define an objective function (\( \Omega = \Pi - \Lambda^i [\Pi - (R^i \dot{p} + Q^i \dot{p}_s)] \)) with a Lagrange multiplier \( \Lambda \) and subject it to the maximum dissipation principle. By satisfying the necessary conditions: the dissipative components are derived as follows:

\[
\dot{R}^i = \dot{\Lambda} \frac{\partial \Pi}{\partial \dot{p}} \; , \; \dot{Q}^i = \dot{\Lambda} \frac{\partial \Pi}{\partial \dot{p}_s} \; , \; \dot{\Lambda} = -\frac{1}{\Pi} \frac{\partial \Pi}{\partial \dot{p}} \frac{\partial \Pi}{\partial \dot{p}_s} \notag
\]

(8)

Different forms of gradient-dependent plasticity/viscoplasticity models can be obtained by assuming proper forms for Helmholtz free energy and rate of energy dissipation.

Results

In this section we apply the presented framework to investigate the size-dependent behavior in uniaxial loading of a plastic thin film on an elastic substrate [Fig. 1(a)] [4]. Therefore, we postulate the following mathematical forms:

\[
\rho \dot{\sigma}^V = \frac{1}{2} \sigma^{(i)} \varepsilon^{(i)} ; \; \rho \dot{\sigma}^p = \frac{1}{2} \sigma^p \varepsilon^p + \epsilon \rho \dot{p} \; ; \; \rho \dot{\phi} = \epsilon \sigma^p \rho \rho^p \; ; \; \Pi = \sigma^p \dot{p}
\]

(9)

Making use of above equations we can easily prove that the yield strength at the interface \( \sigma_y \) is size-dependent (i.e. \( \sigma_y = \sigma_y^0 \left( 1 + \ell_d \right) \)). The size-dependent interfacial yield strength is shown in Fig. 1(b).

Fig.1. (a) thin film on an elastic substrate subjected to uniaxial tension. (b) normalized yield strength vs. \( \ell / \ell_d \) for different values of \( \ell / \ell_d \).

Conclusions

In this work, a thermodynamic based higher-order gradient plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces is presented. It is shown that the interfacial length scale, \( \ell_x \), is responsible for size-dependent yield strength of thin metal films on substrates, size and interfacial hardening effects in metal matrix composites, and nonuniform size-dependent deformation of micro-pillars under uniform stressing. It is also shown that decomposition of thermodynamic conjugate forces into energetic and dissipative components is necessary for accurately estimate the rate of energy dissipation.

References

Degradation Kinetics of Aerospace Wire Insulation Material

Peter R. Hondred¹, Sungho Yoon¹, ², Nicola Bowler¹, and Michael R. Kessler¹*

¹Department of Materials Science and Engineering, Iowa State University
2220 Hoover Hall, Ames, IA, 50011, USA
E-mail address: mkessler@iastate.edu
²School of Mechanical Engineering, Kumoh National Institute of Technology
Yangho-Dong, Gumi, Gyeongbuk, 730-701, KOREA

ABSTRACT

The past conventional wisdom that aerospace wire insulation failures such as cracks, fraying, and degradation are atypical and harmless has proven to be a costly liability exhibited in the tragic accidents of Swissair 111 (Nova Scotia, 1998) and TWA 800 (Long Island, NY 1996). These accidents have been attributed to damaged wiring insulation caused by degradation, cracking, and fraying; a problem for many miles of wire buried deep within their structures. As the aerospace industry matures, hundreds of failures are being discovered in typical aircrafts. Consequently, it is imperative to understand the cause of the failures. However, despite the importance of understanding the mechanisms and kinetics of wire degradation under various thermal, environmental, and mechanical loadings, no systematic studies has been reported on the thermal degradation kinetics of typical wire insulation materials.

This work investigates the thermal degradation kinetics of three commonly used wire insulation materials, poly(ethylene-alt-tetrafluoroethylene) (ETFE), poly(tetrafluoroethylene) (PTFE), and poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-c:4,5-c']dipyrole-2,6(1H,3H)-diyl]-1,4-phenyleneoxy-1,4-phenylene] (Kapton) through the use of thermogravimetric analysis (TG).

TG measures the degree of degradation (as measured by mass loss) with respect to time (t) and temperature (T). The degree of degradation (α) can be defined as:

\[ \alpha = f(t,T) = 1 - \frac{\text{wt}\%}{100} \]  

where wt\% is the relative mass obtained directly from the TG experiment.

When modeling, two separate functions are assumed, \( K(T) \) and \( f(\alpha) \), such that the governing differential equation has the following form:

\[ \frac{d\alpha}{dt} = K(T) \cdot f(\alpha) \]  

where \( \frac{d\alpha}{dt} \) is the rate of degradation, \( K(T) \) is the temperature-dependent rate constant, and \( f(\alpha) \) corresponds to the reaction model. The temperature-dependent rate constant is commonly described by the Arrhenius equation:

\[ K(T) = A \cdot e^{-\frac{E}{RT}} \]  

where \( R \) is the universal gas constant, \( E \) is the activation energy, and \( A \) is a pre-exponential factor. The reaction model is chosen based on isoconversional analysis techniques.

When heating at a constant rate, the equation can be redefined to eliminate the time-dependence by dividing through the differential equation by the heating rate:
where \( \beta = {dT/dt} \) is the heating rate.

Derivative thermograms (DTG) and isoconversional analysis techniques, which provide information about how activation energy changes with the degree of degradation, provide the number of steps and elucidate the type of mechanism in the formulation of mathematical kinetic models of these insulation materials. The DTG provides insight into the minimum number of reaction steps. A Friedman analysis, which is the first step in the isoconversional method, contains information on the activation energy. This analysis can also indicate the speed of each reaction step—accelerated, normal, or retarded. Through the direction of the isoconversional method, the degradation kinetics for each insulation material was mathematically modeled and the fittings are presented below in Figure 1. Table 1, the model steps and statistical fit, show the variability and complexity in the degradation kinetics of PTFE, ETFE and Kapton.

![Figure 1. Model fit TG experiments in air for (a) PTFE, (b) ETFE, and (c) Kapton. Experimental data is represented by points and model by the solid line.](image)

Table 1. The reaction steps for each model.*

<table>
<thead>
<tr>
<th>PTFE Model</th>
<th>ETFE Model</th>
<th>Kapton Model</th>
</tr>
</thead>
<tbody>
<tr>
<td>A ( \rightarrow ) B</td>
<td>A ( \rightarrow ) B ( \rightarrow ) C ( \rightarrow ) D</td>
<td>A ( \rightarrow ) B ( \rightarrow ) C ( \rightarrow ) D ( \rightarrow ) E</td>
</tr>
<tr>
<td>( R^2 = 0.99482 )</td>
<td>( R^2 = 0.99958 )</td>
<td>( R^2 = 0.99991 )</td>
</tr>
</tbody>
</table>

*All steps modeled with \( n^{th} \) order with autocatalysis

During the onset of degradation, catastrophic failure due to subsequent short-circuiting of electrical wiring insulation may result. Therefore, it is our goal to correlate the degradation mechanism and model predictions to dielectric breakdown through life theory and TG theory as seen in the work by Toop. Through the use of the TG model activation energies and the failure voltage, the weight loss life prediction can be correlated to the electrical breakdown voltage as seen in equation 5:

\[
\log T_f = \left( \frac{E_{A}}{2.303R_f} \right) + \log \left( \frac{E_{A} \nu (x_f)}{\beta R} \right)
\]

(5)
where $T_f$ is failure time, $E_{ac}$ is activation energy, $R$ is the gas constant, $\theta$ is the absolute temperature, $p(x_f)$ is empirical correlation, and $\beta$ is the heating rate.

Oxidation and Hole Formation in Aluminum Nanoparticle

Hamed Attariani¹ and Valery I. Levitas²
¹PhD students, Departments of Mechanical Engineering, Iowa State University, Ames, Iowa
²Schaefer 2050 Challenge Professor, Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, Iowa State University, Ames, Iowa

This work is concerned with modeling of thermo-mechanochemical processes that occur in aluminum nanoparticles covered by oxide shell during heating. This study is important for understanding and optimization of synthesis and application of Al nanoparticles, in particular pre-stressed nanoparticles and nanoparticles with holes. Aluminum nanoparticles have a broad range of application as nanoenergetic material. They are being considered for overlapping technologies such as: materials synthesis application, explosive additives, and propellant rate modifiers; MEMS energy sources, as well as thermites, nanobarics, and reactive materials for ordnance applications. In manufacturing process or during oxidation, solid nanoparticle may change its structure to hollow sphere due to the Kirkendall effect [1]. The difference in diffusion of metal and oxide layer causes the migration of atoms from core to shell, which leads to supersaturation of vacancy in the core and nanovoid nucleation.

Additionally, aluminum reacts with oxygen and form the growing oxide layer [2]. Coupled system of equations for diffusion of Al, oxygen, and vacancies, oxidation reaction and elasticity theory is formulated and solved using finite element method and COMSOL code. Conditions for void nucleation and growth are determined depending on particle’s parameters. Depending on the achieved level of supersaturation, void can disappear, grow or first shrink and then grow.

![Vacancy concentration at the initial time steps](image1)

![Evolution of the radius of void during the diffusion process](image2)

The vacancy concentration at the initial time step is depicted in Fig.2-a. The void shrinks until the vacancy concentration at the void surface is higher than the core (0.82 s). Then the void starts to grow when the vacancy concentration in the core exceed. Thermodynamically consistent volumetric reaction kinetics with finite reaction rate is used. Reaction occurs inside of alumina shell where diffused Al and oxygen meet. Diffusion is coupled to mechanics through diffusion expansion (for atoms) and contraction (for vacancies), contribution of the stress gradient into diffusion equation, and through pressure-dependence of equilibrium vacancy concentration and diffusion coefficient. Surface energy of all interfaces (hole, Al-alumina, and alumina-oxygen) is taken into account. Fig.2-a shows the Al and oxygen concentration in the system during oxidation. The migration of Al atoms from core to the shell increases the vacancy concentration and consequently prepares the suitable condition for void growth.
Fig. 2-a) Concentration of diffusive species (aluminum and oxygen) in nanoparticle. b) Radial stress distribution in a nanoparticle

Also, the radial stress distribution in coupled system is plotted in Fig. 2-b. The diffusion induced the tensile stress in the system, which in turn affects the diffusion process. Reaction is coupled to mechanics through misfit (reaction) strain, change in properties and pressure-dependence of reaction kinetics. Expression for misfit strain is determined. Misfit strain creates large stresses, which lead to expansion of the reaction zone. Various diffusion and oxidation scenarios are investigated.

Effect of surface tension and energy on multi-variant phase transformations based on phase field approach

Mahdi Javanbakht¹ and Valery I. Levitas²
¹PhD students, Departments of Mechanical Engineering, Iowa State University, Ames, Iowa
²Schaefer 2050 Challenge Professor, Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, Iowa State University, Ames, Iowa

Phase-field or Ginzburg-Landau modeling represents a unique approach for simulation of various aspects of stress-induced multi-variant martensitic phase transformations, especially at nanoscale. In this approach, each $i$-order parameters varies from 0 (corresponding to austenite) to 1 (corresponding to martensitic variant $M_i$). However, despite the significant progress in the field, such as the development of a much more sophisticated Landau potential to make the theory conceptually consistent with known experimental data for shape-memory alloys, steel, and ceramics, a lot of fundamental physics is missing in the phase field equations. In the present work, the Ginzburg-Landau theory for multivariant martensitic phase transformations is advanced in three directions:

First, a potential is developed that introduces a thermodynamically consistent expression for surface tension, which is consistent with a sharp interface limit. Previous approaches to introduce surface tension for liquid-liquid and liquid-solid interface are not completely consistent with a sharp interface limit because they result in additional hydrostatic pressure. Nontrivial point in our new potential is that, even for negligible small strains we have to use a large strain formulation, consider the gradient of the order parameters with respect to a deformed configuration, and introduce ratio of mass densities in the nondeformed and deformed states in some terms.

Second, a mixed term in gradient energy is introduced by considering the product of gradients of different order parameters corresponding to different martensitic phases. Previous forms of the gradient energy result in the energy of the $A-M_i$ interface to be half of energy of $M_i-M_j$ interface, while in reality it is significantly larger. This mixed term allows us to control the energy of martensite-martensite interface. The resultant Ginzburg-Landau equations become coupled through Laplacians, in addition to traditional coupling.

Third, a noncontradictory expression for variable surface energy is suggested. The main drawback of previous works is that the expression for surface energy does not allow homogeneous solution for the product phase- i.e. the product phase always has a surface structure toward the alternative phase, even when this phase is completely unstable. This also leads to unphysical regions in the phase diagram. Here, we derive the expression that does not possess the above problem, generalize it for multi-variant phase transformations, and study surface-induced pre-transformation and barrierless nucleation of multiple martensitic variants.

Combining all the above advancements, the coupled system of time-dependent Ginzburg-Landau equations for all order parameters, the continuum of mechanical equations, and the boundary conditions are formulated. The finite element method approach, algorithm, and subroutines are developed using COMSOL code. Model problems of surface-induced pre-transformation, barrierless multivariant nucleation and nanostructure evolution in a nanosize sample are solved, and the effect of the above contributions is elucidated. As an example, Fig. 1 demonstrates the stationary solutions for a sample with the boundary condition related to the variable surface energy with surface tension and without it, respectively. Also, the nanostructure evolution from a pre-existing nucleus is considered and the
internal stress-induced nucleation is revealed. As shown in Fig 2, the sample without surface tension transforms to the second martensitic variant while with surface tension transforms to the first martensitic variant. The obtained results represent a much more detailed and precise model for coherent solid-solid interface than current phenomenological models.

Fig 1. The stationary solution for the nanostructure evolution after barrierless surface-induced nucleation from the right-hand site of the sample. (a) Without surface tension; (b) With surface tension.

Fig. 2. The nanostructure evolution in the sample from the initial embryo without and with surface tension.

H. Kodali, B. Ganapathysubramanian
Departments of Mechanical Engineering, Iowa State University, Ames, IA

Introduction: Organic solar cells (OSC) offer a promising low-cost strategy for harnessing solar energy. Additional advantages include mechanical flexibility and light-weight. Efficiencies of ~ 7.8% have been achieved recently in conjugated polymer based organic solar cells. These devices were fabricated by spin coating an active layer from a blend of p-type photoactive polymer and n-type derivatives of fullerenes into the so called “blend-heterojunction” architecture.

Experimental evidence suggests that a key property determining the solar efficiency of such devices is the final morphological distribution of the organic phases. Furthermore, there is a complex relationship between device topology (device scale), morphological distribution of the polymers (nano-scale) and the device efficiency. Computational techniques can help unravel these relationships to accelerate the fabrication of high efficiency OSC.

We showcase a computational engine that efficiently interrogates virtual organic solar cell devices to investigate relationships between the morphology at the nano-scale and topology at the device scale with the electrical and optical characteristics.

Methods: Simulation of OSCs requires determination of electrostatic potential and electron/hole densities, which is described by Boltzmann Transport Equation (BTE). As the direct solution of BTE is computationally challenging, the drift-diffusion model is used for modeling these devices. We utilize the Finite element method to model the topological and morphological details. A 'Streamline Upwind Petrov Galerkin' (SUPG) based stabilization method is used to minimize numerical instabilities.

The generation rate of excitons depends on the amount of radiation absorbed, which in-turn depends on the dielectric constant of the materials in the blend. The absorptivity is calculated by solving Maxwell's equations using 'finite difference time domain' (FDTD) method.

A method of continuation is used to aid convergence of the strongly coupled nonlinear equations. In this method, initially spatially averaged material properties are used for calculating the variables. The morphological variations are introduced gradually, one property at a time. Domain Decomposition is utilized to solve the large computational problem arising (out of the necessity to resolve the microstructure details).

Results: The effect of microstructure on the distribution of electrons, holes and electrostatic potential is investigated. The electron density was observed to be diminished in the polymer rich regions (PRR) and enhanced in fullerene rich regions (FRR). This results in uneven current density in FRR and PRR at electrodes. The effect of geometry (topology) and morphology on the generation rate is shown. The accumulation of electric field at corners due to undulations in the topology of the polymer-fullerene film has been captured.

Conclusions: The scalability studies show the effectiveness of the domain decomposition strategy. A method of continuation is proposed to solve the stiff drift-diffusion problem with morphological property variation. Trends between the metrics associated with morphology and overall current generated reveals the property-performance relationships for OSC.
Molecular Dynamics Simulation of Conformational Transition and Associated Frictional Performance of Self-Assembled Monolayers

Xiao Ma, Pranav Shrotriya
Department of Mechanical Engineering, Iowa State University, Ames, IA
Email: xma@iastate.edu

Recently Self-Assembled Monolayers (SAMs) of organic molecules such as Poly Ethylene Glycol (PEG) terminated alkanethiols have attracted considerable attention in Micro/Nano tribology, microfluid and biomedical applications, due to their unique and flexible structure upon which conformational transition can be generated under various conditions, such as temperature, solvent, electro-chemical surface modifications and external electrical field. Applying electrical fields is an effective and feasible method to control the conformational transition without any detrimental harm on the chemical stability of SAMs.

By application of Molecular Dynamics (MD) simulation, the structural conformation transition of PEG terminated SAMs and associated frictional performance transition due to the polarity alteration of external electrical field were investigated and reported in this research. The MD simulation study helps to explore the desired information and quantities that are not available through experiments.

The interatomic potential model was applied to simulate the atomic and molecular interaction during the conformational transition. The potentials include bonded, nonbonded and electrical field parts, as shown in equation (1). For bonded part, Harmonic/Class2 potentials with consideration of gold-thiol interaction as a Morse potential were applied in the model.

\[ V = V_{\text{bond}} + V_{\text{nonbond}} + V_{\text{electrical field}} = (V_{\text{bond}} + V_{\text{angle}} + V_{\text{dihedral}}) + (V_{\text{lj}} + V_{\text{coulombic}} + V_{\text{morse}}) + V_{\text{electrical field}} \]  

(1)

The PEG terminated alkanethiol chains \( -\text{S-(CH}_2\text{)}_{11}-(\text{O-CH}_2\text{-CH}_2\text{)}_{7}-\text{O-CH}_3 \) were attached to \( \text{Au}(1 1 1) \) plane with \((\sqrt{3} \times \sqrt{3})\) R30° lattice structure and close packed coverage density. Initialization and thermalization were performed with NVT ensemble at first to generate the initial random vibration and achieve the required temperature and system stability, then electrical fields of different polarities were exerted onto the SAMs respectively to induce the conformational transition. In the end, a repulsive indenter was applied to the system to generate frictional force, and the contact force is shown in equation (2)

\[ F(r) = -k(r - R)^2 \]  

(2)

Simulation results indicate that significant conformational transition of close packed PEG terminated SAMs formed due to the force couple of electrical fields with different polarities. Under positive electrical fields, the PEG groups were compressed and twisted into the helical form which is known as the “Gauche” conformation. While under negative electrical fields, the PEG groups were stretched into the straight form which is known as the “All-trans conformation, as shown in Fig.1. More quantitative analysis of radial distribution function shows that the characteristic distance between two oxygen atoms in OCCO dihedral groups was 2.7Å under positive electrical field, which corresponded to “Gauche” conformation, however was 3.5Å under negative electrical field, as shown in Fig.2. Such conformational transition can be profoundly related to the frictional performance transformation of PEG terminated SAMs.
Interaction of SAMs with the repulsive indenter upon penetration and sliding shows that under positive electrical field, “Gauche” conformation caused the stiffness declination of the molecular chain, thus led to a comparatively lower frictional coefficient level. While under negative electrical field, “All-trans” conformation increased the stiffness of the molecular chain, and generated a higher frictional coefficient level, as shown in Fig.3. In order to observe the dimensional influence, cylindrical and spherical shape indenters were applied respectively in the simulation.

During the simulation of interaction of SAMs with indenter, two kinds of frictional phase were observed. Under shallow indentation and sliding, a lower level of frictional coefficient was obtained and the whole configuration of the molecular chains was not influenced by the indenter. While under deep indentation and sliding, the higher loads caused a higher level of frictional coefficient and the backbone chains can be dragged along with the indenter away from their original locations.

The Molecular Dynamics simulation in this research provides meaningful insights and application potential upon the structural characteristics and frictional performance of the PEG terminated SAMs.
An Experimental Study of Pulsed Micro Flows Pertinent to Continuous Subcutaneous Insulin Infusion Therapy

Bin Wang¹, Ayodeji Demuren², Eric Gyuricsko³ and Hui Hu¹
1. Aerospace Engineering Dept., Iowa State University, Ames, Iowa Email:huhui@iastate.edu
2. Mechanical Engineering Dept., Old Dominion University, Norfolk, VA
3. Children’s Hospital of the King’s Daughters, Eastern Virginia Medical School, Norfolk, VA

Introduction
Continuous subcutaneous insulin infusion (CSII) therapy, also known as insulin pump therapy, has become an important advancement in diabetes therapy to improve the quality of life for millions of diabetes patients. Insulin delivery failures caused by the precipitations of insulin within micro-sized CSII tubing systems have been reported in recent years. It has also been conjectured that the flow of insulin through an insulin infusion set may be reduced or inhibited by air bubbles entrained into the capillary CSII tubing system during the typical three- to five-day operation between refills. Currently, most solutions to insulin occlusion related problems are based on clinical trials. It is of great value to elucidate underlying physics of insulin infusion process, from the pump action to the catheter delivery, and from a fluid dynamics perspective, in order to provide a better guidance for troubleshooting.

In the present study, an experimental investigation was conducted to quantify the transient behavior of the unsteady micro-flow driven by an insulin pump commonly used in CSII therapy to elucidate the underlying physics for a better understanding of the microphysical process associated with the insulin delivery. A microscopic Particle Image Velocimetry (μ-PIV) system was used to provide detailed flow velocity field measurements inside a $300 \mu m \times 300 \mu m$ microchannel to characterize the transient behavior of the micro-flow upon the pulsed excitation of the insulin pump. The effects of the air bubbles entrained into the micro-sized tubing system on the insulin delivery process are also assessed based the detailed -PIV measurements.

Experimental Setup and μ-PIV Measurements
Fig. 1 shows the schematic of the experimental setup used in the present study. A Medtronic MiniMed Paradigm 512 insulin pump was used to drive the flow passing through a standard Paradigm Quick-Set infusion set (inner diameter=356 m) at the flow rate of 2.0 U/H (~20 L per hour). A transparent microchannel (L×W×H: 38mm×300 m×300 m) was used to be a part of the tubing system for -PIV measurements. For simplicity, DI water premixed with ~1 μm FluoSpheres® beads was used as the working fluid in the present study.

For the -PIV measurements, a double-pulsed Nd:YAG laser at the second harmonic wavelength (532nm) was used to provide illumination for the micro-PIV measurements. The repetition rate of the laser pulses was 10 Hz. A high-resolution 12-bit CCD camera mounted on an inverted microscope with a 10X objective lens (NA=0.4) was used to acquire PIV images. The timing of the CCD camera and the pulsed laser illumination was controlled via a Digital Delay Generator. After micro-PIV images were acquired, instantaneous flow velocity vectors were obtained by using a frame to frame cross-correlation technique. The measurement uncertainty level for the measurements of the instantaneous velocity vectors was estimated to be within 2.0%.

Experimental Results and Discussions
Fig. 2 shows a frame of the typical -PIV measurement results obtained when the insulin pump operated in basal mode at the flow rate of 2.0 U/H. Based on time sequences of the instantaneous -PIV measurement results as that shown in Fig. 2, the time variation of the flow velocity inside the CSII tubing system in response to the pulsed action of the insulin pump can be derived, which is given in Fig. 3. As expected from the basal rate setting (2.0 U/H) and the minimum controllable dose (0.1 U) of the pump, the period of the pulsed operation cycle of the insulin pump was found to be 180s. It can be seen clearly that the fluid would creep slowly through the CSII tubing system most of the time during each pump operation cycle; all of a sudden a flood would be generated upon the pulsed action of the insulin pump. While the time-averaged flow velocity at the centerline of the channel was only found to be about 0.098 mm/s as indicated by the red dash line in Fig. 3, the instantaneous maximum flow velocity inside the microchannel can be as high as 26.4 mm/s, which is two orders of magnitude higher than the time-averaged flow velocity. The zoom-in view of the flow velocity history right before and after the pump operation pulse reveals clearly that the duration of the pump operation was as short as about 0.25 seconds. The subsequent decay process of the flow velocity inside the CSII tubing system can be fitted reasonably well by an exponential function.
It has been suggested that air bubbles entrained into the micro-sized CSII tubing system may reduce or inhibit insulin delivery in CSII therapy. In the present study, an experimental study was also conducted to assess the effects of air bubbles entrained inside the CSII tubing system during the insulin delivery process. From the μ-PIV measurement results shown in Fig. 4, it can be seen clear that, due to the entrainment of air bubbles, the liquid flow would decelerate and diverge along the rear meniscus of the air bubbles, and accelerate and converge towards the centerline near the advancing tip. It was also observed that the insulin delivery pattern appeared to be much “noisier” with several “secondary bumps” riding on the initially smooth decay curve due to the existence of the air bubbles, as shown quantitatively in Fig. 5. Moreover, the characteristic time of the initial flow decay after each pump operation pulse was found to increase significantly compared with the case without air bubble entrainment. Such observations may be attributed to the compressibility of the air bubbles enabling them to act as shock-absorbers to change the dynamic response of the micro-flows inside CSII tubing system to the pulsed action of the insulin pump.
Phase Field Modeling of Melting of Aluminum Nanoparticles

K. Samani and V. I. Levitas
Departments of Mechanical Engineering
Iowa State University, Ames, Iowa

Surface pre-melting and melting of nanoparticles are fundamental problems, which are currently under intense study. For aluminum nanoparticles, this study also has applied aspects. Aluminum nanoparticles represent important class of nanoenergetic materials that are used in rocket propellant mixtures and other energetic applications. They possess significantly enhanced burning rate and reduced ignition delay time. Aluminum nanoparticles usually have a several nanometers thick oxide layer.

According to the recently developed melt-dispersion mechanism of reaction of Al anoparticles, one of the processes that determines the reactivity of Al nanoparticles is melting of Al and stress development in Al core–shell system due to volume increase during melting. Melt nucleation, melting temperature and rate of melting at high heating rates (10^8 K/s and above) determine mechanics of deformation and fracture of alumina shell, which are important for the melt-dispersion mechanism.

We expanded a phase field approach for the pre-melting (surface melting) and melting of nanoparticles by introducing correct expression for surface tension at the solid-melt interface and correct description of variation of surface energy of the external surface. New definition of surface tension yields results that are consistent with sharp interface approach, in contrast to previous theories. Suggested description of variation of surface energy eliminates drawbacks of known approaches to surface melting.

Coupled phase field and mechanical equations are solved using finite element method and COMSOL code. Melting, without and with mechanics, is considered. Calculated results for the thickness of the molten layer versus temperature (Fig. 1) and melting temperature versus particle size are in good correspondence with known experiments. Surprisingly, for the particles with radius from 2 to 5 nm, melting temperatures are even in better agreement with experiments than the molecular dynamics results (see Fig. 2). For heating rates greater than 10^{13}K/s, homogeneous nucleation competes with interface propagation. It is also found that classical expression for the interface velocity based on sharp-interface equation is well reproduced in our calculations even for temperatures for which solid is completely unstable and for particle radii exceeding interface width, which is approximately 4 nm. For spherical particle, interface energy is independent of interface radius down to 4 nm.

Classical relationship for pressure jump across the interface, \( \Delta \sigma = 2\Gamma/r \), where \( \Gamma \) is interface energy and \( r \) is the interface radius, is confirmed for \( r > 5 \text{ nm} \) and neglected internal stresses. The effect of alumina shell is also considered. Alumina shell increases melting time and melting temperature considerably. Large hoop stresses and strain rates developed in the shell can yield spallation of the shell.
Undergraduate Student Abstracts/Presentation Awards

ORGANIZERS:
Pranav Shrotriya, Iowa State University
Scott Beckman, Iowa State University
Quantifying the Effect of Pulsatile Fluid Flow on Drug Distribution in the Spinal Canal

Ying Hsu
University of Illinois at Chicago, Department of Bioengineering, Laboratory for Product and Process Design (LPPD)
851 S. Morgan St., SEO - Office 218 (Advisor: Dr. Andreas A. Linninger), Chicago, 60607, US
Phone: (312) 413-8201, Email: yhsu3@uic.edu

Timothy J. Harris Jr.
University of Illinois at Chicago Laboratory for Product and Process Design, Chicago, IL

Sukhi Basati
University of Illinois at Chicago Laboratory for Product and Process Design, Chicago, IL

Dr. Andreas A. Linninger (Advisor)
University of Illinois at Chicago Laboratory for Product and Process Design, Chicago, IL

Abstract:

Treatments of cerebral diseases such as Parkinson’s, Alzheimer’s, and cancer require the efficient delivery of therapeutic drugs to the brain. These drugs could be delivered by oral or intravenous administration. Unfortunately, due to the large sizes of most drugs, these macromolecules cannot effectively reach the affected brain tissue via the circulatory system, as they cannot cross the blood brain barrier. Intrathecal drug delivery uses the cerebrospinal fluid to transport macromolecules via the interconnected subarachnoid space in the spinal canal and the brain, bypassing the blood brain barrier. Clinical studies have shown that drugs delivered intrathecally experience a greater distribution than that accounted for by pure diffusion. Neurosurgeons have hypothesized that the pulsations of the cerebrospinal fluid could have caused the accelerated distribution. These pulsations stem from the pulsatile motion of the vasculature of the brain due to the elasticity of the vessel walls. Hence, the cerebrospinal fluid is driven into the spinal canal with each cardiac cycle. The total cerebral spinal fluid displaced into the spinal canal per cardiac cycle is between 1-3mL. An experimental apparatus was devised to emulate and investigate the accelerated distribution of species within the spinal canal. The experimental set-up examined the effects of pulsations on the dye distribution. The results of these experiments suggest that the pulsations cause a greater than 30% increase in the overall dye distribution. Experimental results also indicate that the pulsations cause forced diffusion, or convection which appears to facilitate the increased dye distribution. Computational fluid dynamics simulations were performed and the phenomenon observed in the previously described experiment was validated. The flow field and species distributions governed by the continuity and Navier Stokes equations were solved iteratively for two dimensional cases. These experimental studies offer valuable insights that will aid in the accurate prediction of the distribution of therapeutic drugs administered by intrathecal delivery.
A Model for Granular Filtration of Polydisperse Particles

Eric Murphy
Iowa State University Multiphase Flow Computational Lab
095E Black Engineering, Ames, 50011, US
Phone: 563-449-6661, Email: ejmurphy@iastate.edu

Ravi Kolakaluri
Iowa State University, Ames, IA

Shankar Subramaniam
Iowa State University, Ames, IA

Abstract:

In the area of granular filtration there remains a discontinuity between empirical correlations and numerical simulation. In this paper we will attempt to bridge the gap between experiments and simulation of polydisperse fine particles in Stokes flow. Conference proceedings by Ritzert et al. explored filtration of fine fly ash particles in a moving granular bed experimentally. The findings showed that a bi-modally dispersed model was a better fit to experimental data than a monodispersed model. Additionally, Araujo et al. introduced a method for predicting the filtration efficiency of monodisperse point particles for the 2D or fibrous case. The prediction method utilizes the dimensionless Stokes number which is parameter related to the inertia of a particle in a carrying fluid. An extension of the monodispersed model to the polydispersed case could serve as a bridge between experimental results and numerical methods.

Validating our Lagrangian particle tracking code with the results of Araujo et al. allows us to produce filtration efficiency curves, which are a relationship between a particles Stokes number and the distance a particle is located in the fluid stream from the axis passing through the center of the granule. Utilizing filtration efficiency curve, we assert that the filtration efficiency of any given distribution of particle Stokes numbers can be predicted for the periodic case. A method was then developed to extend the filtration efficiency curves from the 2D case to the 3D axisymmetric case present in deep bed granular filtration.

We extend the method further, using the filtration efficiency curves developed from the ordered filter to the disordered filter. Araujo et al. showed that the penetration length \( \lambda \) in a disordered filter is related to the flow in an ordered filter, and thus dependent on the particle Stokes number. Using a similar method as with the ordered filter, the filtration efficiency for polydisperse particles entering the 2D disordered filter is predicted. Lastly, we propose a method for predicting the filtration efficiency for the 3D axisymmetric case and a plan to incorporate other physics as necessary to bridge the gap between the present experimental work and numerical simulations.
Error analysis for 3-D shape measurement with projector defocusing

Ying Xu
Iowa State University
2025 Black Engineering, Ames, IA
Phone: 515-203-1849, Email: xuying@iastate.edu

Song Zhang
Iowa State University, Ames, IA

Abstract:
This paper analyzes the phase error for a 3-D shape measurement system that utilizes our recently proposed projector defocusing technique. By defocusing binary structured patterns, seemingly sinusoidal ones can be generated, and 3-D shape measurement can be performed by fringe analysis. However, there are still significant errors if the object is not within a certain range. In this research, we experimentally studied a large range of defocused fringe patterns, from close to be binary to to be severely blurred, and its associated phase error is analyzed and is compensated. To quantify the phase error, a uniform flat board is placed in front of the system with different distances from the system. The phase error is analyzed for each position and stored into a look-up table (LUT). This LUT is then used to compensate for the phase error when a real experiment is performed.
The Destruction of Biofilms Using Ultrasound Treatment

Benjamin Rusk  
Truman State University, Kirksville, MO  
Email: bdr560@truman.edu

Jin Xu  
Iowa State University, Ames, IA

Timothy A. Bigelow  
Iowa State University, Ames, IA

Larry Halverson  
Iowa State University, Ames, IA

Abstract:

Even under the most sterile conditions, medical implants used by hospitals are often infected by bacteria. These bacteria can sometimes form communities on the implant, called biofilms. Biofilms create a slime-like encasing that protects the bacteria as they lay almost dormant on the implant surface. Because of this protection, antibiotics are usually unsuccessful in treating the patients' infection. The only solution to the problem that currently exists is to surgically remove the implant and replace it with another sterile implant. This replacement implant is even more likely to be infected than the original, and the procedure costs time, resources, and can be life threatening to the patient. There is a major need to develop a noninvasive technique to combat these biofilm infections in vivo.

Various studies have shown that ultrasonic treatment can be used to increase certain biofilms susceptibility to antibiotics. The goal of this study was to determine whether ultrasound induced cavitations was a feasible method for destroying biofilms. It is known that high intensity ultrasound focused in tissue can cause microbubbles. These microbubbles are capable of destroying the nearby tissue by breaking it down into sub-cellular components. Therefore, it may be possible to destroy the biofilm infection on an implant without invasive surgery using high-intensity ultrasound.

The first goal for this study was to prepare consistent biofilms. A flow cell system needed to be constructed which could repeatedly produce robust biofilms. An exposure chamber also needed to be designed with the intent of holding the graphite disk that the biofilms were grown on while the high intensity focused ultrasound (HIFU) treatment was performed. Calibrating the ultrasound transducer was necessary in order to achieve a certain pressure on the disk surface. After these objectives were met it was possible to perform a HIFU treatment on the biofilm covered graphite disks.

Using a specific strain of Pseudomonas aeruginosa bacteria that was tagged with green fluorescent protein, it was found that robust biofilms required 2-3 days of growth in the flow cells. Less time produced patchy biofilms and longer time periods resulted in biofilms with significant amount of dead or dying cells. The final signal used for treatment was 1.1 MHz at 20 cycles with a 5ms burst period which produced the desired pressure of 13 MPa at the disks surface. The transducer producing the signal scanned at 1 mm intervals over the disk in a rectangle 7 mm by 13 mm, giving 112 points total. A computer program controlled the scanning of the disk and allowed to adjust the pause time at each point, meaning the total treatment time was the sum of the 112 points and the time spent at each point.
To test the effects of the ultrasound treatment three biofilm covered disks were exposed for varying amounts of time. One disk received no HIFU treatment, one disk received 28 minutes total, and the other received 56 minutes total. After the treatment all three disks were examined under a microscope using fluorescence microscopy to determine the extent of biofilm destruction and if remaining cells were dying or dead using a viability stain. The control disk receiving no ultrasound treatment showed a mostly robust biofilm, while the other two disks had very little biofilm and most of the remaining cells were dead. No distinction could be made between the disks receiving 28 and 56 minutes total. From these results it could be concluded that the high intensity focused ultrasound treatment successfully removed the majority of the biofilm from the graphite disks. Future work will need to determine whether these results can be achieved with lower exposure times and to examine if the biofilms are being completely destroyed or just dislodged.
3-D Shape Measurement of Liquid Droplet with a Structured-light Technique

William Lohry
Iowa State University
Department of Chemical Engineering, Ames, IA
Email: wflohr@iastate.edu

Bin Wang
Iowa State University, Ames, IA

Hui Hu
Iowa State University, Ames, IA

Song Zhang
Iowa State University, Ames, IA

Abstract:

Aircraft icing remains a fundamental problem today. Moisture buildup in cold weather can freeze, causing damage to aircraft wings and engines. Studying how this ice forms can lead to improvements in design to avoid such problems. Fluorescent imaging is commonly used to evaluate fluid thickness. In this method, UV lights shine on a liquid dyed with a fluorescent dye while a camera captures the fluid. Since thick areas will transmit more light than thin areas, the system can convert pixel intensity into fluid depth. Such a setup assumes constant distribution of fluorescent dye in the fluid, so any variations will cause unavoidable systematic error. In this paper, we use a structured light technique to achieve high-spatial and temporal resolution without worrying about the density of the fluid. In this method, a DLP projector is used to project structured patterns on the object, a CCD camera, viewing from another angle is used to capture the scattered structured patterns, from which, the 3-D information can be recovered by triangulation.
Surface Coverage and Hybridization Density of Double Thiolated Molecules on Surfaces for Microcantilever Sensors

Alex Avendano
Iowa State University
Department of Mechanical Engineering, 2025 Black Engineering, Ames, IA 50011
Email: alexavch@iastate.edu

Lillian Johnson
University of Arkansas at Pine Bluff, AR

Kyungho Kang
Iowa State University, Ames, IA

Pranav Shrotriya
Iowa State University, Ames, IA
Abstracts by Symposium
Track 1
Horner Symposia
A Symposium in Honor of the Contribution of Ray Ogden,
The Recipient of Prager Medal

ORGANIZERS:

Luis Dorfmann, Tufts University, Medford, MA
Jose Merodio, Polytechnic University of Madrid, Spain
A 3D Pseudo-Elastic Model for Mullins Effect with Residual Strains in Filled Polymers

Gal deBotton
Ben-Gurion University
Dept. Biomedical Engineering, P.O.B. 653, Beer-Sheva, 84105, IL
Phone: (972) 73 277 7105, Email: debotton@bgu.ac.il

Abstract:

In common filled elastomers the stresses that develop during a deformation from a virgin state are markedly higher than the ones developing during subsequent loading cycles. Damage mechanisms that are associated with this phenomenon result in residual strains and hence, upon unloading, the stress-free configuration of the material is different from the virgin one. This stress-softening phenomenon is often referred to as the Mullins effect. A pseudo-elastic model that allows to account for this effect in a straightforward manner was proposed by Ogden and Roxburgh (Phys. and Engng. Sci., 455:2861, 1999) and was later extended by Dorfmann and Ogden (Int. J. Solids Struct., 41:1855, 2004).

In this study we extend these works and develop a three-dimensional pseudo-elastic model that can be easily implemented in various numerical simulations. It is assumed that the amount of damage accumulated at a given material point depends on the history of the deformation at this point. The dependency is through a set of “internal variables”. As a special case we assume that the dependency is only on the most recent state at which one or more of the internal variables was modified. A constitutive relation is proposed for the relation between this extremal state and the associated stress-free state. In terms of derivatives of the proposed pseudo-elastic energy density function with respect to the deformation gradient, subsequent unloading and reloading stress-strain relations are derived. To demonstrate the applicability of the model a few experiments with industrial grade silicon rubber were performed. The predictions of the proposed model were favorably compared with the experimental stress-strain curves up to 300% deformation.
Theoretical and Experimental Investigations to Characterize Volume Change of Rubber-Like Solids

Luis Dorfmann  
Tufts University  
200 College Avenue, Medford, 02155, US  
Phone: 617-6276137, Email: luis.dorfmann@tufts.edu

Francesco Pancheri 
Tufts University, Medford, MA

Abstract:
In this talk we discuss the isothermal phenomenological theory to describe the elastic and inelastic response of rubberlike solids. We begin with an overview of newly obtained experimental results to characterize the mechanical response. In particular, we examine the volume change accompanying the deformation and characterize the change in material behavior associated with the Mullins effect. In the second part of the lecture we discuss the mathematical theories to illustrate these phenomena. Two approaches are conventionally used to develop stress-strain relations. According to the phenomenological approach, the mechanical properties are usually represented in terms of a strain-energy function, $W$. The second approach is based on the molecular theory of rubber elasticity, which treats elastomers as a network of long chains bridged by permanent and temporary junctions. Much theoretical work is available where the material is considered incompressible and the corresponding theory used to solve representative boundary value problems. However, the incompressibility constraint no longer holds for highly compressible elastic materials and volumetric changes must be accounted for. We describe the phenomenological theory necessary for modeling the change in volume during arbitrary deformations. Using the multiplicative decomposition of the deformation gradient into dilatational and isochoric parts, we discuss briefly some representative decoupled strain-energy formulation. The theory is used to fit experimental data describing the change in volume during uniaxial extension. A good correspondence between the theory and the data is obtained.
Analytical Solutions for the Onset of Cavitation in Rubber under General 3D Loading Conditions

Oscar Lopez-Pamies
State University of New York, Stony Brook
139 Light Engineering, SUNY Stony Brook, Stony Brook, 11794-2300, US
Phone: 6316328249, Email: oscar.lopez-pamies@sunysb.edu

Abstract:

Physical evidence has shown that sufficiently large tensile loads can induce the sudden appearance of internal cavities in elastomeric solids. The occurrence of such instabilities, commonly referred to as cavitation, can be attributed to the growth of pre-existing defects into finite sizes. Because of its close connection with material failure initiation, the phenomenon of cavitation has received much attention from the materials and mechanics communities. Cavitation has also been a subject of interest in the mathematical community because its modeling has prompted the development of techniques to deal with a broad class of non-convex variational problems. While in recent years considerable progress has been made via energy minimization methods to establish existence results, fundamental problems regarding the quantitative prediction of the occurrence of cavitation in real elastomeric materials remain largely unresolved.

In this work, we concern ourselves with studying the effect of loading triaxiality on the onset of cavitation in rubber. Specifically, by means of a new iterated homogenization method, we derive analytical solutions for the onset of cavitation in a Neo-Hookean solid when subjected to arbitrary 3D loading conditions. In this connection, it should be emphasized that the vast majority of cavitation studies to date have been almost exclusively limited to hydrostatic loading conditions, presumably because of the simpler tractability of this relevant but overly restricted case. However, as indicated by our solutions, the occurrence of cavitation is expected to depend very intricately on the triaxiality of the applied loading conditions, not just on the hydrostatic component.
The Problem of Computing 3D Residual Stress Distributions in a Neo-Hookean Tube

Roger Bustamante
Universidad de Chile
Departamento de Ingenieria Mecanica, Universidad de Chile, Beaucheff 850, Santiago Centro, Chile
Phone: 56-2-9784543, Email: rogbusta@ing.uchile.cl

Gerhard Holzapfel
Institute of Biomechanics, Center of Biomedical Engineering, Graz University of Technology, Graz, Austria.
Department of Solid Mechanics, Royal Institute of Technology (KTH), Stockholm, Sweden.

Abstract:

Recent works in biomechanics have shown the importance of having detailed models of residual stresses for arteries [1,2]. It is well known that when a piece of artery is cut axially and radially, it deforms by showing the presence of residual stresses in the in vivo situation [3,4].

For the case of a radial cut of a cylindrical section, an important assumption being used is to consider the opening angle constant along the axial position. In this way, closed-form solutions for the boundary-value problem have been found, see, e.g., [5]. However, recent experiments [4] show that the opening angle also depends significantly on the axial position. Due to the big influence that residual stresses have on the behavior of arterial tissue in vivo, it is necessary to study the above phenomena in the distributions of these stresses.

For the case that we are only interested in studying the behavior of arterial tissue when stretches and stresses are not too large, a good approximation is based on the assumption of isotropy. Therefore, we consider, in a first approximation, the problem of calculating residual stresses for a non-homogeneous neo-Hookean tube.

We explore two boundary-value problems, where we have radially opened tubes, and where the opening angle depends on the position along the tubes [6]:

- In the first case we work with a straight tube, and an opening angle that depends on the axial position along it.

- In a second more general case, we assume that in the reference configuration we have an opened tube which is also bent in the axial direction. This bending has actually been observed in recent experiments [4].

Using the semi-inverse method, we study the problem when these tubes are closed, and we explore some considerations about the boundary-value problem, and also the nonlinear partial-differential equations that need to be solved to find the current configuration.
References


A Rigorous Derivation of Hemitropy in Nonlinearly Elastic Cosserat Rods

Tim Healey
Cornell University
Department of Mathematics, 432 Malott Hall, Ithaca, 14853, US
Phone: 607-255-4373, Email: healey@math.cornell.edu

Abstract:

We consider a class nonlinearly hyperelastic rods with helical symmetry. Such a rod is mechanically invariant under the symmetries of a circular-cylindrical helix. Examples include idealized DNA molecules, wire ropes and cables. We examine the limit as the pitch of the helix characterizing the symmetry approaches zero and show that the resulting model is a hemitropic rod. The former is mechanically invariant under all proper rotations about its centerline and generally possesses chirality or handedness in its mechanical response. An isotropic rod is also rotationally invariant but, in addition, enjoys certain reflection symmetries, which rule out chirality. Isotropy implies hemitropy, but the converse is not generally true. We employ both averaging methods and methods of gamma convergence to obtain the effective or homogenized (hemitropic) problem, the latter not corresponding to a naïve average.
Analysis of Stiffness Variations in the Context of Strain-, Stress-, and Energy-Controlled Processes

William Mars
Cooper Tire & Rubber Company
701 Lima Ave., Findlay, 45840, US
Phone: 419 423 1321, Email: wvmars@coopertire.com

Abstract:

In compounded material systems such as rubber, a wide range of properties can be achieved by design. This flexibility poses a challenge - how to balance stiffness against other considerations such as energy dissipation under dynamic loading, fatigue, etc. Negotiating this balance requires that adequate account be taken of how a given mechanical input (ie strain, stress, energy) is controlled, and how other mechanical outputs vary as the stiffness changes. We outline here a simple analysis by which these considerations can be managed. The analysis is based on a novel split of the elasticity law into work-conjugate parts: one representing generally that which is to be held constant, and the other representing that which occurs in reaction to imposed control. The split gives rise to a scalar parameter suitable for quantifying the degree to which a given 1D mechanical process is strain-, energy-, or stress-controlled. The physical sense of the parameter is illustrated through the example of a two spring system, where one spring represents the subject material, and the other represents the mechanical environment in which the material operates. The example shows that the parameter concisely summarizes the effects of the environment on the operating conditions of the material. Some forward-looking comments are then offered regarding how the analysis might be extended to the 3D case.
Anomalous Mechanical Behavior of Ultrathin Polymer Films

Gregory McKenna
Texas Tech University
Department of Chemical Engineering, Texas Tech University, Lubbock, 79409-3121, US
Phone: 806-742-4136, Email: greg.mckenna@ttu.edu

Shanhong Xu
Texas Tech University, Lubbock, TX

Jinhua Wang
Texas Tech University, Lubbock, TX

Abstract:

The mechanical response of ultrathin polymer films is of considerable fundamental and practical interest. There are reports, for example, that at thicknesses below 50 nm the glass transition temperature can drop by as much as 80 K. Furthermore, in our labs we have found that the rubbery plateau modulus of such films seems to stiffen by up to 3 orders of magnitude. Here we describe results from work on polymer microbubble inflation of both circular and rectangular shape and for film thicknesses as small as 3 nm. We show that the reduction of the glass transition is 'non-universal', i.e., it can exceed 60 K for polystyrene and polycarbonate but does not decrease for poly(vinyl acetate). In addition, the dramatic rubbery stiffening observed in polystyrene and poly(vinyl acetate) is considerably reduced in poly(n-butyl methacrylate). Finally, novel ultrathin dewetting experiments will also be discussed.
Indentation of a Nonlinear Viscoelastic Circular Membrane

Alan Wineman
University of Michigan
Department of Mechanical Engineering, Ann Arbor, 48109, US
Phone: 734-936-0411, Email: lardan@umich.edu

Anthony Waas
University of Michigan, Ann Arbor, MI

Abstract:

Measurements related to the indentation of a circular membrane can be used to identify the material response of a wide variety of materials, including biological tissue. In this paper, the axisymmetric deformation of an initially planar membrane that is supported along a circular boundary and indented by a spherical indentor is considered. The membrane is composed of a non-linear viscoelastic material whose constitutive equation is of nonlinear single integral type. This problem is formulated by examining two regions (contact and noncontact) of the deformed membrane. The noncontact region is governed by three first-order integro-differential equations, while the contact region (with a known geometry as a spherical surface) is described by two first-order integro-differential equations. The boundary between these two regions is unknown, but the stress and deformation there satisfy continuity conditions. With the nonlinear viscoelastic constitutive equation, and appropriate boundary conditions, these two sets of governing equations can be integrated by a numerical method for two-point boundary value problems. This paper analyzes the time dependent distributions of the stress, stretch, thickness variation and indentation force for various indentation histories. The common boundary between the contact and noncontact regions is also determined as a part of the solution process. Numerical results are presented for a constitutive equation that embeds the features of a Mooney-Rivlin elastic material in the Pipkin-Rogers nonlinear single integral viscoelastic framework. These illustrate the important features of the obtained solution. A discussion related to material property identification using the numerical results in conjunction with experimental results is also included.
Composites with Imperfect Interfaces at Finites Strains

Qi-Chang HE
Universite Paris-Est
MLV, MSME, Batiment Lavoisier, Paris, 77454, FR
Phone: 0033160957786, Email: he@univ-mlv.fr

J. Yvonnet
Universite Paris Est, Paris, France

Abstract:

The mechanical response of a composite consisting of two isotropic incompressible Neo-Hookean materials separated by an imperfect interface is investigated. In particular, the interface stress model under consideration is the coherent model in which the displacement field is continuous while the jump of the stress vectors is governed by the generalized Young-Laplace equation involving a surface energy. Exact results are provided for a fiber-reinforced cylinder undergoing a simple axial extension and a simple torsion. The analysis is also carried out for a hollow sphere subjected to internal and external pressure. To perform numerical simulations, a computational technique combining the level set method and the extended finite element method is developed and implemented for large deformations. The results are compared and discussed with respect to the relevant analytical ones.
Linear Theory for the Bending and Stretching of a Thin, Residually Stressed, Fiber-Reinforced Lamina

David Steigmann
University of California
Department of Mechanical Engineering, Berkeley, 94720, US
Phone: 510-684-5380, Email: steigman@me.berkeley.edu

Abstract:

The Euler equations of a thickness-wise expansion of the potential energy of a thin elastic body, truncated at a specified order, furnish a model for the bending and stretching of plates and shells. We develop a well-posed truncation for a uniform, pre-stressed, fiber-reinforced lamina. A pedagogically useful derivation of classical plate theory is obtained as a special case. This recovers results obtained via the method of gamma convergence, but without the need for functional analysis.
Buckling of Structures Under Tensile Dead Loading

Davide Bigoni  
University of Trento  
Via Mesiano 77, Trento, 38050, IT  
Phone: +390461282507, Email: bigoni@ing.unitn.it

Daniele Zaccaria  
University of Trieste, Trieste, Italy

Giovanni Noselli  
University of Trento, Trento, Italy

Diego Misseroni  
University of Trento, Trento, Italy

Abstract:

Possibility of bifurcations for structures subjected to tensile loads are investigated. Examples of such structures are shown. Theoretical findings are successfully compared to experimental results.
Buckling and Finite Deformation of a Hyper-Elastic Tube under External Pressure

Xiaoyu Luo
University of Glasgow
Department of Mathematics, University of Glasgow, Glasgow, G12 8QW, GB
Phone: +441413304746, Email: x.y.luo@maths.gla.ac.uk

Raymond W Ogden
University of Glasgow, Glasgow, UK

Abstract:

Cylindrical tube deforms in a strongly nonlinear fashion when subject to large external pressure, a problem that frequently appears in many biological applications. Engineering approaches to this problem often adopted small strain linear deformation, which can give very inaccurate predictions. In this work, a geometric and material nonlinear analysis is conducted for axisymmetric deformation of a thick-walled cylindrical tube subject to external pressure, and the results are compared to the linear predictions. The formulation is fully nonlinear and the governing system of nonlinear partial differential equations is derived and solved numerically using the C++ based object-oriented finite element library Libmesh. The weighted residual-Galerkin method and the Newton-Krylov nonlinear solver are employed for solving the governing equations. Since the nonlinear problem is highly sensitive to small changes in the numerical scheme, convergence was achieved using the analytical Jacobian matrix. It is found that for small deformation, both linear and nonlinear models give very similar results. However, cylindrical tubes behaves very differently under large external pressure, and the dominate features are the corner bulging and higher modes. This is the first time that a totally nonlinear analysis is carried out for thick walled tubes, and the results may have significant implications to many physiological applications involving soft vessels undergoing large deformation.
Mechanics of Novel Biohybrid Structures

Katia Bertoldi  
Harvard University  
317 Pierce Hall, 29 Oxford Street, Cambridge, 02138, US  
Phone: 6174963084, Email: bertoldi@seas.harvard.edu

JongMin Shim  
Harvard University, Cambridge, MA

Anna Grosberg  
Harvard University, Cambridge, MA

Kevin K. Parker  
Harvard University, Cambridge, MA

Abstract:

Nature makes extensive use of structures characterized by well defined design to achieve different functionalities. The mimosa folds its leaves when touched; the jellyfish controls its vertical movement contracting and expanding its umbrella. The natural world offers a great model for imitation and also an inspiration for new technologies. Flying was inspired by birds and the new generation of adhesives is designed mimicking highly fibrillated microstructure that control adhesion in many organisms.

Recently biohybrid materials from engineered tissues and synthetic polymer thin films were grown successfully [1]. Spatially ordered, two-dimensional myogenesis are built on thin elastomeric films, making the structure capable to adopt functional, three-dimensional conformations in response to a stimulus. These structures pave the way to the development of a new generation of structures capable to perform biomimetic tasks as diverse as gripping, pumping, walking, and swimming. However, such functionalities may be achieved only through a careful design of the structure and currently the design process is a bottleneck in the development of biohybrid structures able to perform specific tasks. This issue may be overcome developing an ad-hoc computational model, able to guide the choice of critical parameters such as the optimal thin-film shape, the tissue architecture and the electrical-pacing protocol. The computational model accounts for the tissue architecture as well as for the interaction of the structure with the surrounding fluid and allows the design of structures capable of specific functionalities.

References

Remarks on the Infinitesimal Stability and Shape Bifurcation of Incompressible, Isotropic Hyperelastic Spherical Shells

Millard F. Beatty
University of Nebraska-Lincoln
Department of Engineering Mechanics, P.O. Box 910215, Lexington, 40591-0215, US
Phone: 859-224-9331, Email: mbeatty2@unl.edu

Abstract:

The infinitesimal stability criterion for the small vibrations about a finitely deformed static equilibrium state of an incompressible, isotropic hyperelastic spherical shell under a constant inflation pressure is studied. This provides a general stability theorem relating the vibrational frequency and the pressure response from which it follows that pressure extrema are unstable or neutrally stable. The formulation is expressed in terms of the general shear response function for a hyperelastic material, and specific results are illustrated for the infinitely extensible Mooney-Rivlin and limited extensible Gent material models. A criterion obtained by others to characterize the possible bifurcation from a spherical to an aspherical shape is cast in terms of the general shear response function and all materials for which an aspherical bifurcation may occur are characterized. The results are illustrated for the classical models and the Ogden model among others.
Instability and Microstructure Evolution in Pseudoelastic Materials

Henryk Petryk
Institute of Fundamental Technological Research (IPPT PAN)
Pawinskiego 5B, Warsaw, 02-106, PL
Phone: +48 22 826 98 34, Email: hpetryk@ippt.gov.pl

S. Stupkiewicz
Institute of Fundamental Technological Research (IPPT PAN), Warsaw, Poland

Abstract:

Pseudoelastic behavior of materials under consideration is related to stress-induced, diffusionless phase transformation in solids. A typical example is the martensitic phase transformation in shape memory alloys. Pseudoelastic behavior incorporates both the elastic deformation of the constituents and the forward or reverse transition from austenite to a variant or combination of variants of martensite. The phase transition is studied as a consequence of intrinsic material instability related to the existence of states of lower energy. The aim of the present work is to examine the effect of interfacial energy and dissipation on the associated microstructure formation and its quasi-static evolution at constant temperature. The well-known notions of ellipticity, rank-one convexity and quasi-convexity of a nonlinear elastic energy function are helpful in analyzing the formation of fine microstructures but are insufficient to study size-dependent effects of interfacial energy and dissipation.

Accordingly, the basic concept of energy minimization is extended to the total energy minimization performed in an incremental manner, in close relation to the thermodynamic criterion of stability. The total energy includes the energy of interfaces on multiple scales and the rate-independent dissipation associated with the transition between different states. The theory has recently been developed by the authors (Petryk and Stupkiewicz, J. Mech. Phys. Solids, 2010). For intrinsic consistency of the approach, it is required that the symmetry restriction be imposed on the state derivative of the dissipation function used. This requirement is satisfied here since the incremental dissipation exhibits a pseudoelastic property of limited path-independence for sufficiently small increments. It is shown how the presence of interfacial energy and dissipation terms affects the thermodynamic condition for quasi-static propagation of a phase transformation front.

With regard to the pseudoelastic behavior of polycrystalline shape memory alloys, the interfacial energy is considered at three scales: of the grain or sub-grain boundaries attained by parallel martensitic plates, of the interfaces between austenite and twinned martensite, and of the twin boundaries within the martensitic plates. The interfacial energy of two origins is considered, namely, the atomic-scale energy of phase or twin boundaries and the elastic micro-strain energy at microstructured interfaces. The latter is calculated with the help of the finite element method applied to a periodic cell with locally incompatible eigenstrains across the boundary of a laminated domain.

Specific calculations have been performed in fully three-dimensional setting for CuAlNi and NiTi shape memory alloys, undergoing cubic-to-orthorombic and cubic-to-monoclinic phase transformation, respectively. Examples of the formation and evolution of a hierarchically laminated microstructure of
finite characteristic dimensions, the lowest in a range from 10 to 100 nanometers, are presented for loading/unloading in uniaxial tension. It is predicted how the characteristic dimensions of microstructure and the respective stress-strain diagram depend on the assumed size of plate-shaped or spherical subgrains.
Creation of Fiber Kinking Surfaces in Transversely Isotropic Hyperelastic Materials

Thomas Pence
Michigan State University
Mechanical Engineering, Michigan State University, East Lansing, 48864, US
Phone: 517 353-3889, Email: pence@egr.msu.edu

Abstract:

We consider surfaces within transversely isotropic hyperelastic materials across which the deformation gradient is discontinuous. As is well known, such surfaces can describe locations of fiber kinking. The purpose of this talk is to characterize the appearance of kink surfaces in terms of three general mechanisms: fade-in, pair creation, and boundary emission. Each has a counterpart for kink surface disappearance. These mechanisms are highly sensitive both to changes in the original fiber orientation field, including spatial variation in this field, and to changes in the nature of the applied boundary conditions. Specific examples of all three mechanisms are simply illustrated in the context of rectilinear shear.
On Mathematics in Ray Ogden's Contributions to Mechanics

Wodzimierz Domański

Military University of Technology, Faculty of Cybernetics, Institute of Mathematics and Cryptology
Kaliskiego 2, Warsaw, 00-908, PL
Phone: 48 22 683 75 52, Email: wdomanski@wat.edu.pl

Abstract:

Ray Ogden has contributed greatly to the field of theoretical mechanics. In all his works of a very broad character, great care for mathematical rigor is visible.

In my presentation I will emphasize some particular aspects of Ray's mathematical contributions in his many papers and books devoted to nonlinear elasticity. More precisely I will briefly discuss the problem of instabilities and loss of ellipticity in fiber-reinforced nonlinear elastic materials [1] and the problem of existence of smooth solutions in nonlinear elastodynamics [2]. I will end up with presenting the extension of my recent work [3] on weakly nonlinear waves in soft solids, inspired among others by Ray's (with collaborators) paper [4].

References

The Transition between Neumann and Dirichlet-Type Boundary Conditions in Elastic Plates

Graham Rogerson
Keele University
School of Computing and Mathematics, Keele University, Keele, ST5 5BG, GB
Phone: 44 1782 733270, Email: g.a.rogerson@keele.ac.uk

Rinat Moukhomdiarov
Keele University, Keele, UK

Abstract:

The transition from Neumann (traction-free) boundary conditions to Dirichlet (fixed-face) boundary conditions is investigated in respect of wave propagation in an elastic layer. Attention is focused on the implications of such a transition on the dispersion curve branches within the long wave region. Various low frequency band gaps are observed. The study includes both a numerical investigation and an multi-parameter asymptotic analysis.
Superposition of Finite-Amplitude Sinusoidal Plane Waves in Deformed Mooney-Rivlin Materials

Elizabete Rodrigues Ferreira
Université Libre de Bruxelles
ULB Campus Plaine CP 218/1, Blvd. du Triomphe, Bruxelles, 1050, BE
Phone: +1 518 9519484, Email: erodrigu@ulb.ac.be

Philippe Boulanger
Université Libre de Bruxelles, Brussels, Belgium

Michael Hayes
University College Dublin, Dublin, Ireland

Abstract:
Here we consider Mooney-Rivlin incompressible elastic materials which are first subjected to an arbitrary homogeneous static deformation. On such a deformation a time-dependent displacement field is superposed, representing a finite-amplitude wave motion. It is assumed that this displacement is along a principal axis of the static deformation and is function of two spatial variables in the principal plane orthogonal to this axis, so that the wave motion is transverse and the incompressibility constraint is satisfied. It is shown that such a displacement is an exact solution of the equations of motion provided it satisfies a two-dimensional anisotropic linear wave equation and a compatibility condition for the determination of the pressure field. In the special case of a plane wave propagating along an arbitrary direction of the principal plane, this compatibility condition is identically satisfied, the wave equation reduces to the one-dimensional vibrating string equation, and we retrieve known results (Ph. Boulanger, M. Hayes, Quarterly Journal of Mechanics and Applied Mathematics, 45, 575-593, (1992)). However, for two-dimensional wave motions, we note that the compatibility condition may be satisfied by requiring that the displacement satisfies a Helmholtz equation. It is seen that the anisotropic wave equation and the Helmholtz equation, which are both linear, may be satisfied together by a displacement field representing a superposition of an arbitrary number of sinusoidal plane waves propagating in different directions of the principal plane. Thus such a superposition is an exact solution of the equations of motion. This extends a result obtained recently by E. Rodrigues Ferreira for the superposition of two plane waves (E. Rodrigues Ferreira, Finite-Amplitude Waves in Deformed Elastic Materials, VDM Verlag Dr. Müller, Saarbrücken, 2009). Here the number of plane waves which may be superposed is arbitrary. These must be of the same wavelength, but each individual plane wave has a different wave speed so that the frequencies are also different. Properties of the corresponding energy flux and energy density are exhibited.
Material Tensors of Weakly-Textured Polycrystalline Materials

Chi-Sing Man  
University of Kentucky  
Department of Mathematics, University of Kentucky, Lexington, 40506-0027, US  
Phone: 859-257-3849, Email: chi-sing.man@uky.edu

Mojia Huang  
Nanchang University, Nanchang, Jiangxi, China

Abstract:

We consider polycrystalline materials whose constituting crystallites are anisotropic, are of the same chemical composition, and assume various orientations in space. We say that a polycrystal carries crystallographic texture if the local crystal lattices in the polycrystal have various preferred orientations. The presence of crystallographic texture, which is quantitatively described by the orientation distribution function (ODF), leads to macroscopic anisotropy of the physical properties of the polycrystal. When the physical property in question is determined by one or by a set of material tensors (e.g., the elasticity tensor, the acoustoelastic tensor, tensors that appear as terms in plastic potentials and yield functions, etc.), the problem of delineating texture-induced anisotropy reduces to that of determining the effects of crystallographic texture on material tensors, i.e., determining the functional dependence of material tensors on the ODF. We say that a polycrystalline material is weakly textured with respect to a physical property if each material tensor characterizing that property can be taken as the sum of an isotropic part and an anisotropic part that is linear with respect to the deviation of the ODF from its isotropic counterpart. In this paper a method is presented by which explicit expressions that delineate the effects of crystallographic texture on material tensors of weakly-textured polycrystalline materials (with arbitrary texture and crystal symmetry) can be derived systematically. The method consists of two steps. First, by one of the familiar methods (e.g., the method of group characters), the given tensor space is decomposed into its irreducible parts with respect to the rotation group. Then a representation formula is derived which expresses the projection of the given tensor onto an irreducible invariant subspace in terms of a specific irreducible tensor basis of that invariant subspace. An algorithm by which the specific irreducible tensor bases can be generated is given. As illustration the representation formula pertaining to the elasticity tensor is presented as an example.
Stability of Electro Active Polymer membranes

Giuseppe Puglisi
Dip. Ing. Civile Ambientale
Politecnico di Bari, Via Re David 200, Bari, 70100, IT
Phone: 0039.080.5963744, Email: g.puglisi@poliba.it

Giuseppe Saccomandi
Dip. Ingegneria Industriale, Università degli Studi di Perugia, Perugia, Italy

Giuseppe Zurlo
Dip. Ing. Civile Ambientale, Politecnico di Bari, Via Re David 200, Bari, Italy

Abstract:
In this note we are concerned with the stability analysis of thin polymeric films subjected to mixed boundary conditions, with special attention to the application of live loads of electrostatic type. Electroactive polymers (EAPs) are thin polymer films, typically prestretched in rigid frames, whose opposite faces are in contact with compliant electrodes. The electrodes are subjected, by means of a control device, to assigned voltage or charge. Coulomb forces between the electrodes determine the film compression. Due to the incompressibility of the polymer layer, this induces an in-plane extension used as a mean of actuation. EAPs based actuation devices have been growingly adopted in several advanced technological applications, due to their lightness, low cost, and fast response. On the other side, EAPs are affected by several failure phenomena of material, electrical, and geometrical type, which represent severe limitations.

In the recent papers ([1], [2]) the stability analysis of electroactive thin layers let us describe the insurgence of different types of instability experimentally observed: wrinkling, pull-in, damage and deformation localization. In particular we described, through an energetic formulation, the possibility of insurgence of all these different instabilities as the geometry of the device changes. Here we extend these results to more general boundary conditions and constitutive assumptions with the aim of the formulation of a more general stability analysis within the framework of problems of stability of membranes under live loading conditions.

References
Dielectric Elastomers Capable of Giant Deformation of Actuation

Xuanhe Zhao
Duke University
Department of Mechanical Engineering And Materials Sciences, Duke University, Durham, 02138, US
Phone: 6172793934, Email: xz69@duke.edu

Zhigang Suo
Harvard University, Cambridge, MA

Abstract:

Subject to a voltage, a membrane of a dielectric elastomer reduces thickness and expands area. This phenomenon is being studied intensely in the emerging technology of elastomeric transducers. Applications include artificial muscles, tunable optics, generators for harvesting energy, and tactile sensors for Braille displays. The elastomeric transducers have remarkable attributes such as high specific energy, fast response, and negligible noise. This talk focuses on the most conspicuous attribute: large deformation of actuation induced by voltage.

While all dielectrics deform under voltage, the attainable deformation of actuation varies markedly. Piezoelectric ceramics attain strains of actuation typically less than 1%. Glassy and semi-crystalline polymers can attain less than 10%. The initial reported values for elastomers were a few percents. By using soft electrodes, strains of actuation about 30% were observed in some elastomers. In the last decade, strains over 100% have been achieved in several ways, by pre-stretching an elastomer, by using an elastomer of interpenetrating networks, by swelling an elastomer with a solvent, and by spraying charge on an electrode-free elastomer.

These experimental advances have prompted a theoretical question: What is the fundamental limit of deformation of actuation? A theory may interpret the diverse and intriguing experimental observations mentioned above, and guide the search for dielectrics of even larger deformation of actuation. Here we present a theory to show that dielectric elastomers are capable of giant deformation of actuation, beyond 100%.
Modelling of Electro-Viscoelasticity - Application to Electrostrictive Polyurethane

Andreas Menzel  
TU Dortmund  
Mechanical Engineering, Leonhard-Euler-Str. 5, Dortmund, 44227, DE  
Phone: +492317556362, Email: andreas.menzel@udo.edu

Matti Ristinmaa  
Lund University, Lund, Sweden

Abstract:

Materials that have the ability to respond mechanically to applied electromagnetic fields are useful in applications such as sensors and actuators. Specifically, electroactive polymers (EAP) show great promise for such uses in, for example, bio-mimetics and robotics. The mechanisms responsible for the electromechanical behaviour in EAP applications vary. Very large strain responses have for instance been reported for dielectric polymer actuators, where attractive charges on the actuator's electrodes make them squeeze the polymer between them. Intrinsic electrostriction, with maximum strain responses of around 5%, has been reported for materials such as P(VDF-TrFE) and polyurethane (PU) elastomers.

As the number of applications grows, the possibility of numerical simulations of EAP is of great interest. The equations of non-linear electromechanical interactions in continua are well established. From the numerical viewpoint, an electromechanically coupled finite element framework is suitable to solve the governing equations of representative boundary value problems. In the case of electrostatics, a suitable approach is to solve for the vectorial displacement field and the scalar electric potential as the nodal degrees of freedom.

An important issue is the use of accurate constitutive models that take into consideration the electromechanical coupling as well as the possibly nonlinear and time-dependent mechanical behaviour of the polymer material. In this work, focus is placed on PU elastomers. Experimental evidence in the literature suggests that inherent electrostriction is present at moderate electric fields. Furthermore, the polyurethane exhibits strong rate dependence and it is therefore necessary to incorporate viscoelasticity into the constitutive model. With viscoelastic effects taken into account, it is shown that good agreement can be obtained between numerical simulations and experimental data. Specifically, the format of the viscoelastic contribution is discussed and also the manner in which it should be included in the energy function describing the material.
Homogenization-Based Constitutive Models for Magneto-Rheological Elastomers

Pedro Ponte Castaneda
University of Pennsylvania
220 S. 33rd. St., Towne Building, Room 235, Philadelphia, 19104-6315, US
Phone: 215-898-5046, Email: ponte@seas.upenn.edu

Abstract:

In this presentation, we propose new constitutive models for Magneto-Rheological Elastomers (MREs) in the finite strain regime. MREs typically consist of a magnetically insensitive, rubbery material that is reinforced with stiff, ferromagnetic particles. Because of magnetic interactions between the particles and the externally applied magnetic field, these materials are capable of undergoing large strains with no mechanically applied loads---they are magnetostrictive, and can therefore be used in applications as active materials. In addition, the externally applied magnetic field can also affect the mechanical response of the composite, leading to a dependence of the incremental modulus on the magnetic field. Making use of a consistent finite-strain homogenization framework, we propose macroscopic constitutive models for the magnetoelastic properties of these materials and explore the effect of various microstructural variables, such as the particle shape, orientation, concentration and distribution on the macroscopic response, including the effect on the magnetostrictive strain.
The Vibration Induced Dissipative Heating of Thin-Wall Structures Containing Piezoactive Layers

Igor Guz
University of Aberdeen
Centre for Micro- and Nanomechanics, Fraser Noble Building, King's College, Aberdeen, AB15 9DW, GB
Phone: +44 1224 272808, Email: i.guz@abdn.ac.uk

Y.A. Zhuk
Timoshenko Institute of Mechanics, Kiev, Ukraine

M. Kashtalyan
Centre for Micro and Nanomechanics, University of Aberdeen, Abedeen, UK

Abstract:

The forced-vibration analysis of structures occupies a significant place in the dynamics of deformable systems. An accurate prediction of the dynamic response is a serious challenge, since the material of a structure may become plastic under intensive loading and/or exhibit viscous properties. Variable viscoelastoplastic behaviour should be studied when designing metal dampers for the vibrations of building structures under wind and seismic loads, devices for suppressing vibrations of pipelines, test specimens in low-cycle fatigue tests, etc.

A modern approach to controlling the vibrations of complex systems suggests introducing additional active elements into a structure being designed. It was demonstrated that distributed piezoelectric elements are efficient in damping vibrations of elastic plates and shells. The overall aim of this research is to improve our understanding of the complex coupled processes in thin-wall inelastic structures that contain both active and passive layers and experience intensive cyclic loading. We analyse the role that the coupling of mechanical and electrical fields can play in defining the structure response. For this purpose, a simplified single-frequency approach is developed to describe the coupled dynamic behaviour under cyclic electric or mechanical loading of layered shells consisting of physically nonlinear passive and viscoelastic active layers. The period averaged dissipative function obtained from the solution for steady-state vibration problem is used to simulate the internal heat sources. Substitution of the dissipative function into the heat-conductivity equation averaged over the period of vibration enables us to address the heating aspect of the problem and estimate the temperature level to prevent the overheating above the Curie point for the piezoelectric material.

As an example, the problem of forced vibrations of a roller supported beam containing piezactive layers is solved. Different aspects of mechanical and electric excitation of the vibration are studied as well as the possibility of suppressing the mechanically induced vibration by means of voltage application to electrodes at the piezactive layer. The interplay between physical and geometrical nonlinearities under transient and steady state processes is investigated. For the mechanically excited vibrations, when piezoelectric layers work as sensors, the electric response of partially depolarised (due to excessive heating above Curie point) beam is considered. The low cycle structural fatigue curves
with respect to the temperature are plotted and safe regimes are determined. The temperature histories are also analysed for the case when the harmonically varied voltage supplied to piezoactive layers suppresses the mechanically excited vibrations.

The single frequency approximation was proved to be an accurate enough and reliable tool for temperature estimation even in the vibration suppression regime when the temperature of dissipative self-heating can reach significant levels due to the dielectric losses in piezoelectric layers. The developed technique is much faster, and demands less computational resources, than approaches involving direct integration of the complicated constitutive equations.
Arterial Modeling Considering the Mechanochemical Response of Smooth Muscle Cells

Gerhard A. Holzapfel
Graz University of Technology
Institute of Biomechanics, Kronesgasse 5-I, Graz, 8010, AT
Phone: 0043-316-873-1625, Email: holzapfel@tugraz.at

Sae Il Murtada
Royal Institute of Technology, Department of Solid Mechanics, Stockholm, Sweden

Abstract:

Arterial modeling at the molecular, cellular and tissue levels is increasing our ability to address multidisciplinary problems of academic, industrial, and clinical importance [1]. An appropriately developed finite element model, for example, may help to better predict mechanobiological processes pertaining to the human body and therapeutical procedures such as balloon angioplasty which is the most frequently used procedure worldwide to reduce the severity of atherosclerotic stenoses. The mechanical properties of the arterial walls are controlled by a complex 3D network of elastin, collagen fibrils and smooth muscle cells, which considerably contribute to the overall mechanical artery behavior. Smooth muscle cells are responsible for the artery contractility, are contained in the middle layer and are responsible for the control of short-term changes in lumen diameter and of the long-term changes in the extracellular matrix turnover. They are composed of thin (actin) and thick (myosin) filaments that are organized into contractile units that appear in a smooth arrangement.

In this presentation we briefly review state-of-the-art models that relate to the matrix material (elastin) and the reinforcement (collagen) of the artery wall. The consideration of the activation of smooth muscles in a constitutive law is also key in order to realistically capture the function of the artery, however, very little work has been documented on the modeling of smooth muscle activation within the continuum mechanics framework. Hence, one focus of this presentation is also the suggestion of a mechanochemical model of a layer of smooth muscle cells which couples the biochemistry with a biomechanical model based on the classical Hill’s model. The biomechanical model of the contracting fibers is described by a strain-energy function, and the active force is due to the increase of intracellular calcium concentration [2].

References


Determination of Residual Stresses in Blood Vessels

Yi-chao Chen
University of Houston
Department of Mechanical Engineering, Houston, 77204-4006, US
Phone: 713-743-4533, Email: chen@uh.edu

Abstract:

Study of residual stresses in blood vessels is of both theoretical and practical importance in biomechanics. The existence of residual stresses in blood vessels has long been recognized. Y. C. Fung is among the first to use both analytic arguments and convincing experimental observation to demonstrate the existence of residual stresses. He shows that after a radial cut was made on a segment of rabbit thoracic aorta, it opened up. This demonstrates indisputably that before the cut, the vessel is in compression near the inner surface, and tension near the outer surface. Fung also elaborates on the possible causes of the residual stress and its effect on the functionality of the blood vessel. Moreover, Fung observes that the change of curvature of the vessel wall in the spring-back process depends on the residual stress and the mechanical property of the wall. This indicates the possibility of quantifying the residual stress from the change of geometry of the vessel.

Much progress has been made on determination of residual stresses from the change of geometry when a section of blood vessel is cut. Most studies assume a specific form of the strain energy function for the vessel wall, assume that the vessel is stress free after being cut, and are confined to numerical solutions.

In this paper, we present an analysis for residual stresses in a blood vessel composed of a general anisotropic, radially inhomogeneous, elastic material. The strain energy function is left in a general form, leading to an analytic expression for the residual stresses. Among other things, no assumption is made that the vessel be stress free after being cut. A class of deformations associated with the cutting process is considered, for which a circular circumferential material line is deformed into a circular arc. The deformed cut surfaces, however, are not necessarily being flat. The class of materials for which the cut surfaces remain flat after cut is identified. For such materials, a general express is derived for the residual stresses. In contrast to the existing models in the literature, the residual stresses are found to depend on both the opening angle and the radius of the cut vessel. Of course, the residual stresses also depend on the form of the strain energy function. To obtain the latter, two deformations of the vessel are considered, corresponding to the inflation of the uncut vessel and the uniaxial stretch of the cut vessel, respectively. These provide possible experimental procedures in determine the residual stresses from one set of experiments without making assumptions on the material properties a prior.
A Two-Scale Collagen Turn-Over Model for Soft Biological Tissues with Application to Abdominal Aortic Aneurysms

T. Christian Gasser
The Royal Institute of Technology (KTH)
Department of Solid Mechanics, School of Engineering Sciences,
Osquars Backe 1, Stockholm, SE-10044, SE
Phone: 0046 8 790 7793, Email: tg@half.kth.se

Martin Auer
Development, VASCOPS GmbH, Graz, Austria

Abstract:

Collagen is the most abundant protein in mammals and gives mechanical strength, stiffness and toughness to many soft biological tissues. Malfunction of collagen turnover is believed to define later stages of Abdominal Aortic Aneurysms (AAAs) disease [1]. AAAs are local, permanent dilatations of the aorta in the abdomen, which are frequently observed in the elderly male population. AAA rupture is lethal in 3 out of 4 cases and predicting their growth and rupture risk could significantly improve their clinical management.

As suggested previously, the vascular wall is modeled as an isotropic matrix material with embedded bundles of collagen, where their alignment is defined by an orientation density function [2]. Specifically, an assemblage of interlinked collagen fibrils defines a bundle of collagen, which structure changes due to a dynamic (continuous) deposition and degradation of fibrils [3]. Consequently, collagen turnover is modeled at the fibril level and each collagen fibril has its own reference configuration. Multiplicative kinematics relates fibril deformation to the (macroscopic) tissue deformation, and a triangular density distribution function is used to capture the distribution of fibrils reference length within a particular bundle of collagen. Finally, similar to micro-plane constitutive models, the stress at the material point is derived by integration over the solid angle [4], i.e. integration over all collagen bundles.

Degradation of collagen is captured by first order kinetics, and, in contrast, a stress dependent rate defines collagen production. Likewise, collagen fibrils are deposited at a fixed stretch in the current configuration of the (macroscopic) tissue, which implicitly defines the collagen fibrils reference configuration. The stretch at collagen deposition is thought to be a characteristic tissue property probably related to fibroblast density.

The proposed model has a strong biological motivation and links collagen fibrils level with the tissues macroscopic length scale. Likewise, the micro-plane approach allows a straightforward Finite Element (FE) implementation (spherical t-designs are used [5, 6]) and examples demonstrate its numerical robustness. Results from representative initial boundary value problems indicate that tissue tends
towards homeostatic conditions, and adding constraints, on the collagen production rate for example, allows predicting saline feature of AAA growth.

References

Statistical Non-Linear Fibre-Reinforced Model for Soft Tissues

Salvatore Federico
Dept of Mechanical and Manufacturing Engineering, The University of Calgary
2500 University Drive NW, Calgary, T2L1Y3, CA
Phone: +1-403-220-5790, Email: salvatore.federico@ucalgary.ca

T. Christian Gasser
Dept Solid Mechanics, KTH Royal Institute of Technology, Stockholm, Sweden

Abstract:

The solid phase of biological soft tissues is comprised of a non-collagenous matrix, reinforced by collagen fibres, the arrangement of which depends on the particular tissue and the physiological loads it undergoes. The elastic strain energy potential for such non-linear fibre-reinforced materials is customarily obtained by superposition of the potentials of the matrix and of each family of fibres [5,3]. For a tissue like articular cartilage, the orientation of the collagen fibres is statistical, i.e., obeys a given probability distribution defined on the unit sphere (the solid angle), the superposition procedure gives rise to an integral term in the elastic potential such that the deformation features in the integrand function. The presence of the deformation in the integral prevents the possibility of calculating the potential a priori, and therefore a direct analytical use of the potential [1]. In this work [2], we implemented the integral term in the elastic potential, called `ensemble fibre potential`, into a numerical procedure that evaluates the potential, the stress and the elasticity tensor at each deformation step. The numerical integration over the unit sphere is performed by means of the method of the spherical designs [4], in which the result of the integral is approximated by a suitable sum over a discrete subset of the unit sphere. Furthermore, we checked the convexity of the ensemble fibre potential, and concluded that the assumption of asymmetric tension-compression fibre behaviour is not only reasonable from the physical point of view, but also required from the mathematical point of view, to guarantee the convexity of the potential.

As an example of application, we modelled the collagen fibre distribution in articular cartilage, and utilised it in simulating displacement controlled tests: the unconfined compression of a cylindrical sample, and the contact problem in the hip joint.

References

Deformation Micromechanisms of Collagen Fibrils under Uniaxial Tension

Roberto Ballarini
University of Minnesota
Department of Civil Engineering, Minneapolis, 55455, US
Phone: 6126252148, Email: broberto@umn.edu

Abstract:

Collagen, an essential building block of connective tissues, possesses useful mechanical properties due to its hierarchical structure. However, little is known about the mechanical properties of the collagen fibril, an intermediate structure between the collagen molecule and connective tissue. Here we report the results of systematic molecular dynamics simulations to probe the mechanical response of initially unflawed finite size collagen fibrils subjected to uniaxial tension. We find that the observed deformation mechanisms, associated with rupture and sliding of tropocollagen molecules, are strongly influenced by fibril length, width and cross-linking density. Fibrils containing more than approximately ten molecules along their length and across their width behave as representative volume elements and exhibit brittle fracture. Shorter fibrils experience a more graceful ductile-like failure. A simple analytical model is constructed and the results of the molecular modeling are used to find curve-fitted expressions for yield stress, yield strain and fracture strain as functions of fibril structural parameters. Our results for the first time elucidate the size dependence of mechanical failure properties of collagen fibrils. The associated molecular deformation mechanisms allow the full power of traditional material and structural engineering theory to be applied to our understanding of the normal and pathological mechanical behaviors of collagenous tissues under load.
A Model of Growth and Mass Transfer in Biphasic, Multi-Constituent Materials

Alfio Grillo
G-CSC Goethe Universitaet Frankfurt am Main, Kettenhofweg 139, Frankfurt am Main, D-60325, DE
Phone: +49(0)6979825225, Email: alfio.grillo@gcsc.uni-frankfurt.de

Michael Lampe
Goethe Centre for Scientific Computing, Goethe Universitaet Frankfurt am Main, Frankfurt am Main, Germany

Gabriel Wittum
Goethe Centre for Scientific Computing, Goethe Universitaet Frankfurt am Main, Frankfurt am Main, Germany

Abstract:
We consider growth and mass transfer in a biological tissue that is macroscopically described by a multi-constituent material. One phase is inviscid fluid, and the other one is an hyperelastic solid. We distinguish between the exchange interactions that occur between the phases, and growth that occurs in the solid-phase. Our purposes are: (i) to discuss possible evolution laws for both mass transfer and growth, and (ii) to characterize the equilibrium of the system. Under the assumption that growth and mass transfer are inelastic processes, the starting point of our approach is the decomposition of the deformation gradient tensor of the solid-phase into an elastic and inelastic part. The time derivative of the latter one is related with the rate of inelastic deformation. The determination of this quantity has become the subject of several investigations dealing with the Thermomechanics of volumetric growth, and is the first purpose of our contribution. We try to determine the rate of inelastic deformation by exploiting the dissipation inequality and accounting for the concept of non-standard dynamics put forward by DiCarlo and Quiligotti (DiCarlo&Quiligotti, Mech. Res. Communication 2002, 29, 449-456). The approach of these authors introduces stress-like second-order tensors which describe generalized forces conjugated to the rate of inelastic deformation. The working of these generalized forces can be understood as the power supplied to the system by its surrounding world in order for changing its internal structure. Our results provide evolution laws for the rates of inelastic deformation related to both growth and mass transfer. We also study the equilibrium of the system. To this end, we regard both growth and mass transfer as non-equilibrium processes, and define the state of equilibrium as the state in which neither growth nor mass transfer take place. In our setting, this implies that the rates of inelastic deformation associated with mass transfer and growth have to vanish independently. We find that, with respect to mass transfer, the non-standard dynamics provide a way for retrieving the Gibbsean characterization of equilibrium in terms of balance of chemical potentials. On the other hand, the condition that switches growth off is that its associated generalized forces attains an equilibrium value, which is given by the negative of Mandel-like stress tensor of the solid-phase. Our study of the dissipation inequality imitates the approach followed for determining the linear constitutive relation linking the non-equilibrium stress with the velocity gradient in visco-elastic materials. The discussion above is presented for the case of isotropic solid-phase. However, a generalization to the anisotropic case is also sought for in order to address, within a similar framework, the problem of remodelling in fibre-reinforced biphasic media.
Theoretical Models for Growth of Melanoma

Martine Ben Amar
Laboratoire de Physique statistique
Ecole normale Supérieure & Université Pierre et Marie Curie, 24 rue Lhomond, Paris, 75005, FR
Phone: 33 1 44 32 34 77, Email: benamar@lps.ens.fr

Abstract:

Melanoma are solid tumors originating in the epidermis before penetration in the dermis and angiogenesis. Destabilisation of the border which occurs at the early stage of development is part of the diagnostic and is currently known as asymmetry and border irregularity. The early evolution of skin cancer is characterized by an increase of the population of cancerous cells at the expense of the interstitial liquid through which the chemical factors diffuse. This explains the spatial inhomogeneity of solid tumours which present a ring of highly proliferating cells enclosing a zone of quiescent and necrotic cells. During the growth process, the basement membrane acts as an elastic substrate and angiogenesis does not occur before its penetration. We model this avascular stage as the growth of a nonlinear gel which has initially the shape of a disc. We show that an elastic instability is enough to explain the destabilization of the border in agreement with our model experiments on swelling gels with varying elastic stiffness. This instability is also present in our simulations obtained using the more sophisticated model of mixtures, which allows to treat the exchange between healthy and cancerous cells, the diffusion of nutrients and the role of the basal membrane. We show analytically that a simplified version of the mixture model exhibits travelling wave solutions which become unstable due to a transverse instability at finite growth rate for the cancerous cells and with a finite wavelength at threshold. This bifurcation occurs for a typical stress- interaction between cancerous cells, commonly used in the literature.

Joint work with C. Chatelain, P. Ciarletta, J. Dervaux and L. Foret
Reading the Mechanical Response of the Skin in its Lines

Melanie Ottenio
Universite de Lyon, INRETS, UMR T9406, Laboratoire de Biomecanique et Mecanique des Chocs, 25, Avenue Francois Mitterrand, Bron Cedex, 69675, FR
Phone: +33472142385, Email: melanie.ottenio@inrets.fr

K. Bruyere
Universite de Lyon, INRETS UMR_T9406, Laboratoire de Biomecanique et Mecanique des Chocs, Lyon, France

M. Gilchrist
University College Dublin, School of Electrical, Electronic & Mechanical Engineering, Dublin, Ireland

Abstract:

Through only a few millimetres, the human skin is able to protect internal organs from external aggressions. But skin can sometimes fail in this rule, especially if it is subjected to severe attacks, as stabbings for instance. As a result, a wound appears such a way that its shape is geometrically depending on the location of the attack. This observation was first made in the 19th century by Langer who mapped the natural lines of tension which occur within the skin. These lines, nowadays known as Langer’s lines, are related to the geometries of the wounds created by puncturing circular awl all over the body. Can these lines be used to propose a constitutive model for the skin which would be easily tuned in order to capture the influence of the location on the sample on the global mechanical response of the tissue.

Tensile tests on skin typically provide J-shaped stress-strain curves, in relation with the strain stiffening effect. This highly nonlinear elastic behaviour is mostly explained by a dense network of collagen fibres that is present in the dermis. We here propose to investigate if any relationship exists between the directions of the collagen fibres and Langer’s lines. As far as authors know, Ridge and Wright are the only one so far to have suggested that such a relationship exists.

To address the question, the authors performed ex-vivo uniaxial tensile tests on human bodies. Eleven standard dog-bone shapes were excised from the back of seven bodies. The specimens were obtained in various orientations to attempt to correlate the samples with the direction of Langer’s lines. Then, data fitting was performed by using different constitutive equations, among which was the fibre-reinforced material model proposed by Holzapfel, Gasser and Ogden in 2004. So, different values of elastic moduli were obtained for each tensile test. In parallel, other mechanical information was extracted from the stress-strain curves, like the ultimate tensile strength, or the failure strain. Finally, the sensitivity between all these extracted mechanical parameters and the direction of Langer’s lines was tested with the help of a statistical approach.

Now, a study is in progress to analyze the 3D network of the collagen fibres from skin biopsies, which has been procured from the tensile tests. It is expected to verify the results provided by statistics from the histological examination. It is also planned to identify some microscopic parameters in order to best tune the anisotropic material models in the case of the skin.

The presentation will try to show how the works of Pr Ogden in nonlinear elasticity and its applications to soft biological tissues inspired the authors in their research.
Advances in DNA Elasticity

Bernard D. Coleman
Rutgers University
Department of Mechanics & Materials Science, Rutgers University, Piscataway, 08854, US
Phone: 732-445-5558, Email: bcoleman@jove.rutgers.edu

Abstract:

This talk will be about advances in cell biology with the emphasis on problems in mechanics. Among the topics to be discussed is the dependence on salt concentration of the equilibrium configuration of circularized, intrinsically curved, DNA molecules, with the emphasis on recent numerical results indicating that changes in salt concentration can lead to large changes in the configuration of DNA minicircles.
Fundamental Solution in Plane Anisotropic Bimaterial with Imperfect Interface

Les Sudak
University of Calgary
Department of Mechanical & Manufacturing Engineering, 2500 University Drive NW, Calgary, T2N 1N4, CA
Phone: 403-220-5779, Email: lsudak@ucalgary.ca

Abstract:

In this talk, a general method is presented for the rigorous solution for the two-dimensional Green’s function in an anisotropic elastic bimaterial subject to a line force or a line dislocation. Most significant is the fact that the bonding along the bimaterial interface is considered to be homogeneous imperfect. Using complex variable techniques the basic boundary value problem for two analytic vector functions is reduced to a coupled linear first-order differential equation for a single analytic vector function defined in the lower half space. The coupled linear differential equation for the single analytic vector function can be subsequently decoupled into three independent linear first-order differential equations for three newly defined analytic functions. Closed-form solutions for the two-dimensional Green’s function are derived. Unlike previous works which involve inverse transform methods to obtain the physical quantities, the key feature of the present method is that the physical quantities can be readily calculated without the need to perform any inverse transform operations.
Well-posedness Results in a Traction Boundary Value Problem from Steigmann and Ogden’s Seminal Paper on Elastic Solids with Boundary Elasticity

Peter Schiavone
University of Alberta
Department of Mechanical Engineering, 4-9 Mechanical Engineering Building, Edmonton, T6G 2G8, CA
Phone: 780 492 3638, Email: p.schiavone@ualberta.ca

Abstract:

In the paper Proc. R. Soc. Lond. A (1997) 453, 853-877, Steigmann and Ogden developed a nonlinear theory of elastic boundary reinforcement in elastic solids subjected to plane strain deformations. This seminal work generated many interesting subsequent studies both in mechanics and in the mathematical analysis of corresponding boundary value problems. In this presentation, we consider the subsequent development of the boundary integral equation method following application to a set of boundary value problems arising from the linearization of Steigmann and Ogden’s theory. We review results obtained by the author and co-workers in the last decade (for example, Proc. R. Soc. Lond. A (1998) 454, 2223-2242; IJES 47 (2009) 1331-1338) and propose a further extension to a particular case arising when only part of the bounding curve of the elastic body is reinforced. Specifically, interior and exterior mixed-boundary problems from the linear theory are formulated and solved using integral equation methods. The boundary value problems are reduced to systems of singular integro-differential equations to which Noether-type theorems are shown to apply. Existence and uniqueness results are presented for both interior and exterior reinforcement problems of plane-strain.

Finally, we mention an interesting result concerning the elimination of the classical stress singularity at a crack tip in linear elastic fracture mechanics and how this is related to the role of boundary reinforcement in the case corresponding to a coating which has only extensibility properties and no bending rigidity (Gurtin-Murdoch).
Simply Unreal: Grassmann Hypercomplex Numbers and Connections Among Geometric Algebra, Tensor Algebra, and Mechanics

Debra Warne
James Madison University
Department of Mathematics and Statistics, MSC 1911, Harrisonburg, 22807, US
Phone: 540-568-2546, Email: warneda@jmu.edu

Paul Warne
James Madison University, Harrisonburg, VA

Abstract:

In this talk, we briefly trace the development of vector algebra and vector calculus (highlighting contributors such as Grassmann, Hamilton, Clifford, Gibbs, and Heaviside) with a view toward the ongoing (re-)emergence of geometric algebra and geometric calculus, a system poised to become an integral tool for mathematics of multiple dimensions. While the algebra of geometric algebra (a Clifford algebra) is well-studied, the same cannot be said for its ease of application or its geometry. Geometric algebra as an approach to foundations for mechanics also presents a radical departure from standard developments and while initially overlooked, has recently generated considerable interest in client fields. Emerging literature contains new expositions tailored toward physicists, engineers, and the computer and computer graphics industries. The well-defined structure of the geometric algebra has not only proven to be notationally more efficient for numerous problems in the sciences, but also better able to capture both the geometric and physical significance of the application. Here, we introduce an approach that provides a simpler departure from and connection to classical mathematical system developments than do many direct treatments of geometric algebra, as the latter have typically been viewed as having too steep a learning curve for common use. We highlight this extended, multi-dimensional number system from a component perspective to capture the algebra (and geometry) of geometric algebra without requiring any high-powered mathematics. We outline the basic mathematical properties of our eight-dimensional Grassmann hypercomplex number system and define a product for such multi-dimensional numbers. This system is then seen to be a simple extension of well-known number systems (the reals, complex numbers, and quaternions, e.g.) that includes and surpasses the standard vector algebra system. We conclude with a bridge to tensor products, highlight the use of the ideas for a few applications (e.g., rotations, reflections, contractions) and demonstrate how Maxwell’s four equations are really just a single mathematical equation.
A Symposium in Honor of the Contribution of Roger Fosdick,
The Recipient of Engineering Science Medal

ORGANIZERS:

Kaushik Bhattacharya, California Institute of Technology
Yi-Chao Chen, University of Houston
Gearoid MacSithigh, Missouri University of Science and Technology
Influence of Fiber Dissolution and Reassembly on Axial Stretch and Torsion of a Fiber Reinforced Hyperelastic Cylinder

Alan Wineman
University of Michigan
Department of Mechanical Engineering, Ann Arbor, 48104, US
Phone: 734-936-0411,  Email: lardan@umich.edu

Thomas J. Pence
Michigan State University, East Lansing, MI

Abstract:

The large deformation mechanical response of materials in which elastic fibers are embedded in an elastic matrix can be modeled in the context of anisotropic hyperelasticity, where the fibrous structure is homogenized and represented by different properties in certain directions. The elastic response of such materials can be considered as arising from a single microstructural mechanism during the entire range of response, namely the distortion of macromolecules in the matrix or in the molecular structure of the fibers. In previous work, the authors have developed a theory in which new microstructural events occur during the response of the fibers. In this theory, fibers undergo dissolution as a result of increasing elongation and then reassemble in a direction defined as part of the model. The case where the fibers reassemble in the direction of maximum principal stretch of the matrix was considered.

This model was previously illustrated for a material having fibers in the reference configuration that are all aligned in a common direction, and subjected to either homogeneous uniaxial extension or simple shear. The present work studies the implications of the model during the non-homogeneous deformation of axial stretch and torsion of a circular solid cylinder composed of an isotropic matrix and families of helically wound fibers. It is shown that the process of fiber dissolution and reassembly produces complex morphological changes in the fibrous structure and hence, in the response of the cylinder. The case of a single family of fibers initially aligned axially is studied in detail. It is shown that the cylinder has an inner core of original material and an outer layer of material in which the fibers have undergone dissolution and reassembly. The interface between these regions can move radially inward as axial stretch and/or twist increase. Gradual reassembly of the fibers with increasing stretch and twist changes their contributions to the torque and axial force and their helical orientation. Different sequences of axial stretch and twist result in different morphologies in the fibrous structure.
On Microstructure Evolution in Fiber-Reinforced Elastomers and Implications for Their Mechanical Response and Stability

Oscar Lopez-Pamies
State University of New York
139 Light Engineering, SUNY Stony Brook, Stony Brook, 11794-2300, US
Phone: 6316328249, Email: oscar.lopez-pamies@sunysb.edu

Abstract:

Lopez-Pamies and Idiart [Lopez-Pamies, O., Idiart, M.I., 2010, Fiber-reinforced hyperelastic solids: A realizable homogenization constitutive theory. Journal of Engineering Mathematics, doi:10.1007/s10665-009-9359-y.] have recently put forward a homogenization theory with the capability to generate exact results not only for the macroscopic response and stability, but also for the evolution of the microstructure in fiber-reinforced hyperelastic solids subjected to finite deformations. In this work, we make use of this new theory to construct exact, closed-form solutions for the change in size, shape, and orientation undergone by the underlying fibers in a model class of fiber-reinforced hyperelastic solids along arbitrary 3D loading conditions. 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 fiber-reinforced elastomers. In particular, we show that the rotation of the fibers may lead to the softening of the overall stiffness of fiber-reinforced elastomers under certain loading conditions. Furthermore, we show that this geometric mechanism is intimately related to the development of long-wavelength instabilities. These findings are discussed in light of comparisons with recent results for related material systems.
On the electro-mechanical response of dielectric polymer composites

Gal deBotton
Ben-Gurion University
Dept. Mechanical Engineering, P.O.B. 653, Beer-Sheva, 84105, IL
Phone: (972) 73 277 7105, Email: debotton@bgu.ac.il

Stephan Rudykh
Mechanical Eng., Ben Gurion Univ., Beer Sheva, IL

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

Abstract:

The class of electroactive polymers have been developed to a point where real life applications are conceivable. While providing attractive advantages, their wide-spread application has been hindered by the need for large electric fields. This work address this issue by developing a systematic framework to characterize the effective electromechanical properties of nonlinearly coupled materials capable of large deformation, together with appropriate simulation tools. The theoretical characterization of the deformation of heterogeneous dielectrics due to electrostatic excitation is initially considered. Within the framework of periodic homogenization it is shown for the first time that the coupled governing equations at the macroscopic level are identical to the ones at the microscopic level. Next, the theory is applied to specific periodic composites where it is shown that the macroscopic coupled response can be extracted from the uncoupled dielectric and mechanical responses. Application of the results to the class of laminates enable to examine optimal microstructures, and to demonstrate that the electromechanical coupling can be intensified by orders of magnitude. To examine the coupled behavior of composites in finite deformation a finite element code (COMSOL multi-physics) was adapted together with a unique implementation of both electrostatic and mechanical periodic boundary conditions. This, in turn, enabled to examine mechanical instabilities under electrostatic excitation. This type of application may result in a practical method for attaining large deformations with relatively small electric fields. In a way of an example we analyze the application of a thick-wall dielectric balloon as a micro-actuator or a micro-pump.
Continuum Theory for the Evolution of Plasticity and Incompatibility

David Steigman
University of California
6133 Etcheverry Hall, Department of Mechanical Engineering, Berkeley, 94720, US
Phone: 510-684-5380, Email: steigman@me.berkeley.edu

Abstract:

The phenomenological theory of elastic-plastic response is reconsidered in the light of recent opinion regarding the constitutive character of the constituent elastic and plastic deformations. The primary role of material symmetry and dissipation in the physics of plastic evolution is emphasized and shown to lead to the clarification of a number of open questions.
On the Importance of Counterion Condensation in Molecular Biophysics

Bernard D. Coleman
Rutgers University
Department of Mechanics & Materials Science, Rutgers University, Piscataway, 08854, US
Phone: 732-445-5558, Email: bcoleman@jove.rutgers.edu

Abstract:
As evidence has accumulated to the effect that G.S. Manning's theory of counterion condensation is not only applicable to separated polyelectrolyte molecules but also yields a verifiable theory of the formation of bundles of polyelectrolyte molecules with the same charge, it becomes clear that a successful theory of the mechanics of processes that take place in the cytoplasm of a cell may be expected to look very different from what we who are familiar with the continuum mechanics of the previous century are likely to expect.
Regularity of Energy Minima in Second-Gradient Nonlinear Elasticity

Tim Healey
Cornell University
Department of Mathematics, 432 Malott Hall, Ithaca, 14853, US
Phone: 607-255-3738, Email: healey@math.cornell.edu

Abstract:

We consider a broad class of problems motivated by nonlinear elastic (Cosserat) structures and solids - including multi-phase. As in the classical 3-d theory, we impose the condition that the energy density grows unboundedly as the local volume ratio approaches zero from above. Assuming convexity of the energy density in the second gradient of the deformation, the existence of minimizers is fairly standard; that of weak solutions is not. Assuming sufficiently rapid growth of the stored energy as the volume ratio goes to zero, we demonstrate that every admissible deformation (including any minimizer) is locally orientation-preserving everywhere throughout the domain. Thus, minimizers are readily shown to be weak solutions for a general class of genuinely mixed boundary value problems.
Energy Balance in Peridynamics

Stewart Silling
Sandia National Laboratories
P.O. Box 5800, Albuquerque, 87185-1322, US
Phone: 505-844-3973, Email: sasilli@sandia.gov

R. B. Lehoucq
Sandia National Laboratories, Albuquerque, NM

Abstract:

The peridynamic model of solid mechanics treats internal forces within a continuum through interactions across finite distances. These forces are determined through a constitutive model that, in the case of an elastic material, permits the strain energy density at a point to depend on the collective deformation of all the material within some finite distance of it. The forces between points are evaluated from the Frechet derivative of this strain energy density with respect to the deformation map. The resulting equation of motion is an integro-differential equation written in terms of these interparticle forces, rather than the traditional stress tensor field.

Recent work on peridynamics has elucidated the energy balance in the presence of these long-range forces. We have derived the appropriate analogue of stress power, called absorbed power, that leads to a satisfactory definition of internal energy. This internal energy is additive, allowing us to meaningfully define an internal energy density field in the body. An expression for the local first law of thermodynamics within peridynamics combines this mechanical component, the absorbed power, with heat transport. The global statement of the energy balance over a subregion can be expressed in a form in which the mechanical and thermal terms contain only interactions between the interior of the subregion and the exterior, in a form anticipated by Noll in 1955.

The local form of this first law within peridynamics, coupled with the second law as expressed in the Clausius-Duhem inequality, is amenable to the Coleman-Noll procedure for deriving restrictions on the constitutive model for thermomechanical response. Using an idea suggested by Fried in the context of systems of discrete particles, this procedure leads to a dissipation inequality for peridynamics that has a surprising form. It also leads to a thermodynamically consistent way to treat damage within the theory, shedding light on how damage, including the nucleation and advance of cracks, should be incorporated into a constitutive model.
Fluid Foams

Cesare Davini
University of Udine, Dip. Georisorse e Territorio, Italy
Dipartimento di Georisorse e Territorio, Via del Cotonificio 114, Udine, 33100, IT
Phone: +39(0)432558750, Email: davini@uniud.it

Abstract:

Fluid foams are complex fluids consisting of small gas bubbles separated by thin liquid walls in a proportion such that the volume fraction of the liquid phase is small. This fine microstructure confers foams peculiar properties that make them precious for a variety of technological applications. Moreover, it is also responsible for a rich phenomenology involving typical mixed liquid-solid behaviour.

While forces playing a role in foam physics are fairly well understood at cell or wall level, to give a phenomenological description is a difficult task, because the phenomena that take place are manifold and not easily separable from one another so as to make modeling affordable. Here I discuss a continuum model thought of for rheological purposes. Ignoring much of the complexity associated to the flow through the Plateau borders (drainage), the gas diffusion through the cell walls (coarsening), viscosity, etc., I concentrate on ideal cells and elaborate a model for monodisperse dry foams in equilibrium. By assuming honeycomb cells, the equilibrium equations and stress-strain relation are deduced. The approach gives also account of topological transformations involving an interchange of neighboring cells (T1 mechanism) and of a mechanism of cell coalescence by wall breakage (coarsening).

The work recasts the current theoretical understanding of equilibrium structure and elastic-plastic response of a dry, perfectly ordered, two-dimensional gas-liquid foam into the mathematical framework of elasticity theory.
On the Modeling of Rheological Behaviors of Weakly Interacting Systems

Junjie Li
Xiamen University
422 Siming Road South, Xiamen, 361005, CN
Phone: +86-592-2187703, Email: yzh@xmu.edu.cn

H.Z. Chen
Xiamen University, Xiamen, Fujian

X. Cheng
Xiamen University, Xiamen, Fujian

Y. Zhang
Xiamen University, Xiamen, Fujian

Abstract:

In recent years, much effort has been undertaken to characterize the flow of such weakly interacting systems as highly viscous emulsions, associating polymers, colloid polymer mixtures and ionomers, of which all show two dispersed phase interactions. It has been shown that polycarbosilane (PCS) melt, an important precursor for preparation of SiC based ceramic fibers, became unstable near its spinning temperature and exhibited strong time-dependent viscoelasticity with a weak thixotropy. Understanding of flow behaviors, microstructure characteristics and material properties is of practical interests to the applied engineers. For the theoretical modeling of weakly interacting systems, coarse-grained models are usually developed by means of physical intuition, simplicity, symmetry and fundamental laws of physics, in particular, in the field of complex fluids. However, the coarse-grained models could not fulfill consistency of different levels of mechanism on the length and time scales involved in such complex fluids, it is necessary to unify these universal properties into a model to be able to illustrate rheological phenomenon like viscosity bifurcation. In this work, a general equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) within a general formalism for the description of weakly interacting systems is developed. This GENERIC formalism includes the weakly interactions due to chain sessions and cross links. The application of this model to PCS melts in shear to predict viscosity bifurcation phenomenon is also discussed.
On the Global Stability of Elastic Bars in Uniaxial Extension

Scott Spector
Southern Illinois University
Department of Mathematics, Carbondale, 62901, US
Phone: 618-453-6577, Email: sspector@math.siu.edu

Abstract:

When a bar is subjected to uniaxial tension, the bar usually deforms (approximately) homogeneously and isoaxially until a critical load is reached. A bifurcation, such as the formation of shear bands or a neck, may then be observed. Suppose one models such an experiment as the extension of a homogeneous, isotropic, hyperelastic material in which the length of the bar is prescribed, the ends of the bar are assumed to be free of shear, and the sides are left completely free. For this model we show that standard, additional constitutive hypotheses on the stored-energy function imply that the experimental observations are not possible due to the fact that the homogeneous deformation is the unique absolute minimizer of the elastic energy. Therefore, either shear bands and necks are not elastic phenomena or the stored-energy function must not satisfy some assumptions in common usage.

The fact that no local bifurcations can occur under our assumptions was known previously [1,3], since these assumptions prohibit the load on the bar from reaching a maximum value. However, the fact that the homogeneous deformation is the absolute minimizer of the energy appears to be a new result.

The proof of our result uses the technique developed in [2] for energy minimization of thick spherical shells. The main idea is fairly simple. We first consider the stored-energy function for a neo-Hookean material. For this function we show that the elastic energy can be bounded below by an integral of a convex function of the deformed length of line segments that were initially parallel to the loading axis. Moreover, this lower bound is an equality when the image curves are straight lines that are deformed uniformly and are parallel to the loading axis. Thus, energetically, the material prefers that each such straight line deform homogeneously into another parallel straight line. The general case then follows from Jensen's inequality.


Acoustoelastic Measurement of Surface and Subsurface Stress in Anisotropic Solids

Chi-Sing Man
University of Kentucky
Department of Mathematics, Lexington, 40506-0027, US
Phone: 859-257-3849, Email: chi-sing.man@uky.edu

Abstract:
Surface conditioning such as shot peening, laser peening, and low plasticity burnishing imparts on the metal parts so treated a thin layer of surface and subsurface compressive residual stress, which provides significant lifetime enhancement against fatigue failure and stress corrosion cracking of the parts. To incorporate the beneficial effect of residual stress in component-life predictions, it is necessary to develop a nondestructive measurement technique which allows monitoring surface and subsurface residual stress retention during the life time of parts.

This talk is a progress report on the efforts of my research collaborators and myself to develop a method that uses simultaneous Rayleigh wave and surface P-wave measurements to evaluate surface stress and to delineate the depth-dependent profile of the subsurface stress. To allow for the effects of crystallographic texture, we formulate our method in the general context of anisotropic elasticity with initial stress. So far, our studies have been restricted to objects with a flat surface, which we model as vertically inhomogeneous half-spaces (i.e., with inhomogeneity only in the direction normal to the surface). In this talk, after outlining the theoretical setting, the work of Moreau and Man will first be reviewed; there, by simultaneous laser-ultrasonic measurements of Rayleigh wave and surface P-wave, they successfully inferred both the surface residual stress and the changes in surface texture induced by low plasticity burning on an AA7075-T651 aluminum sample block. Then some highlights of the work of Tanuma, Man, Nakamura, and Wang on measurement of subsurface stress will be presented. The vertical inhomogeneity of the incremental elasticity tensor and of the initial stress will lead to dispersion of Rayleigh waves. By extending the Stroh formalism to vertically inhomogeneous half-space, we have derived a high-frequency asymptotic formula for the frequency dependence of phase velocity of Rayleigh waves, which relates the dispersion to the normal derivatives of the incremental elasticity tensor and of the initial stress at the surface. Applications of the formula in estimating subsurface stress will be discussed.
Periodic Bifurcations for an Incompressible Elastic Tube Subject to Pure Circular Shearing

Pilade Foti
Politecnico di Bari
Dipartimento di Ingegneria Civile e Ambientale - Politecnico di Bari, Via Re David, 200 - 70125 - Bari, Italy, Bari, 70125, IT
Phone: +390805963502, Email: p.foti@poliba.it

Aguinaldo Fraddosio
Politecnico di Bari, Bari, Italy

Salvatore Marzano
Politecnico di Bari, Bari, Italy

Abstract:
4
In the recent paper [1], we investigated the possibility for a compressible, isotropic elastic solid to support a periodic displacement bifurcation, induced by a shear stress state. We were interested in the analog of the classical planar Couette sinusoidal instability pattern observed in the flow of viscous fluids and/or the swirling motion in the longitudinal cells. Specifically, we studied the case of an infinitely long block of generalized Blatz-Ko material confined between, and attached to, parallel plates which are subject to a relative rectilinear shear. Our analysis centered on an appropriate choice of periodic incremental deformations superposed upon the primary equilibrium simple shear. We determined a critical value of the applied shearing strain corresponding to the occurrence of a planar Couette-like instability mode. We adopted the Hadamard energy criterion of infinitesimal stability, and showed that as the simple shear load is increased a planar Couette-like field corresponds to the first form of instability within the set of admissible incremental displacements. Finally, we discussed a suitably restricted form of the strong ellipticity condition for the incremental elasticity tensor and showed that this condition is first violated at the critical shearing strain.

The study summarized above represents a precursor to the problem of annular shear-driven instabilities for an elastic tube, briefly discussed in [2]. This corresponds to the analog for solids of the classical Taylor-Couette bifurcation problem associated with the laminar steady shearing flow of a viscous fluid confined between two concentric cylinders, each rotating with different angular velocity (cf. [3]). In this talk we consider a compressible elastic tube with Levinson-Burgess strain energy function subject to a relative annular shear at its inner and outer boundaries. We argue, based on a suitable incremental boundary-value problem, the possibility of a bifurcation from a pure circular shear to an axially periodic toroidal twist-like deformation. The condition for determining the critical bifurcation load depends on the solution of a non-autonomous linear matrix ordinary differential equation for which the Magnus expansion is introduced (cf. [4]).
Time permitting, we consider the Taylor-Couette-like bifurcation for the case of an incompressible, isotropic elastic tube. This bifurcation analysis exhibits analytical features somewhat different from that developed for the compressible case due to the presence of the incompressibility constraint.

Numerical examples are presented for the compressible Levinson-Burgess material, as well as for an incompressible material of a common constitutive form.

References


Aguinaldo Fraddosio
Politecnico di Bari, Dipartimento di Ingegneria Civile e Ambientale - Politecnico di Bari, Via Re David, 200 - 70125 Bari, Italy
Phone: +390805963502, Email: a.fraddosio@poliba.it

Mario Daniele Piccioni
Politecnico di Bari, Bari, Italy

Abstract:
A fundamental goal in the analysis of bifurcation for non-linear elastic solids during a static loading process is to accurately estimate the threshold at which the primary deformation ceases to be stable and a new configuration emerges. To address this goal, it is common to introduce the Hadamard energy criterion of infinitesimal stability (cf. [1]). This criterion is adopted in many classical studies of bifurcation, together with the vanishing of the first variation of the total energy, but this approach yields only necessary conditions for a weak local minimum. On the other hand, the vanishing of the first variation accompanied by the uniform Hadamard stability condition (which corresponds to the uniform positiveness of the second variation) are sufficient conditions for a weak local minimum. Some significant results on stability issues and conditions for weak local minimizers recently have been recorded in [2]. Moreover, a useful tool for checking the uniform Hadamard stability condition has been proposed in [3]: the uniform Hadamard stability condition holds if the strong ellipticity and the complementing conditions hold, and the Hadamard functional is strictly positive. Thus, it is important to seek optimal conditions which ensure that the Hadamard functional is strictly positive. While optimality is the goal, it is of practical importance to determine a lower bound for the critical load, i.e., a value of the load below which the Hadamard functional is definitely positive. Such a lower bound estimate for the critical load recently has been analyzed in [4] for compressible elastic solids. Here, we extend the study to the case of incompressible elastic solids and we show that our procedure generally improves other lower bound estimates that have been proposed in the literature.

References
Effect of Nonlinearity on the Steady Motion of a Twinning Dislocation

Anna Vainchtein
University of Pittsburgh
Department of Mathematics, University of Pittsburgh, 301 Thackeray Hall, Pittsburgh, 15260, US
Phone: 412 624 8309, Email: aav4@pitt.edu

Abstract:

We consider the steady motion of a twinning dislocation in a Frenkel-Kontorova lattice with a double-well substrate potential that has a non-degenerate spinodal region. Semi-analytical traveling wave solutions are constructed for the piecewise quadratic potential, and their stability and further effects of nonlinearity are investigated numerically. We show that the width of the spinodal region and the nonlinearity of the potential have a significant effect on the dislocation kinetics, resulting in stable steady motion in some low-velocity intervals and lower propagation stress. We also conjecture that a stable steady propagation must correspond to an increasing portion of the kinetic relation between the applied stress and dislocation velocity.
Interatomic Potentials, Forces and Stress

Ellad Tadmor
University of Minnesota
107 Akerman Hall, 110 Union St SE, Minneapolis, 55455, US
Phone: 651-646-0092, Email: tadmor@aem.umn.edu

Nikhil C. Admal
University of Minnesota, Minneapolis, MN

Abstract:

At the molecular level there are atoms and forces, whereas continuum theories deal with fields and stress. To connect between these models of reality it is necessary to obtain expressions for continuum variables, such as stress, at the molecular level. To date, many different expressions have been proposed and some confusion exists in the literature as to which is "correct". We show that a unified framework, based on the work of Irving and Kirkwood and later Noll, can be established from which all other expressions can be derived. Interestingly, it turns out that subtle arguments related to the nature of interatomic potentials play an important role in the derivation. The theoretical framework as well as numerical results will be presented.
Is Step-Flow Epitaxy Ever Stable?

Michel Jabbour
University of Kentucky
Department of Mathematics, Lexington, 40506-0027, US
Phone: 859-257-8836, Email: jabbour@ms.uky.edu

Paolo Cermelli
University of Turin, Torino, Italy

Abstract:

Recent experiments have established that bunching and meandering instabilities (the former referring to the formation of regions with high step density separated by wide terraces; the latter designating the evolution of initially rectilinear steps into wavy ones) can occur simultaneously during step-flow growth on metallic vicinal surfaces. This is in contrast to the predictions of existing models that trace back to the seminal 1951 work of Burton, Cabrera, and Frank (referred to hereafter as BCF). Indeed, in the BCF framework, meandering is contingent upon the existence of an Ehrlich-Schwoebel (ES) barrier, one that favors adatom attachment to ascending steps, whereas bunching requires an inverse ES effect (whereby the barrier to adatom incorporation to a descending step is lower than that which characterizes ordinary diffusion). Bunching and meandering appear therefore to be a priori mutually exclusive. In this talk, an extension of the BCF theory, one that ensures consistency with the second law of thermodynamics, is presented that resolves this apparent paradox, in the sense that it yields simultaneous bunching and meandering under the assumption of an ES barrier. Central to the theory is the step chemical potential for which a generalized Gibbs-Thomson relation is derived via a direct energy-rate calculation, resulting in boundary conditions along step edges that couple adjacent terraces. Specialization to the case of a periodic train of initially equidistant steps reveals a competition between the stabilizing ES effect and a destabilizing energetic correction that, for sufficiently high adatom equilibrium coverage, leads to step collisions. The underlying physics can be understood in terms of the tendency of the thin solid film to minimize its total free energy.
Damage-induced Instabilities in Rubber Films

Giuseppe Puglisi
Politecnico di Bari
Dip. Ingegneria Civile e Ambientale, Politecnico di Bari, Via Re David 200, Bari, 70100, Italy
Phone: 0039.080.5963744, Email: g.puglisi@poliba.it

Salvatore Marzano
Dip. Ingegneria Civile e Ambientale, Politecnico di Bari, Via Re David 200, Bari, Italy

Giuseppe Zurlo
Dip. Ingegneria Civile e Ambientale, Politecnico di Bari, Via Re David 200, Bari, Italy

Abstract:

In this paper, by using a recently proposed approach for damageable amorphous materials [2, 3], we deduce a two-dimensional model for polymeric membranes. Our main focus is the analysis of damage-induced instability effects. Since the pioneering works of Treloar on the instability of thin rubber sheets under dead loading at the boundary, much work has been done toward a comprehension of this type of phenomena. Following [2, 3], we assume that the bulk filled rubber is constituted by a mixture of different materials: an elastic fraction and an amorphous breakable fraction, constituted by a distribution of materials with variable activation and breaking thresholds. The model well describes the response of filled rubbers undergoing damage and healing, during classical experiments such as combined extension and torsion of cylinders [4] and inflation of thin rubber balloons [1]. In particular, in [1] the effects of damage and healing in rubber balloons has been analyzed. Well documented inflation experiments on initially spherical, thin rubber balloons, show the occurrence of asphericity during inflation in correspondence with precise pressure ranges. Moreover, in successive inflations from the natural configuration, the occurrence of asphericity may be attenuated or even disappear. This striking effect suggests that distortions may be strictly related to the occurrence of damage-induced softening in rubber films. In this note we give some insights on these phenomena which may help toward the formulation of a finer phenomenological continuum theory for filled rubbers.

References

Entropy of a Constrained Hamiltonian System and Mesoscale Dislocation Mechanics

Amit Acharya
Carnegie Mellon University
119 Porter Hall, Civil and Env. Engg., Pittsburgh, 15215, US
Phone: 412 268 4566, Email: acharyaamit@cmu.edu

Abstract:

In classical statistical mechanics, there is a formula for the entropy of a finite dimensional constrained Hamiltonian system. It seems that this idea can be combined in a systematic way with space-time averaged, kinematically rigorous PDE models of dislocations or voids to produce mesoscale models of plasticity or damage, respectively. The energetics and driving forces for dissipative mechanisms in these models can be precisely linked to atomistic behavior through well-defined, material-specific, one-time calculations that are expected to be possible on modern computers. This presentation will discuss the details of this formalism.
Predicting Fracture Nucleation at Grain Boundaries in TiAl using Evolving Mesoscale Metrics

Darren Mason
Albion College
611 East Porter Street, Albion, 49224, US
Phone: 5176290826

Tom Bieler
Michigan State University, East Lansing, MI

Philip Eisenlohr
2Max Planck Institut für Eisenforschung, Düsseldorf, Germany

Martin Crimp
Michigan State University, East Lansing, MI

Abstract:

A well characterized patch of a polycrystalline TiAl is used to evaluate the ability of fracture initiation parameters (fip) to predict the relative resistance of grain boundaries to microcracking when subjected to a defined global stress state. Prior work examined the development of grain boundary microcracks that developed during 4-point bending. A variety of metrics based on the mesoscopic quantities of initial grain orientation, grain boundary normal orientation, alignment of slip/twin systems, as well as the macroscopic tensile stress state, identified some boundaries as being more susceptible to cracking than others. In the current study fip concepts are generalized to a local fip at the mesoscale that evolves in both space and time during deformation. Local lattice curvature near the grain boundary, local elastic and plastic stress evolution, and compatibility at the grain boundary are among the quantities considered. The evolution of these local fip models are then evaluated using data generated from a three dimensional crystal plasticity finite element (CPFE) simulation of the same experimental TiAl region to identify how the fip evolves with deformation using the local stress and slip accumulation provided by the CPFE results.
The Volume Derivative and Fracture Surfaces in Strain Space

Jeyabal Sivaloganathan
University of Bath
Department of Mathematical Sciences, Claverton Down, Bath, BA2 7AY, GB
Phone: +44 (0)1225 386003, Email: js@maths.bath.ac.uk

Pablo Negron Marrero
Department of Mathematics, University of Puerto Rico, Humacao, Puerto Rico

Abstract:
In this talk we present a novel variational approach to predicting when local fracture is energetically favoured in a hyperelastic material based on a new notion of the derivative of a stored energy function with respect to discontinuous deformations. Theoretical results and numerical examples will be presented.

Let B denote the region occupied by a ball of nonlinear, hyperelastic material in its reference state. We consider the displacement boundary value problem in which the admissible deformations $u(x)$ of the ball must satisfy the linear boundary condition $u(x)=Ax$ for $x$ on the boundary of B, where $A$ is a general constant matrix.

We seek minimisers of the total stored energy amongst all such admissible deformations that have at most one point of discontinuity located at the centre of B. Under suitable assumptions, it is known that for small $A$ the unique energy minimising deformation is the homogeneous deformation $u(x)=Ax$ (and in this case we say that the stored energy function is stable at the matrix $A$).

However, for large $A$, it is known that the homogeneous deformations are not minimising and that any energy minimiser must produce a (not necessarily spherical) hole at the centre of the deformed ball (the phenomenon of cavitation). (See, e.g., [1], [2])

We denote by $S$ the stable region (within the set of all matrices $A$) inside which the stored energy function is stable in the above sense. The boundary of this set $S$ then represents a fracture surface in the space of strains in the following sense: given a body, of any shape, and a smooth equilibrium solution $u(x)$, if $u(x)$ produces a strain at any point in the body which lies outside (the closure of) the stable set $S$, then that equilibrium is energetically unstable in the sense that forming a hole (ie a local fracture) will further lower the stored energy.

In this work we present a novel approach to the problem of calculating the boundary of the stable region $S$ in strain space. For each boundary displacement matrix $A$ we define a new variational derivative, denoted $F(A)$, of the total stored energy with respect to hole producing deformations which we call the volume derivative. We are able to show in a number of cases that:

(i) the stable set $S$ is the set on which $F(A)>0$, 

(ii) \( F(A) < 0 \) on the unstable set and

(iii) the boundary of \( S \) consists of matrices \( A \) for which \( F(A) = 0 \).

Hence the bifurcation equation \( F(A) = 0 \) appears to characterise a fracture surface in strain space.

References


The Anomalous Behavior of Material Overlapping in Elasticity and a Possible Cure

Adair Aguiar
University of São Paulo
Av. Trabalhador são-carlense, 400, Cx. P. 359, São Carlos, 13566-590, BR
Phone: (011-55-16) 3373-9463, Email: aguiarar@sc.usp.br

Abstract:

We present theoretical and numerical results concerning the imposition of the injectivity constraint on a class of elastic solids. In classical linear elasticity, solutions to these problems are not injective inside the solids, yielding the unrealistic behavior of material overlapping. To find a cure for this behavior, we formulate a problem in this class as a constrained minimization problem, which consists of finding a displacement field that minimizes the total potential energy of the solid subject to the constraint that the associated deformation field be locally invertible. We show that the solution of this constrained problem is everywhere injective. Another approach to impose the injectivity constraint consists of assuming a proper nonlinear elastic behavior of the material. The material behavior near the corners of the punch is such that, while still singular, prevents material overlapping. Away from these points, this material behaves like the classical semi-linear material of John introduced in 1960. This work is part of an ongoing collaboration with Professor Roger Fosdick in the area of Singularities and Constraints in Elastostatics.
The Variational Approach to Fracture Mechanics-New Advances

Gianni Royer Carfagni
University of Parma
Department of Civil-Environmental Engineering and Architecture, Viale G.P. Usberti 181/A, Parma, Italy
Phone: +39-0521-905917, Email: gianni.royer@unipr.it

Abstract:
According to the seminal work by Francfort and Marigo (1998), the stable equilibrium configurations of a body amenable to fracture are associated with minimizers of an energy functional composed of a bulk and a surface energy term, where crack-opening is represented by a discontinuity in the displacement field. Later on the same authors, together with Bourdin (2000), proposed a regularized approximation of this free-discontinuity problem with a regularized two-field functional à la Ambrosio Tortorelli (1990), where the relationship with the parent problem was corroborated by a Gamma-converge result. To account that crack opening is irreversible, the load history was divided into small steps and the crack path was associated with the evolution of the minimizers of the corresponding variational sub-problems at each loading step, under the constraint that crack surface is a non-decreasing function of time. Here, two generalizations of this approach are presented.

In the first one, the bulk energy term of the regularized functional is modified by combining it with structured deformation theory, to model that when the material microstructure is loosened and damaged, peculiar inelastic (structured) deformations may occur in the representative volume element at the price of surface energy consumption. This approach unifies various theories of failure because, by simply varying the form of the class for admissible structured deformations, different-in-type responses can be captured, incorporating the idea of cleavage, deviatoric, combined cleavage-deviatoric and masonry-like-fractures. The model is numerically implemented using a standard finite-element discretization and adopts an alternate minimization algorithm, adding an inequality constraint to impose crack irreversibility (fixed crack model). Numerical experiments for some paradigmatic examples are presented and compared for various possible versions of the model.

In the second proposed approach, the substantial modification is in the surface energy term because what is presented is a model in which any displacement jump can only occur while a cohesive stress bridges the crack lips, the stress remaining constants whatever the crack opening displacement is. This, on the one hand, represents a particular type of Dugdale-Barenblatt cohesive crack theory but, on the other hand, can also interpret the response of a perfect plastic body, where the onset of inelastic deformations is modeled as the consequence of displacement jumps occurring along slip surfaces of the crystalline lattices at constant yielding stress. Moreover, it is also shown that the proposed energy functional, which leads to a free-discontinuity problem set in the space of SBV functions, can be approximated by a sequence of regularized elliptic functionals following Ambrosio-Tortorelli (1990) within the framework of Gamma-convergence. Comparisons between the results obtainable with the free-discontinuity model and its regularized approximation, in particular the stability of the pure elastic phase, the irreversibility of plastic slip and the response under unloading, are presented, in general, for the 2-D case of antiplane shear and exemplified, in particular, for the 1-D case.
Energy Release Rate of Dielectric Materials with Evolving Defects under Electric Fields

Yi-chao Chen
University of Houston
Department of Mechanical Engineering, Houston, 77204-4006, US
Phone: 713-743-4533, Email: chen@uh.edu

Abstract:

Defects always occur during manufacturing processes of polymer-matrix composites. These defects may grow and evolve into damages during operation, and drastically affect the performance and service life of the material. In a curing process, thermoset resins pass through aggregation phase, percolation phase, and cooling phase. It is known that micro-cracks and voids nucleate at late stage of percolation phase, and grow in the cooling phase. Controlling the nucleation and growth of defects at these stages can significantly improve the quality of the material.

The formation and growth of defects can be described by the work/energy exchange. On one hand, the breakage of the atomic bonds lowers the potential energy of the material. Such a reduction of potential energy is usually described by energy release rate. On the other hand, certain energy is required to break the atomic bonds. This energy supply could be due to mechanical loads, temperature inhomogeneity, or residual stresses during manufacturing processes. These physical effects are often described as the “driving force” for the onset and growth of defects. When the supplied energy exceeds the release energy, defects will initiate and continue to grow. When the supplied energy is lower than the released energy, the existing defects will not grow, and no new defect will be generated.

This work/energy exchange process may be altered by the presence of other physical sources than those of thermal and mechanical nature. In this paper, we study the possible effect of electric fields on the nucleation and growth of defects in dielectric material. In the defect region, the material has different properties from those of the virgin material. When the material is subjected to an electric field, various field quantities in the material are determined by Maxell's equations. Due to the presence of the evolving defect region, the electric permittivity is a function of position and time. The rate of work done by the electric field on the material can be calculated by integrating Maxell’s equations. It is found that the rate of work of the electric field on the material is of the same sign as the partial derivative of the electric permittivity with respect to time. For dielectric materials, the value of electric permittivity in the defect region is always smaller than that of the virgin material. Hence, the time derivative of the electric permittivity is negative in the defect growth region. As a result, the rate of electric work done by the field on the material is negative. In other words, the material does positive work on the electric field during the growth of defects, that is, the electric energy release rate is negative during the growth of defects. It is known that a positive energy release rate is a driving force for the growth of defects. It can be then argued that the application of electric field has an effect of suppressing defect growth. This indicates the possibility of using electric fields to control defects a priori during manufacturing processes.
TRACK 2
Bioengineering Materials, Mechanics and Structures
Cell Mechanics

ORGANIZERS:

Christian Franck, Brown University
Three-dimensional Quantitative Measurements of Cells in their Surrounding Environment

Christian Franck
Brown University
182 Hope St, Providence, 02912, US
Phone: (401) 863-2863, Email: franck@brown.edu

Stacey A. Maskarinec
California Institute of Technology, Pasadena, CA

David A. Tirrell
California Institute of Technology, Pasadena, CA

Guruswami Ravichandran
California Institute of Technology, Pasadena, CA

Abstract:

In recent years, the importance of mechanical forces in directing cellular function has been recognized as a significant factor in biological and physiological processes. In fact, these physical forces are now viewed equally as important as biochemical stimuli in controlling cellular response. Not only do these cellular forces, or cell tractions, play an important role in cell migration, they are also significant to many other physiological and pathological processes, both at the tissue and organ level, including wound healing, inflammation, angiogenesis, and embryogenesis. A complete quantification of cell tractions during cell-material interactions can lead to a deeper understanding of the fundamental role these forces play in cell biology. Thus, understanding the function and role of a cell from a mechanical framework can have important implications towards the development of new implant materials and drug treatments.

Previous research has contributed significant descriptions of cell-tissue interactions by quantifying cell tractions in two-dimensional environments; however, most physiological processes are three-dimensional in nature. Recent studies have shown morphological differences in cells cultured on two-dimensional substrates versus three-dimensional matrices, and that the intrinsic extracellular matrix interactions and migration behavior are different in three dimensions versus two dimensions. Hence, measurement techniques are needed to investigate cellular behavior in all three dimensions.

This talk presents a full-field imaging technique capable of quantitatively measuring cell traction forces in all three spatial dimensions, and hence addresses the need of a three-dimensional quantitative imaging technique to gain insight into the fundamental role of physical forces in biological processes. The technique combines laser scanning confocal microscopy (LSCM) with digital volume correlation (DVC) to track the motion of fluorescent particles during cell-induced or externally applied deformations. This method is validated by comparing experimentally measured non-uniform deformation fields near hard and soft spherical inclusions under uniaxial compression with the corresponding analytical solution.

Using this technique, the full three-dimensional substrate displacement fields are experimentally determined during the migration of individual fibroblast cells on polyacrylamide gels. This is the first
study to show the highly three-dimensional structure of cell-induced displacement and traction fields during cell locomotion. These new findings suggest a three-dimensional push-pull cell motility, which differs from the traditional theories based on two-dimensional data. These results provide new insight into the dynamic cell-matrix force exchange or mechanotransduction of migrating cells, and will aid in the development of new three-dimensional cell motility and adhesion models.

As this study reveals, the mechanical interactions of cells and their extracellular matrix appear to be highly three-dimensional. It also shows that the LSCM-DVC technique is well suited for investigating the mechanics of cell-matrix interactions while providing a platform to access detailed information of the intricate biomechanical coupling for many cellular responses. Thus, this method has the capability to provide direct quantitative experimental data showing how cells interact with their surroundings in three dimensions and might stimulate new avenues of scientific thought in understanding the fundamental role physical forces play in regulating cell behavior.
Focal Adhesion Strength and Lifetime Depend on Substrate Stiffness and Directionality of Detachment Forces

Sangjin Ryu
Brown University
182 Hope Street, Box D, Providence, 02912, US
Phone: 617-861-7625, Email: sangjin_ryu@brown.edu

Christian Franck
Brown University, Providence RI,

Abstract:
Motile cells interact with their extracellular matrix (ECM) through focal adhesions (FAs). A cell crawls by anchoring its protruding membrane to the ECM or planar substrata through FAs, pulling its body and then detaching FAs behind. During this process, the cell exerts a force on the substrate via FAs in the lateral direction (the direction of movement) as well as in the normal direction. On the other hand, cells sense mechanical changes in ECM through FAs: they show different morphology and motility depending on the elastic properties of the substrate. Therefore, investigating the dynamics of FAs promotes a better understanding of cell-ECM interactions.

In this study, we study FA contacts through the interaction between cellular integrins and extracellular ligands (fibronectin) and measure their rupture force with the atomic force microscopy (AFM) as a function of substrate elastic modulus and detachment force orientation. Integrins are one of most abundant transmembrane receptors of FAs, and they specifically bind to fibronectin ligands of the ECM. In our model system FAs are represented by colloidal AFM probes functionalized with human $\alpha5\beta1$-integrin, and the ECM by planar substrata patterned with human plasma fibronectin. To simulate changes in the elastic property of the substrate, we employ materials of various elastic moduli including glass, polydimethylsiloxane (PDMS) and polyacrylamide (PAAM). To mimic the lateral component of the force that crawling cells exert on the substrate, we disengage the probe from the substrate in the lateral direction as well as in the normal direction.

Our measurements show that bond strength between the integrin and fibronectin clusters are dependent on both changes in the elastic modulus of the substrates and the direction of pulling. Furthermore, rupture force curves between the ligand and receptor clusters show a similar behavior that is influenced by the direction of the AFM probe disengagement as well as the substrate elastic modulus. This seems to be due to differences in the association/dissociation behavior between integrin and fibronectin molecules. In the normal disengagement, chance of rebinding decreases as the probe recedes from the substrate because the distance between the receptor and ligand increases. By contrast, the receptor can find new ligands to bind in the lateral disengagement because the distance between the bead and substrate is kept constant. Understanding the observed behavior of our model system will provide us with a better understanding how cells might modulate their internal forces during crawling and how force directionality and the elastic properties of the underlying matrix influence the cell’s ligand-receptor interactions during cell locomotion and adhesion.
Chemomechanics at the Cell-material Interface: Molecular Manipulation of Adhesion and Migration

Krystyn Van Vliet
Massachusetts Institute of Technology
MIT Room 8-237, 77 Massachusetts Avenue, Cambridge, 02139, US
Phone: 6175489947, Email: krystyn@mit.edu

John M. Maloney
MIT, Cambridge, MA

Ranjani Krishnan
MIT, Cambridge, MA

Adam Zeiger
MIT, Cambridge, MA

Abstract:

There exists strong coupling between local biochemistry and mechanics at the cell-material interface. This chemomechanics can be altered to change cell shape and mechanical resistance to deformation, as well as biological behaviors such as adhesion and migration of cells within extracellular matrices (ECM). Here, we will discuss the mechanisms by which the adhesion and migration of adherent cells can be altered via local changes in extracellular material stiffness, extracellular pH, and extracellular protein concentrations. We and others have found that the mechanical stiffness of materials or tools used to understand cell mechanosensitivity can directly impact intermolecular kinetics, cell shape, and downstream function. However, the mechanisms by which this coupling proceeds are still to be elucidated. Interestingly, the majority of in vitro cell studies employ materials that are orders of magnitude more stiff and more dilute in proteins that in vivo microenvironments. Thus, understanding of the effects of such shifts is of interest to the study of cell mechanics, and the design of in vitro environments that may better sustain cell functions in a laboratory setting. The level of changes in ECM and extracellular niche properties discussed here are relevant to both wound healing and metastasis of tumor cells, which can further impact immunity responses and stem cell proliferation and function. To study the effects of chemomechanical cues on cell mechanics and function, we employ multiscale mechanical experiments, quantifying the effects of stiffness, pH, and local molecular concentrations on adhesion receptor kinetics and cell-level adhesion and migration. We then present integrated simulations that predict whole-cell consequences of molecular unbinding under applied force or mechanical constraint. We find that propensity and rates of ligand-receptor unbinding at the cell-material interface can predict these effects, and connect these molecular-scale findings to altered changes in mechanics and function at the whole-cell level for three cell types critical to vascular function.
Probing Molecular and Cellular Mechanics in a Coupled Stochastic-elastic Modeling Framework

Huajian Gao
Brown University
Division of Engineering, Providence, 02912, US
Phone: 4018632626, Email: Huajian_Gao@Brown.edu

Abstract:

The coupling between elasticity and stochastic behaviors is at the center of many problems in molecular and cellular biomechanics. One example is that cell-matrix adhesion depends on the collective behaviors of clusters of receptor-ligand bonds called focal contacts between cell and extracellular matrix. While the behavior of a single molecular bond is governed by statistical mechanics at the molecular scale, continuum mechanics should be valid at a larger scale. Another example is the contractile mechanisms of cytoskeleton or skeletal muscles depend on synchronous actions of many myosin motors. In this talk, I will give an overview of some recent theoretical studies aimed at probing the basic mechanical principles of focal contacts in cell-matrix adhesion via stochastic-elastic models in which stochastic descriptions of molecular bonds and elastic descriptions of interfacial traction/separation are unified in a single modeling framework, as well as stochastic-elastic modeling of the constitutive behaviors of skeletal muscle contraction. The objective is to illustrate these principles using simple analytical and numerical models.
Interplay between Cell and Matrix Stiffness

Paul Janmey
University of Pennsylvania
Philadelphia, US

Abstract:

Many cell types respond to the mechanical properties of their substrate stiffness and can tune their own stiffness to match that of the substrate to which they adhere, at least over a limited range of stiffness near that of the tissue in which these cells normally reside. This response depends on the non-linear viscoelasticity of both the cytoskeleton and the extracellular matrix. It also requires signaling from specific transmembrane receptors and the functions of actin crosslinkers such as filamin A. Fibroblasts and human mesenchymal stem cells on fibrin or collagen gels deform the matrix by several microns up to five cell lengths away from their plasma membrane through a force-limited mechanism. Atomic force microscopy and rheology confirm that these strains locally and globally stiffen the gel, depending on cell density, and this effect leads to long distance cell-cell communication and alignment. Thus cells are acutely responsive to the nonlinear elasticity of their substrates and can manipulate this rheological property to induce patterning.

References:
Mechanical and Chemomechanical Properties of HbAA and HbAS Erythrocytes via AFM

George Lykotrafitis
University of Connecticut
191 Auditorium Road, Unit 3139, Storrs, 06269, US
Phone: 8604862439,   Email: gelyko@engr.uconn.edu

George Lykotrafitis
University of Connecticut, Storrs, CT

Abstract:

Sickle cell disease (SCD) is an inherited blood disorder marked by polymerization of deoxygenated Hb, which results in long, stiff, rodlike fibers which force red blood cells (RBCs, erythrocytes) to assume a sickle shape. Sickle cell trait (SCT) is characterized by the presence of sickle hemoglobin (HbS) and normal hemoglobin (HbA). While usually regarded as a benign condition, under extreme conditions, individuals with SCT can develop a syndrome resembling SCD with vaso-occlusive sequelae resulting from rigid erythrocytes. It has been suspected that the interaction of Lu/B-CAM with LAMA5 can contribute to vaso-occlusion in sickle cell disease (SCD). Lu/B-CAM is a glycoprotein that binds to the α5 chain of laminin, an extracellular matrix (ECM) protein, and has been shown to be over expressed in sickled red blood cells (RBCs).

In the current work, atomic force microscopy (AFM) was employed to investigate morphological, material, and chemomechanical properties of abnormal human RBCs from patients with the genotype for SCT to investigate the presence of HbS. AFM allows for high-resolution topography studies of biological cells, measurement of their mechanical properties at the nanometer scale in physiological conditions, and quantification of single molecule adhesive bonds.

The Young’s modulus from a sickle trait erythrocyte was compared with that obtained from measurements of erythrocytes from healthy subjects. The results showed that the Young’s modulus of pathological erythrocytes was approximately three times greater than found in normal cells. Observed differences indicate the effect of HbS as well as possible changes in the organization of the cell cytoskeleton associated with the sickle cell trait. In addition, it was found that while the magnitude of the bond was the same in both SCT and healthy RBCs, Lu/B-CAM receptors appear to have a homogenous distribution in healthy RBCs and concentrate themselves around the perimeter and in 100-200 nm crevices on the SCT erythrocyte. These results suggest changes in the spectrin-based cytoskeleton, associated with the cytoplasmic domain of Lu, resulting from the presence on HbS in SCT erythrocytes.
A Coarse-Grain Molecular Dynamics Model for Sickle Hemoglobin Fibers

George Lykotrafitis
University of Connecticut
191 Auditorium Road, Unit 3139, Storrs, 06269, US
Phone: 860-486-2439, Email: gelyko@engr.uconn.edu

Abstract:

The intracellular polymerization of deoxy sickle cell hemoglobin (HbS) has been identified as the main cause of sickle cell disease. Polymerized HbS fibers are stiff and able to create protrusions and generate vesiculation on the red blood cell (RBC) membrane, leading to the deformation of the RBC. Therefore, the material properties and biomechanical behavior of polymerized HbS fibers have been the subjects of a large amount of experimental and theoretical studies. In this work, a solvent-free coarse-grain molecular dynamics (CGMD) model is developed to represent a single HbS fiber with four tightly bonded chains, each of which comprises 1000 soft particles. The four-chain model is preferred to the one-chain model because a directional vector that measures the torsional angle of the fiber can be easily defined. The total length of the simulated HbS fiber is 1 μm and the radius of the fiber is approximately 10 nm, which are consistent with the geometry of single hemoglobin fibers described in former experimental studies. A harmonic spring potential, a bending potential, a torsional potential, and a Lennard-Jones potential are introduced between the particles to model the behavior of a polymerized HbS fiber in the cytoplasm. The Langevin thermostat is employed in the simulation. The simulation results demonstrate that the proposed model is able to represent a single HbS fiber with the length-scale at order of μm and simulation time at order of μs. Significant mechanical properties of a single HbS fiber, such as bending rigidity, torsional rigidity and persistent length are obtained from the simulations and the data make a good agreement with published experimental results. Microscopy observations have shown that individual HbS fibers are able to interact with each other and form various X-shaped junctions, Y-shaped branches, and side-to-side coalescence ("zippering") cross-links. In the last part of this paper, the developed model is used to study two cases of fiber cross-links formation from two single HbS fibers. First, two single fibers start zippering from a ‘V’ shape initial configuration. Second, the zippering process of two initially parallel fibers is simulated.
Dissecting Cellular Mechanics from In Vitro Actin Assembly to Neutrophil Migration

Jay Tang
Brown University
182 Hope Street, Box 1843, Providence, 02912, US
Phone: 4018632292, Email: jxtang2001@gmail.com

Abstract:

Actin filaments are the primary component of the cellular cytoskeleton, endowing eukaryotic cells their 3-D shape, mechanical strength and compliance. A dynamic actin network is also vital for force generation and migration of many cell types. My laboratory focuses on characterizing actin networks reconstituted in test tubes and microscope slide chambers, in order to capture the fundamental biomechanics responsible for their similar properties in live cells. The techniques we employ include direct imaging of trace labeled filaments, recording the actin based structures induced by micro-sized beads functionalized by polymerization stimulating enzymes, and non-interacting particles as probes of local mechanical properties, known also as the particle tracking micro-rheology. Measurements using this range of techniques provide essential information on the material and mechanical properties of cellular components that are vital in defining cell mechanics and motility.

More recently, we have started to study mechanics and motility of human neutrophils, which are white blood cells whose primary function in our body is to fight infection. Neutrophils perform their function by converting biochemical cues into mechanical response. Upon stimulation, they can adhere to substrate, spread, and migrate towards source of infection. Our study focuses on neutrophil mechano-sensing, by applying a specific biophysical technique of traction microscopy. By coating glass surface with a uniform gel functionalized with extracellular matrix proteins, we investigate neutrophil adhesion, spreading, traction and migration on controllable soft substrate. The tractional stress field mapping, in particular, has revealed some amazing insights in regard to how a crawling cell pushes and pulls as it muscles its way forward on the surface of a squishy substrate, much like the materials they encounter within our body. The over-arching goal of our studies is to gain insights to certain physiological processes such as leukocyte migration and phagocytosis, for which actin assembly plays key roles. Understanding the mechanical aspects of these processes has implications on infection control, wound healing, as well as intervention of diseases involving aberrant cellular motility.
Contact Mechanics of Circular Membranes

Kenneth Liechti
University of Texas at Austin
210 East 24th Street WRW 110C, 1 University Station C0600, Austin, 78712, US
Phone: 512-471-4164, Email: kml@mail.utexas.edu

Joshua McNalley
University of Texas at Austin, Austin, 78712

Abstract:

Thin membrane adhesion, contact and deformation have played important roles in many fields. For instance, in biological science, cell membrane and substratum adhesion is vital in normal cell functioning and locomotion and vesicle membrane fusion is of practical importance for targeted drug delivery. In micro-or micro-opto-electro-mechanical systems (MEMS or MOEMS), electrostatically driven bridges or diaphragm membranes operate over trillions of cycles in their life span and the study of reliability and durability of such MEMS/MOEMS devices relies on a quantitative understanding and determination of change in adhesion and contact over time. Furthermore, an accurate determination of contact size is necessary to evaluate contact resistance, heat dissipation and contact temperature in DC-contact-switch MEMS. Consequently, it is of great interest to study the contact and adhesion mechanics of thin films.

The contact mechanics of two elastic solids is well established through the Hertz, JKR, DMT and Maugis theories. The application conditions and selection guidelines of these theories are summarized in the Johnson-Greenwood map based on the dimensionless parameter initiated by Tabor. However, these theories for elastic solids are not applicable to thin membranes in contact. In the latter case, the elastic strain energy is determined by the membrane stresses which result from the large out-of-plane deflections of the thin membrane. Consequently, geometrical nonlinearity has to be considered and exact closed-form solutions are not feasible.

In this study we focus on a pressurized circular membrane contacting a rigid substrate. Plaut et al. numerically investigated this contact configuration extensively. Wan et al. studied a similar contact configuration, an axisymmetric flat punch on a thin flexible membrane from the first principles. However, no experimental verification has been reported in these studies. In this project, a combination of experiments and analysis is pursued. Analytical solutions which are reminiscent of Hertz, JKR, DMT and Maugis contact theories for two elastic bodies are developed for thin membranes in contact. It is further shown that a Maugis-type analysis recovers both the DMT and JKR limits. An apparatus modified from a bulge tester based on moiré deflectometry is used to measure both the contact radius and the slope of the deflection of the hanging membrane simultaneously. The direct measurement of the slope of the deflection during contact, which has not been reported in the literature, is critical for thin membrane contact since the membrane strain and the corresponding stress are best determined from the slope of the deflection rather than the deflection itself. The agreement between the solutions and measurements was quite reasonable.
Collagen Fibrils: Multifunctional Nanoscale Components in Bone Structure

Majid Minary
University of Illinois at Urbana-Champaign
1206 West Green Street, Urbana, 61801, US
Phone: 2177146776, Email: mminary2@illinois.edu

Min Feng Yu
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Type I collagen, as the most abundant protein in mammals, is the main organic component of bone, tendon, dentine, skin, and cornea. Functioning in such diverse tissues shows the multifunctional capability of collagen fibrils. The alternating gap and overlap regions in axial direction of a single fibril with a characteristic period of ~67 nm is believed to be an important factor in microstructure of the fibrils enabling its multi-functionality. For example, in bone mineral nano-crystals are deposited specifically in the gap region. In this study, we focus on studying mechanical (structural) and electromechanical properties at different scale levels, from sub-fibrillar microstructure of single isolated collagen fibrils with below 100 nm in diameter up to bone samples.

In terms structural and mechanical properties of elastic and viscoelastic properties, implementing near-surface static and dynamic nanoindentation technique with AFM, we show that the gap and overlap regions in single collagen fibril have significantly different elastic and energy dissipation properties, correlating the significantly different molecular structures in these two regions. We further show that such subfibrillar heterogeneity holds in collagen fibrils inside bone and might be intrinsically related to the excellent energy dissipation performance of bone.

It is long known that bone and tendon show piezoelectric behavior, and it is believed that the piezoelectric charges produced under mechanical deformation in these tissues has a potential role in mechanoelectric transduction leading to their growth and remodeling. With high resolution PFM we probe piezoelectric properties in bone and show that single collagen fibrils are responsible for piezoelectric behavior of bone and behave predominantly as shear piezoelectric materials. Furthermore, we show that there is an intrinsic electromechanical heterogeneity in axial direction of each single fibril that holds even for the collagen fibrils embedded in bone matrix. Such heterogeneity may have implications in regulating ionic environment in bone responsible for bone remodeling.
Fibroblast Elongation, Dendritic Extensions and Failure in Constrained Versus Unconstrained Microtissues

Vivek Shenoy
Brown University
Brown University, Division of Engineering, Providence, 02912, US
Phone: 401-863-1465, Email: Vivek_Shenoy@brown.edu

Peng Chen
Brown University, Providence, RI

Jeff Morgan
Brown University, Providence, RI

Abstract:

Cytoskeletal tension is fundamental to many biological processes, including germ layer sorting during embryogenesis. In vitro, such tension influences cell sorting in self-assembled, 3D microtissues and can be of sufficient magnitude to cause complex-shaped microtissue failure. To examine the process of failure under cell-derived tension Morgan and coworkers [1] subjected normal human fibroblasts (NHFs) to directed self-assembly in micro-molds designed to yield self-constraining microtissues. As cells contracted in this assay, the constrained microtissues narrowed, thinned and ultimately failed at their midpoints. We have developed a micromechanical model of tissues that accounts for the contractility of cells induced by myosin. Our model is used to simulate fibroblast elongation and failure in constrained geometries and to extract fundamental material and mechanical properties of microtissues.

Mechanical Model of Neuronal Cell Injury

Guoxin Cao
University of Nebraska-Lincoln
w407 Nebraska Hall, Dept. of Eng. Mech., University of Nebraska-Lincoln, Lincoln, 68508, US
Phone: 402-4728857, Email: gcao2@unl.edu

You Zhou
University of Nebraska Lincoln, Lincoln, NE

Jung Yul Lim
University of Nebraska Lincoln, Lincoln, NE

Namas Chandra
University of Nebraska Lincoln, Lincoln, NE

Abstract:

The mechanism of mild traumatic brain injury (mTBI) is directly related to the neuronal response to the mechanical loads, e.g. impact or blast. The hypotheses is that the external mechanical load will firstly cause the mechanical deformation of neurons and then, when the mechanical deformation of neurons reaches to a critical point (threshold), it will initiate the neuronal injury. Since the mTBI is what we are interested, the nonlethal neuronal injury in focused. Therefore, understanding the critical deformation level to cause the nonlethal neuronal injury is an important first step to understand the mechanism of mTBI.

The neuronal injury can be also termed as the chemical/ biological responses to the mechanical load, which can be monitored using the fluorescence method. In the tests, the fluorescent dye are loaded with the deformed neurons, such as propidium iodide (PI) and ROS indicator, 2,7-dichlorofluorescin (DCF). PI is the viability indicator, which is used to check whether or not the cells are dead after the deformation. DCF is used to check the ROS level of the living cells.

In the current work, two loading limits are defined to show the critical nonlethal injury of neurons: (1) the lower limit-- the critical strain of the nonlethal injury, which is defined to be a uniaxial tensile strain which causes about 80% of the tested neurons to have nonlethal injury (the neurons are still alive but shows the response to DCF); (2) the upper limit--the maximum strain of the nonlethal injury, which is defined to be a uniaxial tensile strain which causes about 30% of tested neurons to die (response to PI).

The neuronal response to the uniaxial stretching is investigated based on in vitro model. In the tests, the SH-SY5Y human neuron are cultured on the PDMS membrane. The uniaxial deformation is applied on the substrate (membrane), and the substrate deformation is considered to be the deformation of neurons. The deformation is applied very slow and thus the loading rate effect is not considered here.

This model can provide a useful guideline of understanding the relationship between the mechanical deformation of neurons and their nonlethal injury.
Applying Controlled Loads to Single Cells Using Hydrodynamically-confined Microfluidics

Kevin Christ
University of Wisconsin-Madison
Phone: 303-775-8659, Email: kchrist@wisc.edu

Kevin Turner
University of Wisconsin Madison, Madison, WI

Abstract:

Biological cells are complex mechanical systems that continually interact physically with other cells and the extracellular matrix. Changes in the cell caused by the onset of disease or exposure to chemicals can alter its mechanical properties, such as adhesion and stiffness, and affect the cell’s functionality. Several methods are available to probe mechanical properties of cells, including atomic force microscopy (AFM) and fluid flow chambers. However, these techniques either require contact between the probe and the cell or do not capture the full heterogeneity of the cell population. There is a critical need for methods that allow the detailed analysis of many single cells in a short amount of time. Our objective here is to investigate the forces applied to cells by hydrodynamically-confined microflows, which provide a controllable loading method to probe the mechanical properties of single cells.

Hydrodynamically-confined microflows (HCMs) allow the physics of microfluidic environments to be brought to traditional cell culture environments. HCMs are microfluidic flows that are confined on the top and bottom by solid walls, but are confined on the sides by a surrounding liquid. The flow is generated by two adjacent ports on the top surface, one of which flows fluid into the system while the other removes the fluid out at a higher rate. The gap between the top and bottom surfaces is less than 100 μm, and the flow between the two ports is laminar and achieves a steady state, creating a flow envelope.

These flows have been used to selectively apply chemicals to a single cell without influencing other cells that are in close proximity. Because the top surface does not contact the cell, many individual cells can be treated rapidly by translating either the top or bottom surface. HCMs can also be used to apply controlled mechanical loads to cells, but this process is complex and has not been described in detail. Here, we provide analysis and experimental measurements of the mechanical forces that are applied to cells that are treated with hydrodynamically confined flows. Using computational fluid dynamics (CFD) simulations, the shear stress and pressure applied to cells using HCM devices is analyzed. Experiments have been performed to verify the pressure and shear stress distributions induced by the HCMs. Overall, this work will provide an understanding of the mechanical loading applied to the cells, which will assist researchers who can then use this method to examine the effects of chemical treatments and diseases on the mechanical properties of cells.
Biomechanics/Bioimaging: Inducing and Tracking Mechanical Deformations in Tissue and Living Cells for Diagnostics and Therapy

ORGANIZERS:
Timothy A. Bigelow, Iowa State University
An Overview of Vibro-Acoustography and Related Techniques

Mostafa Fatemi
Mayo Clinic College of Medicine
200 First St. SW, Rochester, 55905, US
Phone: 507-284-0608, Email: fatemi@mayo.edu

Invited Presentation

Abstract:

The concept of vibro-acoustography was first introduced in 1998 in a paper in Science under the title of “Ultrasound Stimulated Vibroacoustic Spectrography.” A subsequent paper, published in Proceedings of National Academy of Science in 1999, described the theoretical aspects of the vibro-acoustography. During the past decade, this technique has flourished in many aspects. This paper summarized the concept, theory, and applications of this and related techniques.

Vibro-acoustography is based on the nonlinear equation of acoustic waves, which describes how the ultrasound wave converts to a low-frequency (kHz-range) acoustic wave. Many aspects and practical advantages of vibro-acoustography result from this conversion. For instance, vibro-acoustographic images are sensitive to both ultrasound and low frequency characteristics of the object. The original implementation of vibro-acoustography includes an ultrasound transducer with two co-focused beams at slightly different frequencies. It is shown that the ultrasound beam can vibrate the object at the difference frequency, which in turn produces a sound at this frequency that is detected by a hydrophone. The hydrophone signal is then used to produce an image of the object as the ultrasound beams scan the object.

Biomedical applications have been the main thrust in the development of vibro-acoustography. In particular, imaging breast, prostate, arteries, and thyroid have been of special interest. Non-medical applications of vibro-acoustography include non-destructive evaluation of materials, flaw detection, and evaluating the vibration modes of the object.

Other implementations of vibro-acoustography include using alternative means for recording and processing of vibration data. An example is to detect object vibrations by a laser vibrometer and use the resulting information to produce an image of the object. In another implementation, inverse problem approach is used to estimate the viscoelastic parameters of the object. Vibro-acoustography provides rich data, including information from the high- and low-frequency portions of the spectrum. This information can be utilized in biomedical or industrial applications to explore the properties of the object being tested. Further research is needed to fully develop explore the potentials of this technique.

Acknowledgements: Work supported by NIH Gants CA127235 and CA91956. Disclosure of Conflict of Interest: Mayo Clinic and the author have a financial interest associated with technology used in this research; the technology has been licensed in part to industry.
Mechanical Destruction of Soft Tissue by Ultrasound Histotripsy: Preliminary In Situ Results in Canine Model

Timothy Bigelow
Iowa State University
2113 Coover Hall, Iowa State University, Ames, 50011, US
Phone: 515-294-4177, Email: bigelow@iastate.edu

Leslie E. Fox
Iowa State University, Ames, IA

Kenneth R. Waller III
Iowa State University, Ames, IA

Elizabeth M. Whitley
Iowa State University, Ames, IA

Jin Xu
Iowa State University, Ames, IA

Viksit Kumar
Iowa State University, Ames, IA

Abstract:

Very high amplitude ultrasound waves can produce bubble clouds in soft tissue. These bubble clouds are then further excited by sound waves to produce inertial cavitation inside the tissue. The collapse of the bubbles in the vicinity of cells will result in large mechanical stresses on the cells which can rip the cells apart leaving no identifiable cellular structures in a process that has been termed histotripsy. In our study, we exposed the spleen of two freshly euthanized dogs to high-intensity focused ultrasound pulses at 1.1 MHz from a spherically focused transducer (f/1, 63 mm focal length). The pulses were 20 cycles in duration and had peak compressional and rarefractional pressures of approximately 60 and 12 MPa, respectively. The period between the pulses was 1 ms for the 1st dog and 2 ms for the 2nd dog, while the dwell time at each exposure location was 30 s for the 1st dog and 60 s for the 2nd dog. Therefore, each dog received the same total number of ultrasound pulses at each location. During the treatment, the focal zone was scanned through a 5 mm x 5 mm section of the spleen in steps of 1 mm. Following the exposure, tissues were collected, fixed, and processed routinely for histopathology. The dog with the 1 ms period had localized destruction of erythrocytes and leukocytes with retention of fibromuscular stroma while the dog with the 2 ms period had total tissue destruction in the treated region. Therefore, the periodicity of pulse parameters is related to tissue destruction in ultrasound histotripsy. (This work was supported in part by a National Science Foundation Career Award ECCS-0901942).
Fracture between Molecules

Kenneth Liechti
University of Texas at Austin
210 East 24th Street WRW 110C, 1 University Station C0600, Austin, 78712, US
Phone: 512-471-4164, Email: kml@mail.utexas.edu

Abbas Hassan
University of Texas at Austin, Austin, 78712

Michael Krische
University of Texas at Austin, Austin, TX

Abstract:
While it is intuitive that molecular interaction should correlate to the mechanical properties of a material, it has only recently become possible to make the measurements necessary to trace the effects of molecular interaction across length scales to properties at the level of the material. The utility of “classical” polymeric adhesives is underscored by their widespread use in primary structural applications ranging from aerospace, automotive, and civil structures to biomedical implants and microelectronic devices. To date, the vast majority of the efforts directed toward improving the strength and durability of adhesives have been largely empirical. At the same time, the drive towards miniaturization in MEMS and NEMS devices and nano patterning means that an understanding of adhesion and fracture at smaller and smaller scales needs to be developed. This actually provides an opportunity to decrease the amount of empiricism as the number of variables is essentially decreased.

The paper describes the development of an experiment with associated analysis to determine the toughness of a molecular level adhesive joining two silicon strips. Si (111) surfaces were coated with amine and carboxy-terminated self-assembled monolayers (SAMs). The silicon beams were pressed together to form miniature laminated beam specimens which were then separated using a specially developed high vacuum fracture tester. The deposition of the SAMs and associated spectroscopic, scanning probe and ellipsometric diagnostics are described. The delaminations between the silicon strips and the associated normal crack opening displacements (NCOD) were measured via infra-red crack opening interferometry.

The fracture toughness of the specimens was measured. Traction-separation laws were extracted from measurements of crack opening displacements and an associated fracture analysis. These compared favorably with traction-separation laws based on potentials for ionic bonding.
Geometrical Settings of Directed Medium by Vector Bundle Description and its Application to Biomechanics

Hidetaka Yamaoka
RIKEN (The Institute of Physical and Chemical Research)
53, Kawahara-cho, Shogoin, Sakyo, Kyoto, 606-8507, JP
Phone: +81(75)751-4854, Email: hyamaoka@riken.jp

Taiji Adachi
Institute for Frontier Medical Sciences, Kyoto University, Kyoto, Japan

Abstract:

An example of the directed media is the so-called Cosserat rod, which is an elastic rod that is thin in two of its dimensions. Its dynamics are expressed in terms of a position vector describing a point on the center axis and an additional vector describing a point in each cross-section. This situation can be, geometrically, interpreted such that the center axis is expressed as a one-dimensional continuum and the points in the cross-section are described as three-dimensional vectors attached to each point of the axis. Therefore, the dynamics of the Cosserat rod are described on a tangent bundle of a vector bundle whose base space is a one-dimensional manifold and whose fiber space is a three-dimensional vector space. In this study, we develop a dynamics on a vector bundle that accurately describes the mechanical behavior of directed medium. The directed medium is a continuum with microstructures, which is described by a deformable vector, called a director. In geometric continuum mechanics, an elastic body is viewed as a differentiable manifold, while a directed medium is viewed as a vector bundle whose fiber denotes a collection of the deformable directors. Then we provide general geometrical settings of the continuum dynamics on a tangent bundle of a vector bundle, and derive a weak form and equations of motion for the directed medium. These resultant equations can be apply to a Cosserat rod, which is an interesting example, because if its one-dimensional axis is extended to the three-dimensional rod, the director can be used to express a smaller microstructure such as the sub-domain of the biopolymers. The resultant equations have formally expressed the deformation behavior of smaller microstructure rather than the cross-sections. This implies that our results are used to investigate the macro-micro interactive mechanisms, if it is necessary to consider geometrical structures of objects using the mechanisms, i.e., corresponding base manifolds and fiber spaces. Such geometrical considerations help us to increase our understanding of the complicated mechanical behavior of various structures associated with the macro-micro interactive mechanisms.
Investigation of Skull Hemorrhage and its Mechanism Due to High Intensity Focused Ultrasound in Nascent Rats and Mice

Viksit Kumar
Iowa State University
2201 Coover Hall, Ames, 50011, US
Phone: 515-509-7576, Email: vkumar@iastate.edu

Timothy A. Bigelow
Iowa State University, Ames, IA

Abstract:
High-intensity focused-ultrasound when targeted on nascent rat skulls has resulted in hemorrhage [T.A. Bigelow et al., Ultrasound Med Biol. 33, 311(2007), D. Dalecki et al., Ultrasound Med Biol. 25, 1139 (1999)]. Although the true mechanism behind the initiation and growth needs to be studied, thermal damage, cavitation damage, radiation pressure or a combination of the three may be responsible for the hemorrhage. Thermal damage is not likely because the study by Bigelow et al. shows that the temperature rise for some of the exposure is too small. Furthermore, hemorrhage is typically not caused by heating. Cavitation is not likely because of the absence of nuclei for cavitation. The current study determines the dependence on energy density; number of pulses; spatial peak temporal average intensity; product of energy density and number of pulses; and product of energy density, number of pulses, and volume of the focal region. The best correlation was found between percentage of hemorrhage occurrence/area of hemorrhage and the product of energy density, number of pulses, and volume of the focal region. The presence of energy density terms indicates that radiation force is a possible mechanism. The dependence on number of pulses suggests that the damage may be mechanical in nature and hemorrhage occurs due to fatigue. Also, as the volume of the focal region increases, the probability of finding a weak spot may increase. The exact mechanism for initiation and growth of hemorrhage needs to be studied in more detail but radiation pressure seems to be the most likely mechanism.
De-correlation of Ultrasound Echoes by Tissue Motion Induced by Acoustic Radiation Force

Jin Xu
Iowa State University
2201 Coover Hall, Ames, 50011, US
Phone: 515-450-0471, Email: xujin@iastate.edu

Yassin Labyed
Iowa State University, Ames, IA

Timothy A. Bigelow
Iowa State University, Ames, IA

Abstract:

Characterization of tissue microstructure has been useful to diagnose between malignant and benign tissue and is accomplished by comparing the backscattered power spectrum averaged over multiple independent echoes to a scattering model for the tissue. Normally multiple adjacent echoes are used resulting in poor spatial resolution when characterizing the tissue. This paper explores the use of acoustic radiation force impulse (ARFI) imaging to produce de-correlated echoes. ARFI imaging utilizes short-duration, high intensity pulses to generate localized impulsive radiation force in tissue. The force results in tissue displacement which can be tracked by monitoring the ultrasound echoes and used to discern the mechanical properties of tissue. In our study, computer simulations were done to simulate the tissue displacement resulting from a 5-millisecond ARFI pushing pulse for tissues with different Young’s moduli. The displacements were then calculated to alter the backscatterered ultrasound signals expected from a tissue region. The computation indicated that echo correlation was a function of time and also dependent of time difference of two instants of concern. Besides, it was also shown that the initial echo was most un-correlated with the one at the 5-millisecond and that after 7-milliseconds, the displacements tended to fade out, giving rise to a trend that the following echoes gradually became correlated again. The de-correlation of the 0-5-millisecond echo pair was achieved successfully and led to a satisfactory estimate for scatterer size with improved spatial resolution. Therefore, this preliminary investigation verifies the viability of this novel diagnostic approach through computer simulation.
Uncovering Morphological and Morphogenetic Features in Epithelia by Eliminating Statistical Bias

Matthew Miklius
Northwestern University
417 Custer Ave, Unit 3, Evanston, 60202, US
Phone: 847-254-8693, Email: mattmiklius@yahoo.com

Sascha Hilgenfeldt
University of Illinois at Urbana Champaign, + Northwestern University, Urbana, IL

Abstract:

Geometric order in quasi-two-dimensional epithelia has been extensively researched in order to identify and classify different tissues to help our understanding of how these tissues form (morphogenesis) and how their formation may be influenced (tissue regeneration). However, the significance of published data -- such as the distribution of numbers of cell neighbors -- has been hard to evaluate and compare because of the persistence of measurement bias. We identify the two primary sources of bias in epithelial tissues, which are (i) the measurement of apparent four-fold vertices, which is method-sensitive and resolution-dependent, and (ii) the selective preference for measuring smaller cells introduced by selecting a finite sampling window. We show that both effects can be corrected retroactively without detailed knowledge of the original samples, and by using only the biased (measured) distributions. This allows for an unbiased, meaningful comparison of data from different sources and with different experimental resolutions. We find conclusive evidence that the distribution and orientation of apparent four-fold vertices are not random, revealing profound differences between proliferating and remodeling tissues. We apply our method to Drosophila wing tissue data and demonstrate how it disentangles distributional moments, allowing for an assessment of their relative importance, independence, and significance in tissue identification and classification.
Internal Fluctuation of DNA in Nanochannels

Tianxiang Su
University of Pennsylvania, 229 Towne Building, 220 S. 33rd Street, Mechanical Engineering, University of Pennsylvania, Philadelphia, 19104, US
Phone: 2677023168, Email: tsu@seas.upenn.edu

Prashant K. Purohit
University of Pennsylvania, Philadelphia, PA

Abstract:
Stretching DNA in nanochannels is an important technique for performing DNA mapping [1]. On the other hand, it also serves as a simplified model for studying single polymer behavior in concentrated polymeric solutions and melts [2]. For these reasons, mechanical behaviors of DNA inside nanochannels have been of great interest to both experimentalists and theorists in recent years. To date, scaling laws for the behaviors of confined DNA in both the de Gennes and Odijk regimes have been well developed, widely used and tested [3,4]. However, fluctuation of the internal segments inside the DNA is still not well understood. This is important for genome mapping because it is the local fluctuation that determines the resolution of the mapping.

In this work, we study the internal fluctuation of confined DNA in nanochannels. We show that for a long DNA molecule whose contour length is much longer than its persistence length, the fluctuation versus mean value data collected from various locations along the polymer collapses onto a single curve with 0.5 power law. This can also be derived by a scaling theory. For short DNA, however, the scaling model fails and the data from different locations does not collapse onto a single curve. Following the framework in reference [5], a more detailed theory is developed. This theory models the DNA as a discrete wormlike chain in a confined channel. The confinement effects are taken into account by quadratic potentials and the internal fluctuation for the confined chain is evaluated.

Further, by considering different boundary conditions, regions that are most affected by the boundary effects are identified. Surprisingly, not all the internal segments close to the boundaries are strongly influenced by the boundary conditions. Fluctuations of short internal segments, for example, are not significantly affected even though they are located close to the boundaries. The model for short DNA is further verified by Monte Carlo simulations.

References:
Microcantilever Based Aptameric Nanosensor for Cocaine Detection

KYUNGHO KANG
Iowa State University
2025 Black Engineering Bldg AMES, 50011, US
Phone: 515-450-0978, Email: kyungho@iastate.edu

Marit Nilsen Hamilton
Iowa State University, AMES, IA

Pranav Shrotriya
Iowa State University, AMES, IA

Abstract:

A new method in label-free cocaine detections performed by the micromachined cantilever based sensor is present. The surface of a microcantilever is functionalized with the thiol-modified cocaine aptamer which synthesized to recognize cocaine. In the presence of cocaine, the aptamer starts conformational change to Y-shape due to the inherent selectivity and affinity while remaining an open structure in the absence of cocaine. The sensing/reference pair is exposed to varying concentrations of cocaine and differential deflection of sensing cantilever with respect to reference is measured to determine the change in surface stress. Varying the cocaine concentration from 25 to 500 μM results in a linear increase of the surface stress changes from 11 to 46 mN/m during the conformational changes of cocaine-aptamer complex. The dissociation constant (Kd) is 86 μM, and this sensor is able to detect cocaine with the lowest detectable concentration down to 5 μM in room temperature.
The Effect of Pia and Dura Matters in the Blast Wave Analysis of Human Head

Mehdi Sotudeh Chafi
University of Nebraska-Lincoln
Dep. of Mechanical Engineering, W118 NH, Lincoln, 68588-0656, US
Phone: 402-472-4221, Email: msotudeh2gmail.com

Linxia Gu
University of Nebraska Lincoln, Lincoln, NE

Namas Chandra
University of Nebraska Lincoln, Lincoln, NE

Abstract:

The blast waves encountered in the current military conflicts have demanded new approaches in the modeling and simulation of biological and geometrical fidelity of war fighters. The question addressed in this paper is the degree of details that are required to be incorporated in the head model to achieved a realistic simulation of blast wave-head interactions. Specifically we examine the rule of pia and dura matters in the validity of numerical results.

A geometrically simplified FE model was developed which includes different layers of the skull, dura, cerebrospinal fluid (CSF), pia mater and the brain. Blast load was directly applied on the skull surface. The model considered the triple layer of the skull (two cortical layers and middle diploe sponge-like layer). ALE formulation was used for the CSF. A hyperviscoelastic material was used for the brain. For dura and pia matters, second order Ogden hyperelastic constitutive models and corresponding parameters were fitted to the published experimental data. The simulations in this study were conducted by using an explicit nonlinear dynamic FE code (LsDyna) capable of simulating high-speed impacts with large deformations. Comparisons of the analysis results regarding linear elastic and nonlinear models showed that nonlinear elasticity does influence on the strain, stress and pressure. The effect of specific inclusion or otherwise of dura and pia matters in the analysis is also examined.
Fluid-Structure Interaction Models of Air Blast on Head

Youn Doh Ha
University of Nebraska-Lincoln
Department of Engineering Mechanics, University of Nebraska-Lincoln, W317 Nebraska Hall, Lincoln, 68588-0526, US
Phone: 402-472-9490, Email: yha4@unl.edu

Shailesh Ganpule
University of Nebraska Lincoln, Lincoln, NE

Florin Bobaru
University of Nebraska Lincoln, Lincoln, NE

Ruqiang Feng
University of Nebraska Lincoln, Lincoln, NE

Abstract:

Traumatic brain injury (TBI) is a critical and complicated phenomenon mostly influenced by strong blast impact. It is also a complex injury with a broad spectrum of symptoms and disabilities. The impact on a person and his or her family can be devastating. Here we investigate fluid-structure interaction models of air blast in shock tube. This study is mostly related to understanding TBI from air blast wave and its main objective is developing more realistic setups for TBI simulation through the calibrations between models and experiments. For modeling of the fluid-structure interaction we firstly propose the way of generating the blast wave. When a pressure wave of finite amplitude is generated in air by a rapid release of energy, such as high-pressure gas storage vessel or the blast from dynamite, instant mixing of two pressurized airs with very different densities makes an air blast wave. The modeling process also includes the investigation of the duration of the peak of the shock wave and modeling of the structure in the shock tube. The computational models for the fluid-structure interaction simulation have been developed using the finite element method with Arbitrary Lagrangian-Eulerian (ALE) technique. For the first step of the calibration with the shock tube, some simple structural models have been developed and the numerical results have been compared with the experiments. Also, the realistic human brain models have been developed and validated with real head experiments. This study will be combined with this real head model for more realistic simulations. The validated results will provide better understanding of the energy transfer characteristics of blast wave through helmet and the injury mechanism of human head.
Mechanical Size Effects in Fracture and Microdamage Accumulation in Trabecular Bone

Thomas Siegmund  
Purdue University  
585 Purdue Mall, Rm 308, West Lafayette, 47907, US  
Phone: 765 494 9766, Email: siegmund@purdue.edu

David B. Burr  
Indiana University School of Medicine, Indianapolis, IN

Matthew R. Allen  
Indiana University School of Medicine, Indianapolis, IN

Abstract:

Failure of bone under monotonic and cyclic loading is related to the bone mineral density, the quality of the bone matrix and the evolution of microcracks. The theory of linear elastic fracture mechanics has commonly been applied to describe fracture in bone. Evidence is presented that bone failure can be described through a non-linear theory of fracture. Thereby, deterministic size effects are introduced. Concepts of a non-linear theory are applied to discern how the interaction among bone matrix constituents (collagen and mineral), microcrack characteristics, and trabecular architecture can create distinctively differences in the fracture resistance at the bone tissue level. The nonlinear model is applied to interpret pre-clinical data concerning the effects of anti-osteoporotic agents on bone properties. The results show that bisphosphonate (BP) treatments that suppress bone remodeling will change trabecular bone in ways such that the size of the failure process zone relative to the trabecular thickness is reduced. Selective estrogen receptor modulators (SERMs) that suppress bone remodeling will change trabecular bone in ways such that the size of the failure process zone relative to the trabecular thickness is increased. The consequences of these changes are reflected in bone mechanical response and predictions are consistent with experimental observations in the animal model which show that BP treatment is associated with more brittle fracture and microcracks without altering the average length of the cracks, whereas SERM treatments lead to a more ductile fracture and mainly increase crack length with a smaller increase in microcrack density. The model suggests that BPs may be more effective in cases in which bone mass is very low, whereas SERMS may be more effective when milder osteoporotic symptoms are present.
Anaylzing Range of Motion in Total Hip Arthoplasty

Dishita Patel
Wright State University
257 Russ Engineering Center,, 3640 Colonel Glenn Hwy,, Dayton, 45435, US
Phone: 937-751-3580,   Email: patel.55@wright.edu

Dr. Tarun Goswami
Wright State University, Dayton, Ohio

Abstract:

Background. Range of motion of hip joint mainly depends on oscillation angle, cup anterior opening, femoral neck anteversion angle, cup abduction and neck-shaft angle. Component placement and prosthetic design parameters affects the range of motion of prosthetic hip. Improper postioning causes prosthetic impingement in Total Hip Arthroplasty (THA). Design parameters affecting the Range of Motion of a specific hip are Neck-Shaft angle, Neck-Head Ratio, Shape & Diameter of Neck and Design of the opening plane.

Aim: The aim of this study is to evalaute the effectiv eness of design parameters of the given prosthetic model by testing a combination of stem and cup positions with respect to neck-shaft angles to achieve desired range of motion after Total Hip Arthoplasty (THA).

Methods: Mathematical models developed by Yoshimine, Ginkayashi, Widmer et.al are used to define the optimal range of motion for Activities of Daily Living (ADL). Solid computational softwares such as Solidworks, ANSYS are used to simulate models and perform stress anaylsis.

Results: Range of Motion obtained for the given prosthetic implants are predicted and compared with optimal range of motion obtained by other authors. Modifications in design parameters are suggested to gain the optimal range of motion.

Discussion: Optimal range of motion would vary based on patient needs and history. Each design parameter and component position are subject specific.
Orthopaedic Bioengineering – Nano-Science to Device Level

ORGANIZERS:

Tarun Goswami, Wright State University
Richard Laughlin, Wright State University
Arthur Ritter, Ph.D., Stevens Institute of Technology
Direct Measurement of Plastic Dissipation During Bone Fracture

Thomas Siegmund
Purdue University, 585 Purdue Mall, West Lafayette, 47907, US
Phone: 7654949766, Email: siegmund@purdue.edu

Torres Denis
Purdue University, West Lafayette, IN

Abstract:
Understanding the factors responsible for changes in the toughness of bone presents a continuous challenge. The present study is based on the general hypothesis that a variety of processes can contribute to bone toughness, and that the individual contributions of toughening mechanisms can vary with the state of bone. Such mechanisms would include the actual creation of the fracture surface, crack path deflection, crack bridging, microcracking and irreversible (plastic) deformation. To date investigations of bone toughness and crack growth resistance have not been able to quantify if and at what level plastic deformation would contribute. We hypothesize that plastic dissipation indeed contributes to bone toughness, and that direct measurements of irreversible deformation would confirm such processes. We also hypothesize that the magnitude of plastic deformation would depend on the state of bone.

Bovine femur bone is employed as a sample material without any selection of specimens with regard to age, gender and anatomical features. Three different state of bone are considered: wet, dehydrated, and ashed. SENB specimens of dimensions (a0=1.0 mm, a0/W=0.55, B=1.5 mm) with side notches were machined such the initial crack is aligned with the periosteal-enosteal direction. Such small specimens allow one to exclude crack bridging with uncracked ligaments from the analysis during fracture testing. The J integral and its elastic and plastic components (Jel and Jpl) were obtained. Post-test, fractured specimens were recovered, and the two fracture surfaces were stained in a solution of black ink to enhance contrast. Corresponding specimen halves were imaged using a compound microscope equipped with a z-stage controlled by a stepper motor. Partially focused image slices were assembled into a height encoded digital elevation model (DEM) by use of the software Helicon Focus. From the DEMs crack surfaces profiles were extracted such that corresponding profiles follow paths through matching points on opposite fracture surfaces. Profiles are aligned to the initially machined pre-notch faces.

The present study presents a protocol for the determination of the contributions of crack path deflection and plasticity to the crack growth resistance of realistically short cracks in cortical bone. In agreement with recent data on human bone, it is found that the initiation toughness of bovine bone measured under high resolution is significantly lower than previously reported values on long cracks. We demonstrate that the crack initiation and subsequent crack growth resistance emerge as the outcome of crack deflection and plastic deformation. Detailed measurements of elastic-plastic fracture parameters agree with the findings from the fracture reconstruction. Fracture reconstruction can be performed independent of instrumented fracture mechanics tests. Such an approach would then allow for an estimation of the contributions to toughening from crack path deflection and confirm the presence or absence of plastic deformation in association with the growth of cracks in cortical bone. As we demonstrate that the mismatch measurement is sensitive to the state of bone, the approach described here could aid in further clarifying the role of the organic matrix in its contribution to bone toughness.
Repeated Freeze-thaw Cycles Do Not Alter the Biomechanical Properties of Fibular Allograft Bone

J. Christopher Gayton
Wright State University, Department of Orthopaedic Surgery, 30 E Apple St, Suite 2200, Dayton, OH 45409
Phone: 937-208-2127, Email: athenscg@yahoo.com

Shawn Hunter
Community Tissue Services, Dayton, OH

Michael J. Coffey
Wright State University Department of Orthopaedic Surgery, Dayton, OH

Michael J. Prayson
Wright State University Department of Orthopaedic Surgery, Dayton, OH

Abstract:
Introduction: Structural allograft bone is commonly used in orthopaedic surgery. Complications relating to unanticipated graft fracture have prompted investigation into possible sources of graft failure, including storage and handling conditions. The objective of this study was to determine the effects of freeze-thaw cycles on the biomechanical properties and structural integrity of fibular allograft bone. Our hypothesis was that the mechanical properties of fibular allograft bone decrease with increasing numbers of freeze-thaw cycles.

Methods: Paired fibulae were recovered from 18 cadaveric donors. Each fibula was thawed, debrided, cut into three 80mm segments, and subjected bioburden reduction process. A control segment was used with the minimum required one freeze-thaw cycle. The remaining segments were randomly assigned to one of the five treatment groups: two, four, or eight freeze-thaw cycles (2FT, 4FT, 8FT), one freeze-thaw cycle plus freeze drying (1FT-FD), or three freeze-thaw cycles plus freeze-drying (3FT-FD). Specimens were tested in three-point bending by loading to failure at a strain rate of 0.5 mm/sec on a materials testing system. Structural and material parameters were derived, and energy was calculated by integrating the force-displacement curve up to the point of failure.

Results: The average ultimate stress for all segments was 174±59 MPa, average modulus was 289±217 MPa, average energy was 2.00±1.83 J, and the average stiffness was 1320±511 N/mm. There were no significant differences between treatment groups (Figs 2 and 3). However, post-hoc analysis revealed a significant difference (p&lt0.05) between 1FT-FD and Control and 2FT and Control in stiffness and energy, respectively. Donor variation was significant for all measures at p&lt0.001.

Conclusions: The results suggest that there is no effect on the failure properties of fibular bone segments when subjected to as many as eight freeze-thaw cycles and/or freeze-drying. However, it is apparent that the donor-to-donor variation is quite large. Analysis of the loading profile implies that the sub-failure fatigue properties of these groups would be markedly different. Moreover, the post-hoc test did indicate a difference between the freeze-dried and the 2FT, 4FT, and 8FT treatments, which implies that freeze-dried bone warrants further study in the sub-failure region.
The Influence of Screw Thread and Tapping on the Fatigue Performance of Pedicle Screws

Arthur Ritter
The Stevens Institute of Technology
CCBBME, Castle Point on Hudson, Hoboken, 07030, US
Phone: 201-216-8290, Email: aritter@stevens.com

Steven Lewis
Toronto Western Hospital,

Joseph Turner
Medtronic's Spinal and Biologics Business,

Abstract:

Introduction: In this study bovine vertebral bodies were inserted with pedicle screws of varying thread/shaft geometry in conjunction with single lead (SL) and dual lead (DL) tapping. It is hypothesized that the under fatigue loading, the effects of screw hole tapping and thread/shaft geometry can be manifested and quantified.

Materials and Methods: For each bovine vertebral body from T11 to L4, bilateral randomized insertions of pedicle screws under various tapping conditions were performed. Three screws were tested: single thread Standard (STD), dual thread (DT) with a wider cortical thread crest (DTW), and a DT with a narrower thread crest (DTN). Single lead (SL), dual lead (DL), and no tapped holes were evaluated. All tapped holes were under-tapped by 1mm. Insertion torque was measured using a calibrated torque wrench. The testing regimen consisted of sinusoidal loading between ±340N to 2600 cycles at 0.5Hz with continuous load and displacement data collected at 100-cycle intervals. The average deflection over each cycle interval was then subjected to a non-linear regression. Following toggle fatigue testing, pullout testing was performed at a rate of 25mm/min with peak load computed. All fitted non-linear regression and static pullout parameters, as well as insertion torque, were compared using a one-way ANOVA and a Tukey post-hoc comparison for determination of statistical differences between groups.

Results: From the plot of deflection versus cycle number, the DTN-Under Tap SL, DTN-Under Tap DL and DTW Under Tap SL display the least amount of deflection increase under toggle fatigue. Plateau values associated with these three groups were statistically different (P&lt0.05) from the remaining groups. With respect to settling rate (K value), the DTN-Under Tap DL displayed a significantly increased rate with respect to all other groups, indicating a rapid achievement of the ultimate settling deformation. Insertion torque was significantly reduced for the STD Screw-Under Tap as compared to all other designs except for the DTW Under-Tap DL group. No statistical differences between screw/tap conditions were detected with respect to the ultimate load sustained in axial pullout.

Discussion: The DL tap displayed a significant increase in K value (faster settling) with respect to the same screw (DTN) using different tapping techniques. The dual lead tap is likely to provide a better
pre-cutting guide into the surrounding bone for dual threaded screws, thereby reducing the incidence of microfracture by virtue of the changing thread on the screw shaft during screw insertion. The DTN No Tap condition displayed the most reduced K value. This reduced settling rate is likely indicative of continuous microfracture under repetitive loading. From these toggle fatigue tests it appears that an narrow crest design coupled with a dual lead tap leads to improved biomechanical performance by virtue of increased thread contact with the surrounding bone. As well, the effect of tapping may provide a pathway for threads to engage and hence reduce the likelihood of microfracturing, which under toggle loading will manifest itself as reduced settling and increased plateau values.
Static Evaluation of Shear Loading Associated With Extension/Compression of the CerviCore® Intervertebral Disc Prosthesis

Arthur Ritter
The Stevens Institute of Technology
CCBBME, Castle Point on Hudson, Hoboken, 07030, US
Phone: 201-216-8290, Email: aritter@stevens.edu

Thomas Errico
NY Hospital for Joint Diseases, New York, NY

Abstract:

Introduction: Migration of intervertebral devices is a multifaceted phenomenon and may be due to prosthesis loading, transfer of motion and clinical factors such as bone quality, site preparation, and sizing. The purpose of this study was to measure compressive and shear loading transfer with the CerviCore® Intervertebral Disc prosthesis under neutral and extension conditions.

Material and Methods: Six caprine functional spinal units (FSUs) were embedded in sleeves and inserted with the CerviCore® Intervertebral Disc prosthesis. The surgical site was distracted at each test angle configuration to permit insertion of Fuji contact pressure film between the prosthesis components. Wedges were fabricated to provide extension angles of 0 (neutral), 5, 10, and 15 degrees to the FSU under a 100N compressive load. The load was maintained for 30 seconds in order to permit film exposure. Pressure film analysis was performed using Topaq software. For each angle, peak and mean values for contact stress, force, and area were computed. The non-zero extension conditions were subjected to computation of shear stress and force through the relationships through vector component analysis.

Results: A significant increase in contact area was detected at 15 degrees of extension as compared to both the neutral and 5 degree condition. The mean and maximum compressive force was significantly increased at 15 degrees of extension as compared to both the neutral and 5 degree condition. No significant difference was detected in maximum compressive pressure or mean compressive pressure regardless of extension angle examined. The mean and maximum shear pressure was significantly increased at all degrees of extension. The mean and maximum shear force was significantly increased at 15 degrees of extension as compared to both the neutral and 5 degree condition.

Discussion: The compressive force and area increased as extension increased and was statistically significant at 15 degrees as compared to the neutral and 5 degree conditions. Compressive pressures were not statistically significant. Shear is indicative of migration propensity and resulted in significant increases in both mean and maximum shear pressure at all angles. The mean maximum shear force was found to be 23±13 N with the maximum shear force ≥40 N. Pull-out strength of cervical bone dowels has been reported to be 199±50 N, while 135 N of anterior force was found to initiate facet capsule injury. In this study, 15 degrees of extension resulted in shear (or anterior migration) forces less than those reported to pull out intervertebral devices.
Distal Third Clavicle Fixation: A Biomechanical Evaluation of Fixation

Kenny Edwards
Wright State University Dept.of Orthopaedic Surgery
30 East Apple Street, Suite 2200, Dayton, 45409, US
Phone: 937 208-2127, Email: kenny.edwards@wright.edu

L. Joseph Rubino, M.D.
Wright State University Orthopaedic Surgery, Dayton, OH

Michael Herbenick, M.D.
Wright State University Orthopaedic Surgery, Dayton, OH

Tarun Goswami, D.Sc.
Wright State University Orthopaedic Surgery, Dayton, OH

Abstract:

Background: Distal third clavicle fractures account for 10-15% of all clavicle fractures, and constitute a much higher proportion of complications in regards to fracture treatment. Neer found that although these fractures are rare, they account for nearly 50% of clavicle non-unions. The rate of non-union is high in fractures treated with both non-operative and operative management. To date there is no agreed upon standard of operative care for these injuries, and they continue to present a significant operative dilemma for the orthopaedic surgeon.

Purpose: The purpose of this study was to compare operative constructs for the treatment of unstable, comminuted, distal third clavicle fractures in a cadaver model. We compared the Distal Third Clavicle Locking Plate (Smith & Nephew, Memphis, TN), the AC Tightrope (Arthrex Corp. Naples, FL), and the Distal third Locking Plate with the AC Tightrope together.

Hypothesis: We hypothesize that the Arthrex AC Tightrope is biomechanically similar to the Distal Clavicle Locking Plate when used to treat unstable distal clavicle fracture.

Methods: Twenty-one fresh cadaveric specimens were used in this study in three groups of seven. Group-1 was implanted with the Distal Third Locking Plate (Smith & Nephew, Memphis, TN). Group-2 was implanted with the AC Tightrope (Arthrex Corp. Naples, FL). Group-3 was implanted with the Distal Third Locking Plate and the Arthrex AC Tightrope together. Each specimen was stabilized for testing with a custom designed clamp to avoid loosening during cyclic testing. An unstable fracture was replicated with an osteotomy of the distal clavicle 20mm from the AC joint in each specimen. The Coracoclavicular (CC) ligaments were cut to allow the medial fragment to become unstable. Biomechanical testing was conducted in an axial compression and torsion biaxial system, Endura TEC Smart Test servo-pneumatic test frame. Axial load of 70N with slight rotation as physiologically seen (± 2°) was replicated, a new feature, and has not been reported in the literature. Frequency was kept from 2 Hz to avoid any adverse affects. Both the peak-load and torque was applied at the same time.
during 5000 test cycles, load drop and displacement was also recorded. Displacement was measured via digital recording acquisition systems.

Results: Load to failure was tested in both compression and displacement tensile strength of each construct. The amount of applied force in each group was measured and averaged as follows: Group-1 830.56 (N) and 396.06 (N), Group-2 N/A and 312.21 (N), and Group-3 1491.1 (N) and 458.51 (N), respectively. The amount of construct stiffness and displacement was also determined at the end of 5000 cycles and was recorded as follows: Group-1 131.63 (N/mm) and 0.72 (mm), Group-2 85.14 9N/mm) and 0.92 (mm), Group-3 319.09 (N/mm) and 0.27 (mm), respectively.

Conclusion: Our study failed to show that fixation with the AC Tightrope alone is biomechanically similar or superior to the distal clavicle locking plate construct. In fact, when used in conjunction with the locking plate, greater fracture stability was achieved, which could lead to increase fracture-healing rates as a result of greater construct strength. However, in a limited setting, the Arthrex AC Tightrope may represent adequate stability in non-comminuted fractures that typically requires less construct rigidity to heal. As well, it could alleviate the problems with painful, prominent hardware; screw breakage and possible implant migration that is frequently encountered with conventional hardware.

Key Words: Shoulder; distal clavicle fracture; biomechanics; anatomic reconstruction
Effect of Compressive Straining on Nanoindentation Elastic Modulus of Trabecular Bone

Vikas Tomar
Purdue University-West Lafayette
3205 ARMS, 701 W Stadium Ave, West Lafayette, 47907, US
Phone: 3172943251, Email: tomar@purdue.edu

Abstract:

Trabecular bone with its porous structure is an important compressive load bearing member. Different structural factors such as porosity, non-homogeneous deformation, varying trabeculae thickness, connectivity, and nanoscale (10 nm to 1 μm) to macroscale (~0.1 mm to 10 mm) composition hierarchy determine the failure properties of trabecular bone. While the above factors have important bearing on bone properties, an understanding of how the local nanoscale properties change at different macroscale compressive strain levels can be important to develop an understanding of how bone fails. In the present work, such analyses are performed on bovine femoral trabecular bone samples derived from a single animal. Analyses focus on measuring nanoindentation elastic moduli at three distinct levels of compressive strains in the bone samples: (1) when the samples are not loaded; (2) after the samples have been loaded to a strain level just before apparent yielding and the macroscale compression test is stopped; and (3) after the samples have been compressed to a strain level after apparent yielding and the macroscale compression test is stopped. Nanoindentation elastic modulus values are two orders of magnitude higher than the macroscale compressive elastic modulus values of all samples. A high variability in macroscale compressive elastic modulus values is observed because of porous architecture and small sample size. Nanoindentation elastic modulus values show a progressive reduction with increase in the extent of macroscale compressive deformation. Apparent yielding has a significant effect on this trend. The decrease in nanoindentation modulus value for all samples accelerates from approximately 20% before yielding to approximately 60% after yielding in comparison to the nanoindentation modulus values at 0% strain level. The level of variation in the predicted nanoindentation modulus values is the lowest for uncompressed samples (~16-18%). However, with increase in the extent of compression, the level of variation increases. It varied between 50% and 90% for the samples tested after yielding showing a widespread heterogeneity in local nanoscale structural order after apparent yielding. Scanning electron microscope (SEM) observations suggest that apparent yielding significantly destroys local nanoscale structural order. However, quantitative results suggest that a significant residual nanoscale stiffness varying from 5 GPa to 8 GPa among different samples still remains for possible repair facilitation.
Nanomechanics of Tropocollagen and Hydroxyapatite Biomaterials With An Account of Collagen Mutations and Varied Hydroxyapatite Textures

Vikas Tomar
Purdue University, West Lafayette
3205 ARMS, 701 W Stadium Ave, West Lafayette, 47907, US
Phone: 3172943251, Email: tomar@purdue.edu

Abstract:

In hierarchical nanocomposite materials (eg. bone, nacre), interfacial interactions between the organic phase (eg. tropocollagen (TC)) and the mineral phase (eg. calcium hydroxyapatite (HAP)) as well as the structural effects arising due to the staggered arrangement, TC mutations, and varied HAP textures significantly affect the strength of such biomaterials. In the present investigation, different idealizations of TC-HAP composite biomaterial system under tensile and compressive loadings are analyzed using explicit three dimensional (3-D) molecular dynamics (MD) simulations to develop an understanding of these factors. Analyses show that maximizing the contact area between the TC and HAP phases result in higher interfacial strength as well as higher fracture strength. Analyses based on strength scaling as a function of structural hierarchy reveal that while peak strength follows a multiscaling relation, the fracture strength does not. The peak strain for failure was found to be independent of the level of structural hierarchy.
An Adhesive System for Bone Bonding Applications

Iwona Jasiuk
University of Illinois
Department of Mechanical Science and Engineering, 1206 West Green Street, Urbana, 61801, US
Phone: 217-333-9259,   Email: ijasiuk@illinois.edu

Ilker Bayer
University of Illinois, Urbana, IL

Eric Loth
University of Virginia, Charlottesville, VA

Abstract:

Current methods for fracture stabilization in bone tissue require the use of metal hardware to be affixed to the bone, resulting in many challenges and limitations in this technology. The need to anchor a metal support that conforms to the tissue structure with enough remaining bone material to support the load does not readily allow for the attachment to small or irregular bone pieces. This problem can be overcome by using an adhesive. However, there are unique challenges present in the bonding of biological material in in vivo conditions. Bonding materials that are bathed in fluid is a difficult task for almost all adhesive systems. In order to overcome the incompatibility between polymers and bone an amphiphilic primer can be used to modify the surface energy and significantly improve adhesion. It is also a requirement that all parts of the adhesive system be biocompatible with no allergic or toxic byproducts from the system.

The chosen system in this study is a single component polymer adhesive. Crosslinking is initiated by the introduction of a small amount of water. The polymerization reaction that occurs with the water results in a release of carbon dioxide gas that promotes the formation of a foam structure. The chosen preparation method can then yield a variety of structures that range from a rigid foam with about 80 percent voids and 2-3 mm pores to a dense foam with microporosity.

Mechanical characterization of the adhesive was investigated in three loading modes: shear, compression, and tension. These modes are the primary modes of interest that occur in the intended application environment. Bulk compression properties of the adhesive were also measured. Finally, the initial in vitro and in vivo tests were conducted. In the in vitro study myoblasts were able to attach to the slides, grow normally, and differential into muscle tissue. Cells appeared to grow and differentiate at their normal rates while on the adhesive. Initial mechanics models were also conducted.
Hip Implant Interfacial Motion, a Finite Element Analysis

Mbulelo Makola
Wright State University
3140 Colonel Glenn Hwy, Dayton, 45435, US
Phone: 9377754989, Email: makola.3@wright.edu

Tarun Goswami
Wright State University, Dayton, OH

Abstract:

Press fit hip implants present marked advantages and disadvantages as compared to cemented hip implants. A key factor in implant fixation is the amount of interfacial motion between implant stem and the femur. A finite element analysis of hip implant stem designs was performed to determine the effect on stem interfacial motion. A femoral finite element model based on the geometry of a composite femur was used. Implants of distinct cross section and stem profile were analyzed. Implant material property effects on interfacial motion were studied by modeling implants as made up of cobalt chromium (CoCr), Stainless Steel (SS316L), and titanium alloy (Ti6Al4V). Each implant was subject to a static loading simulating the weight of an average U.S. male (189 lb) taking a step forward. Implant profile and stem design along with material property played an important role in the amount of interfacial motion observed. Implant stems of circular cross section showed the lowest amounts of interfacial motion. Ti6Al4V showed the greatest difference in implant interfacial motion as compared to SS316L and CoCr. The study has shown that stem profiles are a key factor in resisting interfacial motion. However, the ability of surgeons to perform hip arthroplasties using press fit un-cemented implant stems and achieving full fixity has not been studied or quantified. As such the continued design and development of implant stems resistant to interfacial motion is needed.

Susanq Schweitzer  
Wright State University  
3640 Colonel Glenn Hwy., Dayton, 45435, US  
Phone: 937-524-9421, Email: schweitzer.6@wright.edu

Mary Kundrat  
Wright State University, Dayton, Ohio

Tarun Goswami, D.Sc  
Wright State University, Dayton, Ohio

Abstract:

The objective of this study was to perform a statistical analysis on the dimensional anatomy of the vertebral bodies present in the cervical spine. This analysis includes the vertebral segments of C3 to C7. The different dimensional aspects that were analyzed were based on the anthropometric measurements completed from a published study on Chinese Singaporeans.

The current study involved the following anthropometric measurements: upper and lower end plate width (EPWu and EPWl), upper and lower end plate depth (EPDu and EPDl), anterior and posterior vertebral body height (VBHa and VBHp), spinal canal width (SCW), spinal canal depth (SCD), left and right pedicle height (PDHl and PDHr), left and right pedicle width (PDWl and PDWr), spinous process length (SPL), transverse process width (TPW), upper and lower end plate area (EPAu and EPAl), spinal canal area (SCA), left and right pedicle area (PDAI and PDAr), upper and lower end plate transverse inclination (EPItu and EPItl), left and right pedicle sagittal inclination (PDIsl and PDIsr), and finally the left and right pedicle transverse inclination (PDItl and PDItlr). Analysis was completed using the concepts of linear regression, ANOVA, and parameter estimation. Investigation into any relationship that might be present between the previous anthropometric measurements in each vertebra was also completed. As an example, a comparison between the EPWu of the C3 vertebra and the PDIsr of the C3 vertebra was analyzed to determine if there was any statistically significant relationship present. Comparison of anthropometric measurements of each vertebra singly was completed (i.e. Comparing C3 measurements to C3 only, C4 to C4 only, and so on). Further analysis was done to see if there was any relationship between the anthropometric measurements as one travels axially down through the cervical spine. As an example the progression of vertebral body height as one moves from C3 to C7.

With the statistical analysis completed for Chinese Singaporeans, projection of these relationships will be applied onto the United States population. The result of this statistical modeling will help provide more accurate modeling of this section of the spine, in order to assist in the development of improved spinal implants as well as more efficient surgical device placement techniques. Additionally, these statistics will lead to a better understanding of cervical spine functionality and its susceptibility to failure.
Mapping Tibial Surface Strains using 3D Stereo Optical System

Jonathan Hein
University of Nebraska-Lincoln
W317.4 Nebraska Hall, University of Nebraska-Lincoln, Lincoln, 68588, US
Phone: 847-420-2191,   Email: jhein3@gmail.com

Brian McMichen
University of Nebraska Lincoln, Lincoln, NE

Dr. Mehrdad Negahban
University of Nebraska Lincoln, Lincoln, NE

Dr. Mohammed Akhter
Creighton University, Omaha, NE

Abstract:

In vivo studies have shown that the bone adaptation response to mechanical stimulus or exercise is proportional to strains during loading. The purpose of this study is to present ex vivo tibial surface strains in three adult mouse genotypes representing HBM [high bone mass with LRP5 G171V mutation], n=5, WT [wild type, nontransgenic littermate n=4], and LRP5-KO [with Lrp5 gene knocked out KO-/-, n=4]. These genotypes represent a full range of bone mass and structural stiffness. We used a full field stereo optical measurement system (ARAMIS, GOM mbH, Germany) that provides tibial surface strain ex vivo (1.5 to 4.5 mm proximal to the tibio fibular junction-TFJ region). Along with quasi-static compression tests (Bose, MN), ARAMIS system provided optical 3D deformation analysis of tibial surfaces. Strain analysis with the ARAMIS system yields the equivalent of hundreds of strain gages on the surface. A set of compressive tibial loads in the longitudinal direction consist of 1, 2, 4 and 6N. Four tests were performed on each bone in order to create a 360 degree view in ARAMIS (example, Figure). The average tibial surface strain was lowest in the HBM mice and highest in the KO mice (Table) for the same axial loads. The data are comparable to direct strain measurements and predicted values presented previously at ASBMR (2009 meeting). Data at 1 N may be prone to error due to the low magnitude of force and bone deformation. These data suggest that the tibial surface strains are sensitive to the structural stiffness. Smaller surface strains are measured in tibiae representing largest cross sectional moment of inertia [MOI] (tibiae from HBM mice have at least 30% greater MOI and KO 30% less than WT). These data suggest that the regional tibial strains mapped with the ARAMIS system (Figure) are comparable to the direct strain gage data at the region 1.5 to 4.5 mm proximal to TFJ. Both ARAMIS and the direct strain measuring technique can complement each other in providing reliable tibial surface strain analyses for compressive loading in small animal model of studying bone adaptation.
Using Finite Difference Methods to Develop the Probability of Neck Injury

Mary Blackmore
Wright State University
330 W 1st Street, Apt 806, Dayton, 45402, US
Phone: 937-775-4989, Email: Mary.Blackmore@wright.edu

Tarun Goswami
Wright State University, Dayton, OH

Abstract:

There is currently insufficient data pertaining to cervical spinal trauma and its associated risks. Various factors contribute to the potential risk of injury to the cervical spine. Gender, height, weight and activity level all have significant impact, along with the types of activities being performed and to what intensity they are carried out. The potential for injury lies in all forms of activities, both work and leisure related. To assess the potential for injury on a per person basis, the objective of this study is to use finite difference methods to develop injury risk curves. The developed curves will have an affiliation with the Abbreviated Injury Scale (AIS), and explain to what degree, a person is at risk of acquiring injuries of differing severities. Causes of cervical trauma will be studied extensively, along with the forces necessary to induce soft tissue damage and vertebral fracture at all levels of the cervical spine. As these two injuries are the most common type of neck trauma, they will be the main focus of the model development. This data will be compiled and plotted to develop injury curves. Various finite difference methods including Forward and Central Difference and the Crank Nicholson Method will be compared to determine which of these provides the most accurate means of estimating the amount and type of force needed to induce injury on various types of human subjects. Once these crucial force values are determined they will be used to derive and plot a function that incorporates the AIS scale, in order to determine what percentage of risk, if any, a person is faced with when subjected to various types of loading. This effort will eventually lead to a better understanding of the potential for cervical spinal injury that faces a person, when undertaking a variety of activities for various lengths of time.
Bone Isotropy Characterization Under Fatigue Loading within the Vertebral Body

Rebecca Chung
Stevens Institute of Technology, Stevens Institute of Technology, Castle Point on Hudson, Hoboken, NJ
Phone: 201-216-8290, Email: rchung@stevens.edu

A. Valdevit
Stevens Institute Of Technology, Hoboken, NJ

A. Ritter
Stevens Institute of Technology, Hoboken, NJ

T. Errico
2NYU Hospital for Joint Diseases, New York, NY

Abstract:
Introduction: Wolff’s Law describes bone response to loading conditions. Although verified under static conditions, bone is clinically subjected to cyclic loading. It was hypothesized that under sinusoidal loading, that the axial or Z direction would display superior mechanical fatigue properties as compared to the X and Y shear directions.
Material and Methods: Cancellous bone cubes were extracted from central regions of six bovine vertebral bodies. For each cube, 500 cycles of compressive loading from -5N to -50N were applied at a rate of 1Hz. Continuous load versus deformation data was acquired at cycle number 5 and at subsequent 25 cycle intervals thereafter. To account for deviations in the cube geometry, normalization in each of the respective X, Y, and Z directions was performed using the individual X, Y and Z dimensions. Mean deformation versus cycle number for each of the X, Y and Z orientations was subjected to a non-linear analysis. The resulting curve parameters were statistically analyzed using a 1 way repeated measures ANOVA.
Results: A non-linear exponential fit was utilized for net deflection versus cycle number. These functions are characterized by a Plateau or asymptotic limit in deformation; K the rate constant and the Span, defined as the change in deformation over the course of the fatigue test.
Discussion: The initial compressive deformation (Y0) plot showed that the samples experienced largest amounts of initial compressive deformation when subjected to loading in the X direction, indicating that the bone is most susceptible to shear. Least amount of initial compressive deformation occurred when loading in the Z direction, indicating that the bone is most resistant to axial loading. The initial compressive deformation experienced by the bone when loaded in the Y direction fell in the range between the X and Z directions. (P<0.05 for all directions) A similar finding was observed with respect to the Plateau values (P<0.05 for all directions). The largest rate constant (K) values were calculated for samples subjected to anterior to posterior shear (X direction), indicating that bone deformation occurred fastest in this direction (P<0.05). No statistical difference was detected between rate constants in Y and Z directions (P>0.05). Wolff’s Law has been studied experimentally under static conditions. This study represents one of the first attempts to validate this concept with clinically relevant fatigue loading. These findings indicate that during insertion of intervertebral device, where shear loading is generated, the underlying vertebral endplate should not be compromised.
Mechanical Comparison of Cadaver Femurs Implanted with Various Intramedullary Nails

Alyssa George Whitney
Wright State University
207 Russ Engineering Center, 3640 Colonel Glenn Highway, Dayton, 45435, US
Phone: 419-340-5519, Email: george.45@wright.edu

Tarun Goswami Ph.D.
Wright State University, Dayton, OH

Abstract:

Intramedullary nails are commonly used for the fixation of femurs that have broken proximally. Even after healing of the initial fracture, failure of the femur bone can occur with intramedullary nail fixation. These failures often happen during a twisting motion of the body while standing or due to falls onto the side of the body. It is important to understand how these failures occur and which devices are more susceptible to such failures in order to prevent them in the future. In order to fulfill this, a cadaveric study is being conducted to simulate both standing (torsion with a constant axial load) and falling (four-point bending) failures so that various intramedullary nail sizes and materials can be compared. For this study, 28 pairs of frozen cadaver femurs are implemented with one of four intramedullary nails. The four types of intramedullary nails include short nails made of stainless steel, short nails made of titanium, long nails made of stainless steel, and long nails made of titanium. Seven femurs for each type of nail are used for torsion testing, and the same is done for bending testing. All tests are completed on an EnduraTEC servo pneumatic machine (Smart Test SP-AT). Two stages are involved in each test. The first involves cyclic loading for 30,000 cycles to simulate normal use of the leg. For torsion testing, 700N of constant load is applied to simulate single-leg stance and ±5Nm of torque is applied cyclically, as seen during walking. Similar testing will be completed for four-point bending. The second stage tests the more extreme scenarios, such as twisting or falling, with displacement to failure tests of the implemented femurs in either torsion or bending. Evaluation of these tests will help to determine how intramedullary nail length and material can affect failure of the bone after initial healing.
Abstract:

Vertebral endplates play an important role in the health and stability of the spinal column. Endplates are a thin layer of bone that act as a boundary between the intervertebral disc and vertebral body. Without the endplate the intervertebral disc would be free to herniate into the vertebral body. Extrusion of the disc into the vertebral body reduces the spinal column height, alters stress distributions inside and outside the vertebral body, impinges on the spinal cord and can cause pain. The endplate also evenly distributes axial spinal column loads.

Endplates have three physical features. They are comprised of a layer of hyaline cartilage that is superficial to a porous bony plate, and the remains of an epiphysial plate, more commonly referred to as the growth plate. The endplate has lots of geometric variations depending on location. The central region of the endplate is typically the thinnest part and increases thickness towards the periphery. There are also variations between the superior and inferior endplates. This variation of thickness is due to the distribution of stresses throughout the vertebral body. Regions with higher stresses will typically be thicker than those with less stress. A convex curvature is also present in many endplates that forms a dish into the vertebral body.

Due to the complex geometry, boundary conditions and load scenarios finite elements methods are used to analyze the endplate for stress and strains. More often then not the endplate is simplified and idealized as a uniformly thick and flat without any curvature. This report will analyze the endplate with more anthropometrically correct geometry and material properties. Comparisons will also be made between curvature and thickness differences.

The goal of this study will be to further understand the biomechanics of the vertebral body endplates. Also an investigation will be conducted into the orthopedic treatment options available for intervertebral disc arthroplasty or fusion.
Mechanics of Soft Materials

ORGANIZERS:

Tian Tang, University of Alberta

Ben Nadler, University of Alberta
On Stress Theory for Fractal Bodies

Reuven Segev
Ben-Gurion University
Department of Mechanical Engineering, P.O.Box 653, Beer Sheva, 84105, IL
Phone: 972-8-647-7108, Email: rsegev@bgu.ac.il

Abstract:

Fractals are used to model the geometry of various objects in nature. Plant parts, snowflakes, cracks and porous materials may serve as examples exhibiting such geometries. Yet, the traditional framework for the formulation of stress theory in continuum mechanics uses smoothness properties, such as the unit normal to the boundary and the Green-Gauss theorem, that do not apply to fractals. While various approaches for the extension of the notions of continuum mechanics to irregular bodies were suggested during the last decades, we follow an approach, suggested in [2], where bodies are represented mathematically as flat chains. This approach, based on Whitney’s geometric integration theory [3], has the following features. (a) It offers a common point of view for various aspects of the analysis such as the class of domains, class of admissible velocity fields, Stokes’ theorem and Cauchy’s theorem. (b) As the analog of Cauchy’s theorem is based on duality, the regularity of the stress objects is automatically the most general possible such that the mechanical power is bounded by the norm of the velocity field.

In the terminology of Whitney’s geometric integration theory, the velocity fields, including the domains on which they are defined, are modeled as vector valued flat chains. Stresses are represented by vector valued differential forms and their existence is implied by a representation theorem for flat cochains-bounded linear functionals defined on the space of flat chains. A weak form of the exterior derivatives exists for the differential forms representing cochains and the principle of virtual work of continuum mechanics may be written in the compact form $s(bdry(w)) = f(w)$. Here, $f$ is the body force, $w$ is the vector valued flat chain representing a velocity field and $bdry(w)$ represents its boundary. In addition, $s$ is the vector, flat cochain representing the stress and the term $s(bdry(w))$ includes also the power that the stress performs due to the velocity gradient. Additional approaches, to the theory of flat chains, e.g., those based on the theory of currents (see [1]), and their mechanical relevance and interpretations will be reviewed. In particular, such approaches enable one to extend the theory to the general geometric setting of Lipschitz manifolds.

References
A Field Theory of Physical Gels

Hanqing Jiang
Arizona State University
Hanqing Jiang,  Tempe, 85286, US
Phone: 480-965-1483,  Email: hanqing.jiang@asu.edu

Abstract:

Physical gels are a class of materials that further extend the range of properties and possible applications of chemically cross linked gels have been extensively investigated and are part of many technological relevant materials and devices. One of the most important applications of physical gels is drug delivery. In contrast with chemical gels, the links between polymer molecules are dynamic and are in constant process of creation and dissolution. Against quick deformations of the gel, the same solid-like behavior of chemical gels can be observed. However, the constant reformation of links allows the gel to release any anisotropic stress imposed on it. That is, it can adapt to the presence of boundaries in much the same way as a liquid. Here we develop a mean-field theoretical model to address the macroscopic behavior (static and dynamics) of physical gels. The large deformation and stress-strain relations are explicated included.
Abstract:

We present applications of a model developed to describe unfolding in macromolecules under an axial force. We show how a variety of experimentally observed force-extension behaviors can be reproduced within a common theoretical framework. We propose that the unfolding occurs via the motion of a folded/unfolded interface along the length of the molecule. The molecules are modeled as one-dimensional continua capable of existing in two metastable states under an applied tension. The interface separates these two metastable states and represents a jump in stretch, which is related to applied force by the worm-like-chain relation. The mechanics of the interface are governed by the Abeyaratne-Knowles theory of phase transitions. The thermodynamic driving force, which is one of the bases of phase transitions theory, has been employed here as the parameter upon which the unfolding velocity depends. The equation which embodies this dependence is the kinetic relation. By choosing an appropriate kinetic relation for the unfolding conditions and the macromolecule under consideration, we have been able to model unfolding processes in a number of molecules.
Experimental Characterization of Magnetically Activated Gels

LeAnn Faidley
Iowa State University
Phone: 515 294-1692, Email: faidley@iastate.edu

Sarah Timmons
Iowa State University, Ames, IA

Wei Hong
Iowa State University, Ames, IA

Abstract:

Ferrogels are compliant materials comprised of a nonmagnetic, flexible matrix with micro- or nano-size magnetic filler. In this study a Poly-Vinyl-Alcohol matrix is chemically crosslinked with Sodium Tetraborate and micro-sized particles of Carbonyl Iron are dispersed randomly in the sample. Ferrogels exhibit active behavior characterized by a deformation, a stiffness increase, and a change in magnetic and other properties when subjected to a magnetic field. Furthermore, since the composition of ferrogels can be easily varied the active properties of these materials can be designed over a wide range of possibilities. In order for this to be possible however, a thorough understanding of the active behavior of these materials and its dependence on external factors is necessary. In this experimental study this magnetically activated behavior is characterized for static and dynamic inputs. First, tests were run to measure the strain of unloaded ferrogels in non-uniform magnetic fields in which gravity acted either with or against the field direction. The ferrogels were observed to strain with a frequency double that of the applied field. The frequency dependency of this strain was characterized for the two test configurations giving indication of the visco-elastic behavior of these materials. Secondly, the effect of loading on the strain behavior of ferrogels in both nonuniform and uniform fields was characterized. Samples of various filler volume percent were exposed to compressive and tensile static loads and the exposed to sinusoidal fields. The output strains were measured. These tests lead to a characterization of the actuator behavior of the material and its work capabilities. Finally, the magnetic properties of the ferrogels were measured at various frequencies under a uniform field. Various sample filler percentages were tested and tests were run with samples that were constrained and unconstrained. A physics based mechanism describing all three of these behaviors is proposed based on the behavior of the magnetic filler in an applied field and the constraining effects of the visco-elastic matrix. These same effects are captured in a lumped parameter spring-dashpot model that captures the behavior observed based on the measurement of 4 parameters.
Abstract:

This paper studies the collapse of a void in an elastomer caused by osmosis. The void is filled with liquid water, while the elastomer is surrounded by unsaturated air. The difference in humidity motivates water molecules to permeate through the elastomer, from inside the void to outside the elastomer, leaving the liquid water inside the void in tension. When the tension is low, the void reduces size but retains the shape, a mode of deformation which we call breathing. When the tension is high, the void changes shape, possibly by two types of instability: buckling and creasing. The critical conditions for both types of instability are calculated. A tubular elastomer collapses by buckling if the wall is thin, but by creasing if the wall is thick. As the tension increases, a thin-walled tube undergoes a buckle-to-crease transition.
The Importance of PG Decorin in the Mechanical Properties of the Corneal Stroma

Hamed Hatami-Marbini
Stanford University
Mechanical Engineering Department, 219 Durand Bldg, 496 Lomita Dr, Stanford, 94305, US
Phone: 518-268-9748, Email: hhatami@stanford.edu

Peter Plinsky
Stanford University, CA

Abstract:

Corneal Stroma is composed of 2 um thick lamellae within which collagen fibrils are regularly arranged and run parallel to the corneal surface at different angles. The maintenance of the regular hexagonal arrangement of collagen fibrils inside the corneal stroma is essential for the transparency of the cornea. In knock-out mice, the cornea becomes opaque because of the omission of the proteoglycan (PG) decorin. In these species compared to healthy mice, the regular fibril diameters and spacings inside the corneal lamella are missing. Decorin is made up of a core protein and a glycosaminoglycan (GAG) side chain which is completely ionized and becomes negatively charged under physiological pH conditions. The electrostatic interaction between GAGs and free ions inside the bath controls collagen inter-fibril spacing and also contributes to the corneal stiffness. Here, we propose a model to capture the contributions of the GAGs to the compressive and in-plane shear properties of a single lamella in the corneal stroma. We postulate that each collagen fibril is locally connected to its next nearest neighboring fibrils by six PGs. The electrostatic contribution of GAGs is modeled by solving the nonlinear PB equation to obtain the electrostatic potential and charge distributions. Moreover, the electrochemical contribution of GAGs is considered by using the experimentally measured forces resulting from their self-adhesion. We compare these theoretic predictions with experimentally measured compressive and shear stiffness values. Since we are interested in the role of the proteoglycans in the mechanics of a single lamella, human cornea samples are cut into three pieces and the mechanical tests of the posterior thirds are used to calibrate and validate the computational model.
Inverse Stress Analysis in AAA Considering Thrombus

Shouhua Hu
The University of Iowa
242 Engineering Research Facility, 330 S. Madison Street, Iowa City, 52242, US
Phone: 3195129298, Email: shouhua-hu@uiowa.edu

Jia Lu
the University of Iowa, Iowa City, IA

Abstract:

Abdominal aortic aneurysm (AAA) is a pathological expansion of the aorta due to gradual wall weakening. AAA represents permanent localized expansions of the aorta that form between the renal arteries and the iliac bifurcation. Their prevalence increases with age, and progressive AAA growth will lead to eventual rupture. AAA is a common vascular problem with fatal implications. Current clinical practice is to evaluate the likelihood of rupture only on the basis of the maximum transverse bulge diameter, ignoring all other factors that contribute to failure. At present, a reliable method to predict AAA rupture is not available. Recent studies have introduced biomechanical analysis to map regions of stress concentrations developing in the aneurismal wall as a much better alternative to the current clinical criterion, which is based on the AAA diameter alone. From a biomechanical standpoint, internal stress is the physical factor that causes wall failure. Rupture can be expected to be increasingly likely as the wall stresses generated by blood pressure approach or exceed the strength of the diseased wall. So the wall stresses distribution in AAA is an important factor to predict the rapture. The usual mechanical study is to take the AAA as a thin-wall without taking the thrombus inside into consideration. Some studies show that intraluminal thrombus can reduce the peak wall stresses in AAA to some extent. Undoubtedly, a better prediction of AAA should include the elasticity of AAA when considering its deformation due to blood pressure.

This work investigates the influence of thrombus in the inverse stress analysis of AAA wall stress. By inverse stress analysis, we mean taking a pressurized geometric data as input to determine the wall stress. The advantage of inverse method is of two folds: one is that it can take into account the pre-deformation in a theoretically accurate manner; and two, for conduit-like structures the method can maximally capitalize on the property of static-determinacy, therefore to predict stress accurately without accurate knowledge of the wall properties. The second property will be compromised by the presence of thrombus so it is of interest to know its influence. Comparing the wall stresses distribution of the AAA with and without thrombus; we can determine how the thrombus in the AAA affect the mechanical behavior. The model can predict the wall stress response the thrombus and also the peak wall stress affected by the thrombus. This may provide more information for predicting the rupture risk.
Experiment and Constitutive Modeling of Tendon and Ligament Viscoelasticity

Roderic Lakes
University of Wisconsin-Madison
541 ERB, 1500 Engineering Drive, Madison, 53706, US
Phone: (608) 265-8697, Email: lakes@cae.wisc.edu

Ray Vanderby, Jr.
University of Wisconsin Madison, Madison, WI

Abstract:
Orthopedic soft tissues such as tendon and ligament display nonlinear viscoelastic behavior [1]. Most of the research supporting the constitutive modeling of such behavior relies solely on a single creep or stress relaxation experiment; this however does not provide enough information to distinguish between viscoelastic models. We have previously reported on the relaxation and recovery behavior of the porcine digital flexor tendon in the physiological strain range (less than 6%); the rate of recovery is less than that of relaxation [2]. We have further examined the ability of three single integral models, quasi-linear viscoelasticity (QLV), nonlinear (modified) superposition, and Schapery’s nonlinear viscoelastic model, to describe the stress relaxation and recovery behavior of porcine flexor tendon and medial collateral ligament (MCL). We found that the rate of stress relaxation increased with strain level for tendon, and decreased with strain level for ligament; neither nonlinear trend is explained by QLV. Examination of the recovery portion of the curve and a subsequent relaxation revealed that the nonlinear viscoelastic model by Schapery was best able to describe the behavior of the tendon and ligament models. The model was flexible enough to fit the opposing viscoelastic trends of tendon and ligament, in this strain region of interest, better than either QLV or nonlinear superposition.

To further determine whether the Schapery model is robust enough to adequately describe tendon behavior, we next attempted to predict creep and creep recovery behavior of porcine flexor tendon. Again, the model was flexible enough to adequately describe tendon behavior. To determine whether the single integral model was robust enough to characterize more complex loading protocols, two strain inputs were devised: the repeated step model, in which the tendon underwent ten seconds of relaxation followed by ten seconds of recovery and repeated ten times, as well as the cyclic model, in which the tendon was subjected to a sinusoidal strain input. In each case, the Schapery model was able to reasonably fit the data, indicating that with this model in this strain region, it is robust enough to describe tendon behavior.

References:
Experimental and Modeling Study to Determine the Turgor Pressure and Cell Wall Thickness of Arabidopsis Plant

Elham Forouzesh
University of Nebraska-Lincoln
W317.4 Nebraska Hall, University of Nebraska-Lincoln, Lincoln, 68588-0526, US
Phone: (402)3268991, Email: elhamf@huskers.unl.edu

Ashwani Komar Goel
University of Nebraska Lincoln, Lincoln, NE

Zoya Avramova
University of Nebraska Lincoln, Lincoln, NE

Joseph A Turner
University of Nebraska Lincoln, Lincoln, NE

Abstract:

The mechanical properties of plant cell walls influence the stability of the plant and also play a major role in plant growth. One important aspect necessary for the plant growth is that the wall should be able to distend under hydrostatic pressure commonly known as turgor pressure. The conventional method for measuring turgor pressure in single cells is using pressure probe but this technique is not very accurate for small cells and it is very time consuming and technically demanding. It also is a destructive test and the tested cells can not be used for further studies. Nanoindentation has proven itself to be a powerful technique for the measurement of mechanical properties and can be used in diverse applications ranging from mineralized tissues to soft tissues. We have used this technique to propose a new non-destructive and in vivo method for determination of the turgor pressure and thickness of cell wall based upon cyclic tests. Due to various unknowns in the problem, which includes shape and morphology of the plant, turgor pressure, instantaneous elastic modulus and viscoelastic material properties of the cell wall, a protocol has been developed that can be used to systematically evaluate the unknown parameters. This protocol combines the cyclic loading unloading experiments, relaxation tests, nano DMA, and finite element simulations. Finally, the effect of turgor pressure is calculated in hypertonic (plasmolyzed in 10% NaCl solution), isotonic and hypotonic (turgid in pure water). The advantage of this method compare to other conventional methods is that it is non-destructive, in vivo, and possible to be applied to very small cells.

Key words: turgor pressure, cell wall thickness, modeling, nanoindentation, hypertonic, isotonic, hypotonic, plasmolyzed
Macroscale and Microscale Structural Characterization of Cephalopod Chromatophores

Keith Kirkwood
Army Research Laboratory
US Army Research Laboratory, Composite and Hybrid Materials Branch, RDRL-WMM-A, Bldg. 4600, Aberdeen Proving Ground, 21005-5069, US
Phone: 410-306-1589, Email: keith.m.kirkwood@arl.army.mil

Keran Lu
US Army Research Laboratory, Aberdeen Proving Ground, MD

Eric D. Wetzel
US Army Research Laboratory, Aberdeen Proving Ground, MD

Abstract:

Cephalopods, the class of mollusks that include squid, cuttlefish, octopus and nautilus, possess skin with dynamic adaptable appearance. The color, iridescence, pattern and texture of the skin can be dramatically altered to match their surroundings. The unique ability to rapidly change the visual appearance is enabled by a sequence of thin layers in its skin. One layer of the skin, approximately 0.15mm thick, is occupied by organs of color change called chromatophores, that contain yellow, red or brown pigments. The chromatophore organ contains a cytoelastic sac (sacculus) of pigment granules surrounded by a spoked array of radial muscles. The chromatophore organs alter their visual appearance through control of the presented optical area of the pigment sac. Contraction of the radial muscles stretches the pigment sac into a flat disc of color, increasing the area of color on the skin. When the radial muscles are relaxed, the elastic sacculus containing the pigment granules relax back to the original size and shape decreasing the presented area. Typical chromatophores are 10-100 μm in diameter when punctate and 0.1-1 mm when expanded. A typical actuation of the chromatophore from ‘off’ to ‘on’ occurs in less than a millisecond for fast pattern execution. To better understand how this complex system of muscles, elastic sacs, and connective tissue performs, we will characterize the structural properties of the skin. We investigated the mechanical properties of the chromatophore layer of live squid skin using a bulge (inflation) technique. The tissue is dissected from the squid mantle with minimal disturbance of the natural tension and kept alive during the tests through submersion in a saltwater bath. The macroscopic bulk elastic properties of the skin are reported as a biaxial modulus and compared against polymeric materials of similar thickness. The linear and non-linear deformation behavior of the tissue is examined using the inflation technique. The strain at which the tissue fails is examined and damage to the network is characterized. Micromechanical characterization of live squid skin was utilized to isolate properties and functions of the tissue structure. Digital image correlation (DIC) was used to image the small-scale mechanical response of individual chromatophore structures to deformation. A random speckle pattern was superimposed on the surface of the skin to determine the local strain field around the chromatophore during deformation in the bulge experiment.
Material Analysis for the Development of a Surrogate Headform to be Tested Under Blast-Induced Shock Loading

SGM Hossain
University of Nebraska-Lincoln
N104 SEC, Lincoln, 68588-0656, US
Phone: 402-419-1967, Email: smgmamur@yahoo.com

Mickael Arnoult
University of Nebraska Lincoln, Lincoln, NE

Thomas Boulet
University of Nebraska Lincoln, Lincoln, NE

Charles Landais
University of Nebraska Lincoln, Lincoln, NE

Abstract:

Modeling of the human head has become a demanding issue recently for performing analysis of impact and shock-wave-induced injuries. To develop a surrogate headform for testing under loading conditions similar to those produced by explosive blasts, a primary design goal was to identify surrogate materials and appropriate geometry for skull, skin and brain matter according to the material properties and their approximate dimensions analyzed from literature. Dynamic mechanical analysis (DMA) (from 0.1Hz to 300Hz) and ultrasonic analysis for both longitudinal and shear waves was performed on two types of PDMS for modeling skin, polyurethane and polycarbonate for modeling skull and two types of silicone gels and one gelatin based colloidal material for modeling brain matter. Preparation of samples for such tests was performed with extra care to maintain required sample sizes and shapes. DMA tests were performed both in compression and shear, and the storage and loss moduli were recorded. As expected, it was found that the mechanical properties of all the materials tested are frequency dependent and that the moduli of polyurethane strongly depend on the applied preload. The PDMS skin samples were tested using ultrasonic contact transducers at different frequencies - 7.5MHz and 10MHz for longitudinal waves and 1MHz and 5MHz for shear waves. The signal was generated using a square pulser-receiver generator. Due to the strong shear attenuation in this material, only meaningful results from longitudinal waves were obtained. For both frequencies, longitudinal wave speed was 802 m/s, and longitudinal modulus was 698 MPa. In the case of the polyurethane skull simulant using a frequency of 1MHz, the longitudinal wave speed found was 2108 m/s and the longitudinal modulus was 4.89GPa. Tests were also performed on structured polycarbonate (containing void meso-channels of various dimensions) using 5MHz focused underwater transducers with a focal length of three inches. Both pulse-echo and through transmission methods were used. The aim was to determine the wave speed and the attenuation in these samples in order to compare these results with data from a real skull. Thus, new structured polycarbonate could be synthesized to match more closely with the properties of a human skull. To match brain matter properties more closely, the stiffness of the silicone gel was varied by mixing different gels in varying ratios, and DMA and ultrasonic tests were performed to find out their corresponding properties. For the most dense and viscous gel samples, the storage modulus has
been found to be around 50 kPa in compression and 6 kPa in shear, whereas the loss modulus was around 8 kPa in compression and 1 kPa in shear. These values tend to decrease as expected for other gel mixtures tested. Based on literature regarding dynamic properties of brain, skull, and soft tissue, the values obtained in these sets of experiments are within the target ranges and indicate the general suitability of these materials for use as tissue simulants in the headform design.
Experimentally Verified Approach for Computation of Contact Stresses in Vocal Fold Collision

Pinaki Bhattacharya
Purdue University
585 Purdue Mall, West Lafayette, 47907, US
Phone: 765 494 9766, Email: pinaki.bhattacharya@gmail.com

Thomas Siegmund
Purdue University, West Lafayette, IN

Abstract:

Damage in vocal fold (VF) tissues has been linked to mechanical stresses arising from collision during phonation. Fluid-structure-interaction (FSI) studies on 3D VFs are limited and have not been validated with experiments. 3D FSI simulations accounting for contact are fewer and the influence of VF adhesion is unknown. A computational experiment that addresses the above concerns is therefore of considerable interest.

We aim to understand the effect of tissue properties and surface adhesion on VF collision and subsequent stress histories. A two-layer VF model, with material properties corresponding to muscle and cover regions is considered. Forced vibrations with a spatio-temporally varying pressure load are considered such that the conditions of arising in FSI are simulated.

FSI simulations are used to calculate the stress and deformation distribution on the superior surface of a reference VF model (M5) and were validated against experimental data obtained by digital image correlation. Pressure profiles on the VF wall obtained from this computation were used to force the structure-only VF model. Adhesion is modeled by use of cohesive zone models. Contact stresses due to collision of the VFs were studied in dependence of the tissue properties (anisotropy, viscosity) and surface adhesion conditions. We assume that the pressure profile obtained from FSI computations for a particular set of tissue properties to be invariant.

The variation in contact characteristics (contact area, surface energy dissipated, maximum tensile and compressive stresses on medial surface) and stress distributions within the folds show a rich structure that was missed in previous studies. We focus the present investigation on particular scalars extracted from the stress tensor that are assumed to play a leading role in determining tissue damage evolution. Tissue anisotropy possesses a significant influence on the distribution of medial-lateral stresses leading to significant localization of stresses in mid-membranous position. In the presence of adhesion, for identical surface adhesion parameters, the medial-lateral stresses also localizes with increasing anisotropy, though the magnitude of maximum stress shows a decrease. This can be attributed to an increase in contact area with increasing anisotropy. As a mechanism of dissipation, the contact area and cohesive energy are seen to be more important parameters compared to cohesive strength, cohesive stiffness and separation length alone.

Viscoelasticity of the cover layer affects the stress-distribution through the decay time-constant parameter. Comparatively the shear- and bulk-moduli relaxation rates are not seen to be important.
Stress localization in compression increases as the creep time increases. In tension however, the stress magnitudes do not alter appreciably with increasing creep, but the localization still increases.

This study contributes to the understanding of stresses in VF during contact. To our knowledge, this is the first attempt to integrate the separate effects of tissue parameters, and surface adhesion properties in the presence of contact. The predicted stress histories are discussed in their role in agent based models aiming to predict the time varying change of biomedical agents in the vocal fold tissue.
A Long-Pulse Kolsky Bar Technique for Dynamic Testing of Soft Biomaterials

Ruqiang Feng
University of Nebraska-Lincoln
W314 Nebraska Hall, 900 North 17th Street, Lincoln, 68588-0526, US
Phone: (402) 472-2384, Email: rfeng1@unl.edu

M. Nienaber
University of Nebraska Lincoln, Lincoln, NE

M. Negahban
University of Nebraska Lincoln, Lincoln, NE

Abstract:

The Kolsky (or split Hopkinson) bar technique has been widely used for measuring the dynamic response of materials subjected to high strain-rate deformation. However, the applications of the Kolsky bar technique to soft and/or porous biomaterials have encountered a number of difficulties: insufficient pulse duration for very long equilibrating process and/or for very large strains necessary to initiate significant flow, poor signal-to-noise ratio due to very low stress response (less than 1.0 MPa), inhomogeneous sample deformation, plastic compaction, and fluid loss while compressing a material containing fluid. To address these issues, we have developed a new compressional Kolsky bar experiment. Instead of using conventional projectile impact, the new technique uses pre-compression and rapid release of part of the input bar to generate low-stress compression pulse with long pulse durations (up to 1.0 ms). The sample is confined in a steel collar so that materials containing fluid can also be tested and the sample deformation is macroscopically uniaxial strain. The use of large-diameter (25.4 mm) thin-wall aluminum alloy tube for the output bar increases significantly the signal-to-noise ratio at low stresses. Experimental results will be presented for several soft and/or porous biomaterials as well as animal tissues. Issues related to dynamic loading and measurement at very low stress levels, sample preparation, and effective prevention of reloading will also be discussed.
Mathematical Models for Creep and Relaxation in Collagenous Tissues

Raffaella De Vita
Virginia Polytechnic Institute and State University
230 Norris Hall, Blacksburg, 24061, US
Phone: 540 231-5905, Email: devita@vt.edu

Ratchada Sopakayang
Virginia Polytechnic Institute and State University, Blacksburg, VA

Abstract:

Collagenous tissues such as ligaments and tendons are characterized by long-term viscoelastic properties. They exhibit a slow continuous increase in strain over time, or creep, when subjected to a constant stress and a slow continuous decrease in stress over time, or stress relaxation, when subjected to a constant strain. Despite the large amount of experimental data collected to quantify creep and relaxation, the micro-structural origin of the long-term viscoelasticity of these tissues remains still unknown and continues to be a subject of debate in biomechanics. It has been suggested by Fung (1993) that creep and relaxation may be determined by the different micro-structural components of the tissues and by their mutual arrangement.

In this study, a simple micro-structural constitutive framework for parallel-fibered collagenous tissues is presented in order to describe their long-term viscoelasticity including nonlinear strain stiffening phenomenon. The collagen fibers, which make up these tissues, are assumed to be all oriented in the physiological direction of loading. They possess different straightening strains defined by a Weibull distribution function. After becoming straight the collagen fibers behave as linear elastic springs. The linear elastic springs are arranged in parallel with a Maxwell-type viscoelastic element that represents the contribution of the proteoglycan-rich matrix that surrounds the collagen fibers. Thus, the overall tissue’s stress is the sum of the stresses of the matrix and collagen fibers.

Relaxation and creep data collected on rabbit medial collateral ligaments by Hingorami et al. (2004) are used to compute the values of the model parameters and evaluate the predictive capabilities. The mathematical framework can successfully illustrate the relaxation and nonlinear strain-stiffening phenomenon and predict creep sufficiently well in parallel-fibered collagenous tissues. The results indicate that the recruitment of collagen fibers determines the response of the tissues during creep while the fluid-like matrix controls such response during relaxation.

References:
Active Porous Scaffolds for Controlled Drug and Cell Delivery

Xuanhe Zhao
Duke University
Department of Mechanical Engineering And Materials Sciences, Durham, 02138, US
Phone: 6172793934, Email: xz69@duke.edu

David Mooney
Harvard University, Cambridge, MA

Abstract:

Porous biomaterials have been widely used as scaffolds in tissue engineering and cell-based therapies. The release of biological agents from conventional porous scaffolds is typically governed by molecular diffusion, material degradation and cell migration, which do not allow for dynamic external regulations. We present a new active porous scaffold that can be remotely controlled by a magnetic field to deliver various biological agents on demand. The active porous scaffold, in the form of a macroporous ferrogel, gives a large deformation and volume change of over 70% under a moderate magnetic field. The deformation and volume variation allows a new mechanism to trigger and enhance the release of various drugs including Mitoxantrone and plasmid DNA from the scaffold. The porous scaffold can also act as a depot of cells, whose release can be controlled by external magnetic fields.
A Finite Element Method for Transient Analysis of Concurrent Large Deformation and Mass Transport in Gels

Hanqing Jiang
Arizona State University
Hanqing Jiang, Tempe, 85286, US
Phone: 480-965-1483, Email: hanqing.jiang@asu.edu

Abstract:

Long-chain polymers may crosslink by strong chemical bonds into a three-dimensional network. The resulting material, an elastomer, is capable of large and reversible deformation. The elastomer may imbibe a large quantity of solvents, aggregating into a gel. The solvent molecules in the gel interact by weak physical bonds and can migrate. The dual attributes of a solid and a liquid make the gel a material of choice in nature and in engineering, such as tissue engineering, drug delivery and soft MEMS.

Many processes in gels involve concurrent deformation and migration. For example, a drug loaded in a gel can migrate out in response to a change in the physiological conditions (i.e., the temperature, the level of pH, or the concentration of an enzyme). The rate of the release may be modulated by the deformation of the gel. As another example, patterns of crease often appear on the surface of a swelling gel, along with many other forms of buckling. Furthermore, swelling may induce stress localization in gels, which leads to cavitation and delamination. Hydrogels with sub-millimeter size have been extensively used as valves in microfluidics due to the short swelling time and large deformation.

This paper studies the concurrent deformation and migration in the gel by a finite element method. We combine the kinematics of large deformation, the conservation of the solvent molecules, the conditions of local equilibrium, and the kinetics of migration to evolve simultaneously two fields: the displacement of the network and the chemical potential of the solvent. The finite element method is demonstrated by analyzing several phenomena, such as swelling, draining and buckling. This work builds a platform to study diverse phenomena in gels with spatial and temporal complexity.
Sensor Behavior of Magneto-Rheological Elastomers

LeAnn Faidley

Iowa State University
Phone: 515 294-1692, Email: faidley@iastate.edu

Abstract:

Magneto-Rheological Elastomers (MREs) are composite materials of an elastomer matrix with a magnetic, micron-sized, powder filler. These materials have gained notoriety because they change stiffness substantially when exposed to a magnetic field giving them the capability of acting as a variable spring for numerous applications. Magnetic field induced strain has also been measured in these materials making them feasible as future actuator materials. However, the inverse effect involving a mechanically induced change in the magnetic properties of these materials has yet to be studied in great detail. This study presents the results of an experimental study of this sensor behavior. Sheets of 5 mm thick MRE are synthesized from silicone rubber (RTV6186) and carbonyl iron power with a diameter of 9 micrometers. The application of a magnetic field during the silicone curing process allows for the creation of samples with particles aligned along the length, width, and thickness of the sample as well as unaligned samples. These samples are then strained while exposed to various constant bias fields. The change in the internal magnetic properties of the sample as it is strained induces a voltage in a pickup coil that surrounds the sample. This voltage is found to closely track the applied strain-rate making these materials promising for large strain, strain-rate sensors. In this study this effect is described in detail both experimentally and theoretically. A mechanism is proposed to describe this sensing ability based on the magnetic interaction between filler particles that is established by the particle alignment and bias field and then changed as those particles are pulled apart when the sample is strained. This effect is enhanced by the change in volume of the sample that is contained in the pickup coil as it is deformed along its axis. The sensing ability of the material is characterized under tensile testing for samples of 4 different filler orientations. Testing variables include strain and strain-rate levels as well as basis field and sample geometry. Their behavior is characterized in terms of the strain-rate sensitivity, linearity, and repeatability. A full factorial design-of-experiments analysis is completed to fully characterize these dependencies.
Experimental Analysis of the Yield Surface of Divinycell H-100 Foam

Murat Vural  
Illinois Institute of Technology  
Mechanical, Materials & Aerospace Engineering Dept., 10 West 32nd St., Chicago, 60616, US  
Phone: 312-567-3181, Email: vural@iit.edu

Ravi S. Ayyagari  
Illinois Institute of Technology, Chicago, IL

Muhammad Shafiq  
Illinois Institute of Technology, Chicago, IL

Abstract:

Cellular solids constitute an important and emerging part of the pool of lightweight engineering materials with their potential advantages in a variety of applications ranging from protective packaging of delicate electronic components (e.g., cell phones) to crash and blast mitigation in automobiles, aerospace and naval structures along with unique multifunctional applications in biomimetic prostheses. There is a critical need to generate experimental data under biaxial as well as triaxial loading conditions to understand their mechanical and failure behavior not only from a design perspective under complex loading scenarios but also for experimental validation of yield criteria proposed in the literature. In this work, we will describe a new experimental tool called Multi-Axial Testing Apparatus (MATA) that we have recently designed and built to probe the yield surface of solid foams along multiaxial stress paths. The MATA uses three servo-hydraulic actuators along three orthogonal axes, three LVDTs, and three controllers along with a unique specimen test bed with six degrees of freedom that enables loading cellular specimens under uniaxial, biaxial and triaxial stress states in compression, tension and any possible combination of tensile-compressive stresses. Maltese-cross and cubic specimen geometries are successfully utilized to extract the yield data of transversely isotropic Divinycell H-100 foam along various stress paths including uniaxial, biaxial, hydrostatic tension and hydrostatic compression states. In order to determine the yield point in an unambiguous and consistent manner, characteristic stress-characteristic strain plots are generated from multiaxial test data and, then, offset technique is used to pinpoint the moment of yield. Experimental yield data are then analyzed in both principal stress space and also mean stress-effective stress space to better understand the physical basis of yielding in solid foams. Finally, experimental data are compared with the predictions of a new energy-based pressure-dependent yield criterion what we have recently proposed. Results show an almost excellent match between experimental data and model predictions. A few phenomenological yield criteria proposed in the literature are also compared to experimental data, and shortcomings of various models are discussed under the light of extensive experimental data that cover all quadrants in principal stress space for the first time.
Slipping Plane Plasticity using the Theory of Material Evolution

Ben Nadler
University of Alberta
5-8R Mechanical Engineering Building, Edmonton, T6G 2G8, CA
Phone: (780) 492 3487, Email: bnadler@ualberta.ca

Marcelo Epstein
University of Calgary, Calgary, AB

Abstract:

The physics of plasticity is related to the motion of dislocation which allows relative slipping along particular planes. In most cases the micro-scale motion of dislocations is not modeled explicitly, but rather a continuum approach is used. We adopt the continuum approach where the motion of dislocations yields a continuum-scale relative slipping.

The theory of material inhomogeneities is a general framework that addresses the question whether two material points are made of the ‘same’ material. For a body made of the ‘same’ material one can define the ideas of material uniformity, homogeneity and inhomogeneity, where the Eshelby stress tensor plays an important role. Material evolution can be viewed in a similar way by allowing the material inhomogeneity to evolve in time.

In this work the theory of material evolution is specialized to model plasticity as a shear-like material evolution along the slip plane associated with the motion of dislocation in the material microstructure. A simple constitutive model is introduced to demonstrate the inelastic (plastic) response governed by this approach. It is shown that perfect plasticity, hardening and softening responses can arise depend on the slipping plane orientation and the loading. Also, this approach is rate dependent which is different than the classic rate-independent plasticity.
A Four Element Model for the Dynamic Response of a Ferrogel under Cyclic Magnetic Fields

Yi Han
Iowa State University of Science and Technology
Department of Aerospace Engineering, Iowa State University, Ames, 50011-2271, US
Phone: 515-294-0089, Email: yihan@iastate.edu

Wei Hong
Iowa State University, Ames, IA

LeAnn Faidley
Iowa State University, Ames, IA

Sarah J Timmons
Iowa State University, Ames, IA

Abstract:

Ferrogels are polymer materials embedded with magnetic powder that drives the deformation in a magnetic field. Some predominant properties of ferrogels, like large strain, fast response, high energy densities, make these materials suitable for various actuator and sensor applications. However, the dynamic behavior of ferrogels are not yet characterized and fully understood. A series of experiments of these materials under various frequencies was carried out to study their dynamic properties. Based on experimental observation, we have developed a phenomenological model that couples the magnetic field with the dynamic response of the material. A simple model constructed by two springs and two dashpots can captures the behaviors of dynamic strains of a ferrogel specimen under cyclic magnetic fields. The prediction of the frequency dependence of the response by this model has a reasonable agreement to the experimental result.
Internal Fluctuation of DNA in Nanochannels

Tianxiang Su
University of Pennsylvania
229 Towne Building, 220 S. 33rd Street, Mechanical Engineering, University of Pennsylvania, Philadelphia, 19104, US
Phone: 2158983870, Email: tsu@seas.upenn.edu

Prashant K. Purohit
University of Pennsylvania, Philadelphia, PA

Abstract:
Stretching DNA in nanochannels is an important technique for performing DNA mapping [1]. On the other hand, it also serves as a simplified model for studying single polymer behavior in concentrated polymeric solutions and melts [2]. For these reasons, mechanical behaviors of DNA inside nanochannels have been of great interest to both experimentalists and theorists in recent years. To date, scaling laws for the behaviors of confined DNA in both the de Gennes and Odijk regimes have been well developed, widely used and tested [3,4]. However, fluctuation of the internal segments inside the DNA is still not well understood. This is important for genome mapping because it is the local fluctuation that determines the resolution of the mapping.

In this work, we study the internal fluctuation of confined DNA in nanochannels. We show that for a long DNA molecule whose contour length is much longer than its persistence length, the fluctuation versus mean value data collected from various locations along the polymer collapses onto a single curve with 0.5 power law. This can also be derived by a scaling theory. For short DNA, however, the scaling model fails and the data from different locations does not collapse onto a single curve. Following the framework in reference [5], a more detailed theory is developed. This theory models the DNA as a discrete wormlike chain in a confined channel. The confinement effects are taken into account by quadratic potentials and the internal fluctuation for the confined chain is evaluated.

Further, by considering different boundary conditions, regions that are most affected by the boundary effects are identified. Surprisingly, not all the internal segments close to the boundaries are strongly influenced by the boundary conditions. Fluctuations of short internal segments, for example, are not significantly affected even though they are located close to the boundaries. The model for short DNA is further verified by Monte Carlo simulations.

References:
Abstract:

Due to their unique electronic properties, carbon nanotubes (CNTs) are valuable candidates for applications in various areas. For example, it is shown that CNTs can be used as improved field-effect transistors (FETs) [1]; as well CNTs can deliver drugs to a particular area [2]. Prior to using CNTs in these applications, it is necessary to resolve the fundamental issue of dispersing and separating CNTs. Zheng et al. showed that using DNA molecules and the method of ion exchange chromatography (IEC), CNTs can be separated according to their electronic properties [3]. During the process of IEC, the negatively charged CNT-DNA hybrids elute from a positively charged surface; and it is experimentally observed that the metallic CNT-DNA hybrids elute earlier than the semiconducting ones. In this work [4], we develop a simplified model for the CNT-DNA hybrid. The DNA is a polyelectrolyte (PE) represented by a thin cylinder and the CNT is modeled as an electronically responsive cylinder of a larger radius, both immersed in an electrolyte solution. In our model, the PE-cylinder complex is located near an oppositely charged wall. We derive analytically tractable expressions for the binding force between the complex and the charged wall for different natures of the electronically responsive cylinder (metallic or dielectric). Our results show that the binding force for the PE-metallic complex is weaker than for the PE-dielectric complex, which agrees with experimental observations.

REFERENCES


Elastomers Embedded with Liquid Filled Microchannels for Sensing and Robotics
Abstract:
An elastomer embedded with microchannels of conductive liquid remains electrically conductive even when stretched to several times its natural length. Moreover, deforming the elastomer changes the electrical resistance and inductance of the embedded channels. Applications include stretchable electronics, hyperelastic strain sensing, and a mechanically tunable antenna.

Another potential application is pressure sensing, in which the electrical resistance of the conductive liquid channels is controlled by the location and intensity of pressure applied to the surface of the elastomer. Because of its low elastic stiffness, the pressure sensor remains functional when stretched and can be used in emerging technologies like wearable computing, flexible tactile interfaces, and soft orthotics. This is in contrast to existing pressure sensors and touch screens, which are composed of stiff inorganic materials and polymers that limit flexibility and/or stretch and prevent biomechanical compatibility.

Liquid filled elastomers for stretchable electronics and sensing may be fabricated from silicone rubber or polyurethane, which are cast in a 3D printed or soft lithography mold. Microchannels are filled with a eutectic, Gallium-Indium alloy (eGaIn), which is conductive and non-toxic. Liquid metals like eGaIn have a low electric resistivity, only one or two orders of magnitude greater than conventional copper and aluminum wires. Moreover, their electrical resistance and inductance follow the same mathematical principles that govern solid-state electronics.

The electronic characteristics of the liquid filled elastomer are controlled by the length, shape, and cross-sectional geometry of the microchannels. A complete predictive model for channel deformation requires mathematical theories for fluid mechanics and three-dimensional finite elasticity. Analysis may be performed with numerical solvers, such as the finite-element-method (FEM), or with approximate modeling techniques from linear elastic fracture mechanics (LEFM).

Additional functionality such as actuation and stiffness control may be possible by replacing eGaIn with electro- or magneto-rheological (MR) fluid. Such materials will have a potentially important role in active orthotics and related biomedical applications, soft robotics, and programmable, multi-functional materials.
A New Variational Procedure for Estimating the Behaviors of Soft Composites

Gal deBotton
Ben-Gurion University
Dept. Mechanical Engineering, P.O.B. 653, Beer-Sheva, 84105, IL
Phone: (972) 73 277 7105, Email: debotton@bgu.ac.il

Gal Shmuel
Mechanical Eng., Ben Gurion Univ., Beer Sheva, IL

Tal Oren
Biomedical Eng., Ben Gurion Univ., Beer Sheva, IL

Abstract:

Frequently soft natural and manmade materials are heterogeneous. The mechanical properties of soft biological tissues are dictated by a network of collagen fibers, and to improve their mechanical behaviors in many industrial applications rubbers are reinforced by stiffer fibers. The spatial distribution of the fiber network has a major impact on the overall response of these composites. Accordingly, a method for predicting the behaviors of these composites in terms of the fibers arrangement and properties is in need. In this work we study hyperelastic composites, and by application of a homogenization technique introduce a variational method for determining their effective strain energy-density function. The new method enables to determine estimates for composites with complicated behaviors of the phases in terms of available estimates for ”hyperelastic comparison composites”. For the class of composites with one family of fibers a recently developed estimate for uniaxial fiber composites with neo-Hookean phases is used. The end result is given in terms of a closed-form expression for the effective strain energy-density function from which the stress-strain relation are extracted analytically. To capture the lock-up effect that is associated with common collagenous tissues explicit estimates for the overall response of composites whose phases behaviors are governed by the Gent model are derived. The results are extended to the class of orthotropic composites with two families of fibers. The analytical predictions are compared with corresponding finite element simulations of periodic models for the composites. A fine agreement between the predictions obtained via the two estimation procedures is revealed even in the limit of large contrast between the properties of the phases.
Coupling of Localized Buckling Deformation and Optical Properties in 2D and 3D Soft Photonic Crystal Materials

Dwarak Krishnan
University of Illinois, Urbana-Champaign
158 MEB M/C 244, 1206 W. Green Street, Urbana, 61801, US
Phone: 2174179933, Email: dkrishn3@illinois.edu

Harley T. Johnson
University of Illinois, Urbana Champaign, Urbana, Illinois

Abstract:

Soft material photonic crystals (PCs) are novel periodic dielectric materials that can be used as optomechanically sensitive, highly flexible structures and devices. They can be fabricated by several processing techniques, including lithography, molding, or etching. Depending on the material used in the structure they can be functionalized by strain, pH, light, heat, or other stimuli. Such systems find use in bio-inspired devices and optomechanical sensing elements. In this work we report interesting pattern transformations facilitated by localized buckling inside 2D or 3D material systems due to applied strain, optical stimuli, or processing constraints. All of these effects change the optical behavior as a consequence of changes in periodicity and filling fraction of the PC.

Following on our work on large deformation and optical properties in 2D PCs [Krishnan and Johnson, JMPS, 2009], we report here on similar pattern transformations in 3D soft material systems undergoing large mechanical strain. In the first part, we analyze the shrinkage of a 3D PC structure patterned in SU-8 photoresist by means of holographic lithography. Our model accurately predicts localized buckling and twisting of ligament like interconnects that induces a macroscopic structural collapse [Chen et al., APL, 2007]. Optical transmittance simulations on the deformed structure correctly model the primary and secondary reflectance spectrum peaks as observed experimentally. In the second part, we analyze a pattern transformation observed in experiments on a swelling hydrogel based inverse FCC opal PC [Lee, Frei, Johnson and Braun, J. Phys. Chem., 2006] and we develop a poroelasticity based FEA model to capture the deformation mode. We also carry out optical transmittance calculations and are able to predict with good accuracy the shift in peak reflectance wavelength and values.

Finally, we introduce simulation evidence for a fully optomechanically coupled soft material PC: a novel azobenzene liquid crystal elastomer (LCE) based 2D PC that can be reversibly optically actuated. Incident light of a certain wavelength induces a trans- to cis- isomerization inside the material in regions experiencing localization of the incident energy. This causes a macroscopic contraction of the structure, a shift in periodicity, and thus a modulation of the optical transmittance through a shift in the photonic bandstructure. We demonstrate that through this mechanism, the material can be made to undergo a fully optomechanically coupled cyclic deformation under steady illumination.
Wave Propagations in Pre-deformed Nonlinear Viscoelastic Materials

Lili Zhang
University of Nebraska-Lincoln
371W Charleston St. 432D, Lincoln, 68528, US
Phone: 402-730-3594, Email: lzhang0528@gmail.com

Jonathan Hein
University of Nebraska Lincoln, Lincoln, NE

Ashwani Goyal
University of Nebraska Lincoln, Lincoln, NE

Mehrdad Negahban
University of Nebraska Lincoln, Lincoln, NE

Y. Wen
University of Nebraska Lincoln, Lincoln, NE

Abstract:

Soft materials are normally non-linear rate-dependent materials. The study of wave propagation properties in such viscoelastic materials under complex finite pre-deformations may be of importance for many applications including the study of human tissue, including the study of injury resulting from improvised explosive devices. This is particularly important since the natural state of many types of human tissue is in a pre-deformed state and the response is viscoelastic. We construct the response from a nonlinear viscoelastic model that is based on a continuous array of parallel relaxation systems. We then study the response through perturbations on pre-deformed configuration. In doing so, we study the development of anisotropic wave motion resulting from the pre-deformation. As particular examples we look at a model constructed two relaxation systems.

Keywords: nonlinear viscoelastic, wave propagation, pre-deformation, anisotropy
An Energy-Based Approach to Capture the Yield Surface of 3D Anisotropic Solid Foams

Murat Vural
Illinois Institute of Technology
Mechanical, Materials & Aerospace Engineering Dept., 10 West 32nd St., Chicago, 60616, US
Phone: 312-567-3181, Email: vural@iit.edu

Ravi S. Ayyagari
Illinois Institute of Technology, Chicago, IL

Abstract:

Solid foams are low impedance materials which are extensively used in diverse engineering applications because of their lightweight, high specific energy absorption capacity, and highly porous architecture that lends itself to multifunctional tasks. Rapid growth in the use of cellular materials necessitates the development of predictive models that capture the initiation and progression of inelastic deformations under not only uniaxial but also complex biaxial and triaxial loading paths. Unlike the majority of bulk engineering materials, cellular solids are often anisotropic and their mechanical response is sensitive to hydrostatic stresses. The present work hypothesizes that yielding of solid foams is governed by total elastic strain energy density and proposes a pressure-dependent yield criterion for transversely isotropic cellular solids. The energy based analytical framework, homogenized to account for material anisotropy, also allows defining new scalar measures of work conjugate stress and strain, called characteristic stress and characteristic strain. These new stress and strain measures play a dominant role in the mechanical response of anisotropic solid foams under multiaxial stress paths in way similar to von Mises effective stress and equivalent strain do in the mechanical behavior of isotropic metals. They are also capable of representing the elastic response of transversely isotropic pressure dependent foams with a unified elastic master line under multiaxial loading. The proposed energy based yield criterion uses elastic constants and yield strengths under uniaxial loading, and does not rely on any arbitrary parameter. It is also demonstrated that it reduces to Deshpande-Fleck phenomenological yield criterion in the special case of isotropic foams.

It is further shown that the pressure dependence in proposed yield criterion is realized through a quadratic mean stress term inherent to energy based approach. However, we have recently obtained extensive computational and experimental evidence showing that yield behavior of solid foams exhibits linear pressure dependence as well. Therefore, proposed yield criterion is extended to include linear pressure dependence, and the physical mechanisms at cellular scale that cause this linear dependence is discussed in relation to subtle variations in load sharing and microstructural deformation modes under hydrostatic tension and compression.
A Thermodynamic-Based Framework for Modeling the Coupled Viscoelastic, Viscoplastic, and Viscodamage Behavior of Soft Materials

Masoud Darabi
Texas A&M University
Zachry Department of Civil Engineering, Texas A&M University, College Station, 77843, US
Phone: 979-739-7504, Email: masouddrb@neo.tamu.edu

Rashid K. Abu Al Rub
Texas A&M University, College Station, Texas

Abstract:

Soft materials show a wide range of different responses depending on temperature, strain rate, and loading conditions. For example, the elastic response could be dominant at low temperatures and low stress levels. However, these materials show viscoelastic and viscoplastic responses at higher temperatures and stress levels. The solid-like viscoelastic models where the viscoelastic strain recovers after large rest periods are usually used for constitutive modeling of solids, whereas the fluid-like viscoelastic models where the viscoelastic strain is not recoverable are usually used for constitutive modeling of fluids. However, depending on the temperature both responses are expected for soft materials. Hence, to accurately model the mechanical response of soft materials, a general constitutive model that can be used at different temperatures and for different loading conditions should be developed. Therefore, in this work we present a general thermodynamic framework that can be followed systematically to derive different viscoelastic, viscoplastic, and anisotropic viscodamage models. It is also shown that an accurate estimation of rate of energy dissipation requires the decomposition of all conjugate forces into energetic and dissipative components. The energetic components should be determined using the Helmholtz free energy, whereas the dissipative components should be determined from the maximum rate of energy dissipation principle. Different mathematical forms are postulated for Helmholtz free energy function and rate of energy dissipation that lead to derivation of different constitutive models. Finally, the general framework is used for deriving well-known viscoelastic models (such as Kelvin-Voigt, Maxwell, generalized Maxwell, and Burger’s models), and different plastic/viscoplastic and anisotropic (visco)damage models.
A Theory of Actuation of Ionic Polymer Conducting Network Composite

Xiao Wang
Iowa State University
Hoover 3313-H2, Ames, 50011, US
Phone: 515-294-3933, Email: xiao@iastate.edu

Wei Hong
Iowa state university, Ames, IA

Abstract:

Ionic polymer conductor network composite (IPCNC) consists of a polyelectrolyte membrane with films of porous electrode composite network on both faces. It is capable of swelling and deswelling in response to the change in electric fields. Due to the large interface area between the network of charged polymer and the network of porous electrode, the actuation strain results from the confined swell in the sandwiched structure is large comparing to that of traditional ionic polymer composites (IPMC). Such an active property is mainly due to the electric double layer that forms at the electrode-solution interface and creates a combined electro-chemical driving force for the interstitial solvent and solution molecules. The migration of particles changes the swelling ratio, leading to macroscopic deformation. To study the coupled electro-chemo-mechanical process, we introduce a homogenized material model that bridges the microscopic details with the macroscopic quantities. By doing so, we model the system within the framework of a newly developed continuum theory of polyelectrolyte gels. The governing equations of the system are derived from the principle of virtual work. By solving the field equations in a quasi-static state, we calculate strain response with respect to actuating potential and exam the crucial role of asymmetric ion sizes in achieving effective actuation strains. Also, in order to understand the mechanisms of instantaneous actuation and relaxation behaviors, the diffusion controlled transient state is studied. This model extends the existing de Levei model for super capacitors by incorporating the coupling of finite deformation. In the limiting case of zero polymer content, our model recovers the phenomenological theory on supercapacitors. With more realistic free energy functions, the theory can easily be modified to be adapted to other systems with similar phenomena.
Experimental Techniques for Multiphysics and Multiscale Analysis

ORGANIZERS:

Sriram Sundararajan, Iowa State University
Three-Dimensional Imaging of Crystal Structure via Atom Probe Tomography

Scott Broderick
Iowa State University
2220 Hoover Hall, Iowa State University, Ames, 50011, US
Phone: 515-520-7617, Email: srbroder@iastate.edu

Krishna Rajan
Iowa State University, Ames, IA

Abstract:
Atom probe tomography (APT) is a revolutionary characterization tool that can provide near atomic scale imaging of materials in three-dimensions, while detecting the chemical identity of the atom. The advent of the local electrode atom probe (LEAP) has enabled higher rates of data acquisition and an increased field of view compared to other variants of three dimensional atom probes. The primary limitation with APT is the detection efficiency, with typically only 50-60% of the atoms being properly captured. This limited detection efficiency results in difficulty in extracting structural information from APT data. We describe two different approaches to address this limitation via informatics: (1) improve determination of structure from available data by developing enhanced spatial distribution maps and (2) improve detection efficiency of APT by mapping relationships between instrument, material, and detection.

Spatial distribution maps (SDM) provide a real-space frequency distribution from which lattice planes for some systems can be identified. However, for other systems noise and aberrations introduce too much noise into the SDMs so that structure cannot be determined. To capture the information embedded within the SDMs, there is a necessity to device a mathematical framework that de-convolutes the several factors that affect the quality of the SDMs. In our approach, we de-convolute the SDMs to classify the data as structurally relevant, noise or aberrations. We accomplish this by correlating the inter-atomic frequency distributions obtained from the spatial distribution map approach using a well established statistical technique, namely the singular value decomposition. We further extend our approach to refine the structural information obtained using the SDMs. To improve detection efficiency, the high-dimensional relationship between instrument parameters, material, and number of ions per evaporation event can be mapped. This mapping across millions of atoms provides the optimum operating conditions so that the detection efficiency can be improved. Both of these approaches develop a mathematical procedure to enhance structural information captured by the atom probe.
Characterization of the Chemistry and Structure of Transfer Films at the Nanoscale

Chris Tourek
Iowa State University
2025 Black Engineering, Ames, 50010, US
Phone: 5152940365, Email: ctourek@iastate.edu

Sriram Sundararajan
Iowa State University, Ames, Ia

Abstract:

Atomic force microscopy (AFM) is used extensively to investigate tribomechanical phenomena on the micro and nano scales. The ability to characterize the structure and chemistry of transferred or newly generated material at the near-apex regions of AFM tips can provide new insights into a range of interfacial phenomena including friction, wear and corrosion. Atom probe tomography (APT) is a technique capable of concurrently determining three dimensional material structure and chemistry at near atomic resolution which has seen expanding use in science and engineering fields. Typical AFM tips can have a conical tip with a tip radius less than 100nm that makes them suitable for analysis by atom probe tomography (APT). By utilizing a suitable holder an AFM tip can be analyzed using APT and 3D reconstructions of the atom positions in the near apex region of the AFM tip can be obtained. We present our investigations utilizing a Local Electrode Atom Probe (LEAP) to study the formation of transfer films during dry sliding experiments involving a Si tip on Cu. The effects of sliding distance and normal load on the formation of transfer film are reported.
In-situ Reconstruction of Tip-sample Interactions for Atomic Force Microscope

David Busch
Iowa State University
1101 Iowa Ave, Ames, 50014, US
Phone: 515-571-6558, Email: eecemath@iastate.edu

Juan Ren
Iowa State University, Ames, Iowa

Qingze Zou
Iowa State University, Ames, Iowa

Baskar Ganapathysubramanian
Iowa State University, Ames, Iowa

Abstract:

The Atomic Force Microscope (AFM), has proven to be a versatile tool in analyzing samples on the micro / nano scale. However, the AFM is limited in its ability to analyze soft aqueous biological material in contact mode. This limitation stems from the difficulty of controlling tip-sample interaction forces. If the tip-sample forces are too small than the signal-to-noise ratio is too small to attain usable data and if the tip-sample forces are too large, the soft biological sample will be destroyed.

With the goal of eventually controlling the tip-sample interaction forces to (a) maximize the signal-to-noise ratio while (b) keeping the force small to prevent sample destruction, a fast reconstruction strategy is developed to accurately extract the tip-sample interaction forces in-situ. The reconstruction problem is posed as an inverse problem. The inverse problem estimates the optimal tip-surface interactions that generate the experimentally observed deflections by solving an optimization problem. A computational model of the AFM cantilever dynamics that include tip-sample interactions, hydrodynamic interactions and base vibrations serves as the direct problem on which the reconstruction strategy is based upon. In-situ reconstruction is achieved by ultra-fast cantilever dynamics and optimization solves by implementing the complete framework on a Graphical processing unit (GPU) utilizing parallel algorithms.

The computational and experimental challenges and insight gained during this process will be discussed. Various cost-functionals investigated in the reconstruction procedure will be showcased and contrasted. Finally, the framework is validated by constructing the tip-sample interaction forces in two complementary systems: stiff easy to analyze samples and a soft aqueous biological material. When completed, this proposed control system will improve the AFM’s ability to analyze aqueous biological material.
An Atomic Force Microscope-Based Technique to Determine Hamaker Constants of Finely Ground Materials

Gilson Lomboy
Iowa State University
136 Town Engineering Building, Iowa State University, Ames, 50011, US
Phone: 515-294-2252, Email: grlomboy@iastate.edu

Sriram Sundararajan
Iowa State University, Department of Mechanical Engineering, Ames, IA

Kejin Wang
Iowa State University, Department of Civil, Construction and Environmental Engineering, Ames, IA

Shankar Subramaniam
Iowa State University, Department of Mechanical Engineering, Ames, IA

Abstract:

A method for determining adhesion forces and Hamaker constants of finely ground materials using atomic force microscopy (AFM) is presented. The materials tested are finely ground (5-40um) SiO2 and CaCO3 as well as Type I Portland Cement. The particles were first mixed in fast set epoxy and cured on a slide. The particle-epoxy composite was then polished flat using sandpaper with grits of 150, 400, 800, 1000, 2000. The surfaces of the sanded particles had roughness of 23.2 to 7.6 nm on a 5 um scan. The pull-off forces in dry air were measured between the ground particles and a silicon nitride tip. From the pull-off forces, the work of adhesion and Hamaker constants were calculated based on the Johnson, Kendall and Roberts (JKR) and/or by the Derjaguin, Muller and Toporov (DMT) models. An uncertainty analysis was performed to qualify the results. The factors considered in the analysis were machine resolution, cantilever stiffness and tip diameter determination, inter-atomic cut-off distance and pull-off deflection. The results are consistent with those obtained from calculation using dielectric spectral data reported by other researchers. This method thus allows for experimental determination of the Hamaker’s constant for ground materials which can subsequently inform modeling efforts to predict mesoscale and macroscale properties of multiphase materials such as fresh concrete/cement paste.
TRACK 3

Fluid Mechanics
Symposium on Nonlinear Mechanics in Celebration of the 60th Birthday of K. R. Rajagopal

ORGANIZERS:

Arif Masud, University of Illinois at Urbana-Champaign

Alan Wineman, University of Michigan
Comments on the Career of Professor KR Rajagopal

Alan Wineman
University of Michigan
Department of Mechanical Engineering, Ann Arbor, MI, 48109, US
Phone: 734-936-0411, Email: lardan@umich.edu
Modeling and Simulation of Magnetoelastic Membranes

David Steigmann
University of California
6133 Etcheverry Hall, University of California, Berkeley, 94720, US
Phone: 510-684-5380, Email: steigman@me.berkeley.edu

Matthew Barham
Lawrence Livermore National Laboratory, Livermore, CA

Dan White
Lawrence Livermore National Laboratory, Livermore, CA

Abstract:

An asymptotic model for thin magnetoelastic films is described. This is used to describe, to leading order in thickness, the nonlinear deformation and magnetization fields existing in a thin body in equilibrium. The model is illustrated through numerical simulations.
Numerical Solutions in Nonlinear Magnetoelasticity

Luis Dorfmann
Tufts University
Tufts University, 200 College Avenue, Medford, 02155, US
Phone: 617-6276137, Email: luis.dorfmann@tufts.edu

Ray Ogden
University of Glasgow, Glasgow, UK

Abstract:

Recently, growing interest in the mechanical and the electromagnetic properties of composites consisting of an elastomeric matrix and a distribution of ferrous micron-sized particles embedded within their bulk has been observed. This interest is motivated by newly developed engineering applications, which involve, for example, sensors, vibration absorbers, and controllable membranes for use in civil and automotive engineering. These materials have mechanical properties that can be altered rapidly by a change in the magnitude or direction of an applied magnetic field.

In this talk we use numerical solutions to analyze representative boundary value problems with finite geometry and solve the governing equations in the material and surrounding space, paying particular attention to the magnetic continuity conditions. We show that the magnetic field cannot be uniform throughout since the boundary conditions on the ends would be incompatible in such circumstances. The distribution of the magnetic field components throughout the body and the surrounding space is determined in order to quantify the extent of the edge effects for both simple shear of a slab and extension and inflation of a circular tube.

To model the nonlinear magneto-mechanical coupling of magneto-sensitive bodies we adopt a formulation based on a total energy function, given in terms of a magnetic field vector (the magnetic field or the magnetic induction) and the deformation gradient tensor. Selected references are the papers by Borcea and Bruno (2001), Bustamante et al. (2007, 2008), Dorfmann and Ogden (2003, 2004a, 2004b, 2005), Kankanala and Triantafyllidis (2004) and Steigmann (2004, 2009).

References:
Mathematical Modeling of a New Class of Elastic Bodies

Roger Bustamante
Universidad de Chile
Departamento de Ingenieria Mecanica, Beaucheff 850, Santiago Centro, Santiago, NA, CL
Phone: 56-2-9784543, Email: rogbusta@ing.uchile.cl

Abstract:

The class of elastic bodies is larger than Cauchy and Green elastic materials. Recently, Rajagopal and co-workers have proposed some implicit constitutive relations for non-dissipative bodies, for which Cauchy and Green elastic bodies are a subclass (see, for example, [1,2]). Using this theory on implicit constitutive relations for elastic materials, Bustamante and Rajagopal [3,4,5] have considered the special case when for elastic bodies the norm of the displacement gradient is assumed to be small, but the relation between strain and stresses is in general nonlinear. In that case, where we have ‘small deformations’ but a nonlinear constitutive relation, it has been demonstrated that the correct form for the constitutive equations should be to express strains as functions of stresses.

We present a general overview of the theory for this new class of elastic bodies, in particular the derivation of the main equations from the theory of implicit constitutive relations. Thereafter, we show the boundary value problem to be solved with some simple examples. A weak formulation for plane problems is also presented and a subclass for these elastic bodies, where there exists a scalar function similar to Green elastic material, is defined.

References
Torsional Divergence of Wings with Nonlinear Viscoelastic Oscillator Properties

Harry H. Hilton
University of Illinois at Urbana-Champaign (UIUC)
104 South Wright Street, 316 Talbot La., MC-236, Urbana, 618012935, US
Phone: 217-333-2653, Email: h-hilton@illinois.edu

Abstract:

The linear torsional divergence problem of viscoelastic wings was first investigated in [1]. It was followed by a limited number of other publications, which are summarized in [2], where the analyses are extended to cover flutter and combined chord wise bending and torsion. In [3] a study was presented on the open loop response and stability of nonlinear viscoelastic oscillators that have elastically equivalent Duffing, Mathieu, Rayleigh, Roberts, van der Pol, etc., mechanisms.

In the present formulation, the viscoelastic shear relaxation modulus is assigned behavioral responses akin to the nonlinear oscillators of [3]. The span wise and chord wise spatial variations are removed by the application of Galerkin’s method. Thus, an ordinary governing closed loop integro-differential equation is realized for the twist angle that is only time dependent.

Nonlinear quasi-static aerodynamic forces are represented in the form of the stall angle. The inertia term is in response to the time dependent viscoelastic properties. It has been shown to lead to significant contributions in the case of linear and nonlinear creep buckling of columns with similar governing relations [4]. This governing equation is solved numerically using MATLAB™ and results are presented for parametric studies associated with the various nonlinear oscillators. Since analytical solutions of this relation are not achievable, no general conclusions can be drawn from the numeral studies.

References:
Mixture Theory to Study Blood Flow

Mehrdad Massoudi
U. S. Department of Energy
P. O. Box 10940, Pittsburgh, 15236, US
Phone: 412-386-4975, Email: MASSOUDI@NETL.DOE.GOV

Jeongho Kim
Carnegie Mellon University, Pittsburgh, PA

Samuel J. Hund
Carnegie Mellon University, Pittsburgh, PA

James F. Antaki
Carnegie Mellon University, Pittsburgh, PA

Abstract:

In this paper we use a modified form of the Mixture Theory to study the blood flow in a simple geometry, namely flow between two flat plates. In this case, the blood is assumed to behave as a two-component mixture comprised of plasma and red blood cells (RBCs). The plasma is assumed to behave as a linear viscous fluid, whereas the RBCs are given a granular-like structure where a simplified form of the model proposed by Massoudi and Rajagopal is used where the viscosity is now also depends on the shear-rate. The interaction forces included in the present study are the drag and lift forces, and a force due to volume fraction gradient. All thermo-chemical effects are ignored.
Modeling and Simulation of Light Activated Shape Memory Polymers

I. Joga Rao
New Jersey Institute of Technology
Department of Mechanical and Industrial Engineering, Newark, 07102, US
Phone: 935965601, Email: raoi@njit.edu

Abstract:

Traditionally Shape Memory Polymers (SMP’s) have used temperature induced phase changes in the polymer to trigger the shape change in the polymer. Newer SMP’s have been developed recently that use different methods of actuation. Light Activated Shape Memory Polymers (LASMP’s), as the name suggests use light to actuate the shape change. LASMP’s have photosensitive molecules grafted on their polymer chains. These photosensitive molecules, when exposed to light at certain wavelengths, form covalent bonds that act as cross links to give this class of SMP’s their temporary shape. On exposure to light at a different wavelength these bonds cleave and the material returns to its original shape. Advantages of LASMP’s over first generation SMP’s such as remote activation and selective exposure open up a whole new range of possibilities for their applications.

Our research concentrates on modeling and analyzing the mechanics of these special LASMP’s. To model the mechanics of LASMP’s we need to be able to characterize different aspects of this material. Starting with models for the original virgin network with a single stress free state and after exposure to light, models to capture the behavior with two or more competing networks with their own stress free states. In addition to this we need to model the initiation criterion, indicating the onset of the formation of the second network and the rate and degree to which this takes place. In a similar manner we need to model the reverse transition resulting in the dissolution of the second network. The models are developed using the framework of multiple natural configurations. The model is then used to simulate results for specific boundary value problems, for both homogenous and inhomogeneous deformations. In addition we will explore more complex shape memory cycles that can be formulated using these materials, in particular cycles which involve sequential exposure and deformation of the polymer.
Phase Field Theory for Phase Transformations at Large Strains and with Surface Effects

Valery Levitas
Iowa State University
Phone: (515) 294-9691, Email: vlevitas@iastate.edu

Abstract:

Using the first and second law of thermodynamics, phase field equations for the description of phase transformations are derived for finite strains and lattice rotations. A criterion for the instability of a crystal lattice with respect to a change in order parameters is formulated for homogeneous states. An explicit relation for lattice rotation is derived. The Landau potential for multivariant displacive phase transformations is formulated in terms of elastic strain, temperature, and order parameters for the most general case of large rotations, elastic and transformational strains, as well as nonlinear and different elastic properties of phases [1]. For small elastic strains, essential simplification of the theory is achieved and the explicit expression for Gibbs potential is obtained [2]. The phase equilibrium and phase transformation conditions are obtained as well. The above theory represents generalization of our small strain theory [3,4] for general geometrically nonlinear case and it satisfies all the same conditions necessary for conceptually correct description of the effect of stress tensor and temperature on martensitic phase transformations. Martensitic phase transformations in NiAl, BN and C are analyzed and the importance of finite-strain corrections is demonstrated. Then this theory was further generalized to incorporate description of the surface effects [5]. Fully geometrically nonlinear formulation is crucial for this generalization, even if strains are small. The generalization includes introducing the surface tension at the internal interfaces and external surface, correct description of the variant-variant interface energy, as well as description of phenomena related to the variation of the energy of the external surface during phase transformations. Various examples of finite element simulations of surface-induced phenomena for solid-solid and solid-liquid phase transformations are presented. A similar approach can be applied for twinning and dislocations.

A New Formulation of Elasticity Theory

Yi-chao Chen
University of Houston
Department of Mechanical Engineering, University of Houston, Houston, 77204-4006, US
Phone: 713-743-4533, Email: chen@uh.edu

Abstract:

The classical theory of continuum mechanics is based on two axioms, one of which claims that the stress at a material point in a continuum is determined by the deformation histories of the continuum. In particular, for an elastic material, the stress tensor at a material point is a function, called response function, of the deformation gradient at the material point. The response function must satisfy certain conditions, such as objectivity. Other conditions are required by hyperelasticity, by internally constraints, or by material symmetries.

There are certain theoretical, experimental, and numerical values to develop a constitutive theory for elastic materials, in which the deformation gradient depends on the stress. In this paper, we present such a theory that is fully compatible with the classical elasticity theory without imposing additional assumptions. Among other things, the response function in the classical theory is not necessarily invertible. By using the concept of multi-valued functions, we define the inverse relation of the response function, yielding a deformation response function, which maps a stress to a family of deformations that correspond to the stress. The deformation response function may be multi-valued.

Various aspects of the deformation response function are studied. The objectivity, the hyperelasticity, the internal constraints, and the material symmetry are formulated for the deformation response function. It is found that the objectivity requires that the deformation response function is invariant under rigid body rotations. This implies that the deformation response function is completely determined by its restriction on a sub-domain which is mapped to symmetric tensors. For hyperelastic materials, the deformation response function can be derived from an energy function. In the context of thermodynamics, this energy function corresponds to the Gibb's energy, while the strain energy function in the classical elasticity theory corresponds to the Helmholtz energy. For an internally constrained material, the response function in the classical elasticity determines only the active part of the stress. The deformation response function in the present theory, on the other hand, determines the generator of an equivalent class of deformation gradients. The equivalent classes for incompressible materials and for inextensible materials are derived. Material symmetry can be expressed using the symmetry group of the stress tensors. The deformation response functions for common classes of anisotropic materials are discussed.
Nonlocal Gradient-Dependent Constitutive Model for Simulating Localized Damage and Fracture

Rashid Abu Al-Rub
Texas A&M University, 3136 TAMU, 710 B CE/TTI Building, College Station, 77843, US
Phone: 9798626603,   Email: rabualrub@civil.tamu.edu

Anthony N. Palazotto
Air Force Institute of Technology, Dayton, Ohaio

Abstract:
Understanding the constraints and limitations of various potential hull structure materials and armor is paramount in design considerations of future civil and military lightweight, safe, and energy efficient vehicles. Developing and applying theoretical and computational models that guide the development of design criteria and fabrication processes of impact/ballistic-resistant material are therefore essential. The ultimate objective is to develop and field a contingency armor that is thin and lightweight, but with a very high level of overpressure protection system that provides low penetration depths. Therefore, performing accurate computational modeling and simulation of the ballistic response of civil and fighting vehicles made of high performance materials under impact loading conditions is invaluable. However, as soon as material failure dominates a deformation process, the material increasingly displays strain softening (localization) and the finite element computations are considerably affected by the finite element (or other numerical method) mesh size and alignment and gives non-physical descriptions of the damaged regions and failure of solids. This study is concerned with the development and application of a novel coupled nonlocal thermo-hypoelasto-viscoplastic and thermo-viscodamage constitutive model within the laws of thermodynamics in which implicit and explicit intrinsic material length scale parameters are incorporated through the nonlocal gradient-dependent viscoplasticity and viscodamage constitutive equations. In formulating the viscoplasticity constitutive equations, the effective plastic strain (for isotropic hardening) and plastic strain tensor (for kinematic hardening) in addition to their first-order gradients are assumed as internal state variables. It is shown that the principle of virtual power can be used to derive nonlocal plasticity yield and damage growth microscopic balance laws and their corresponding microscopic boundary conditions at free surfaces, interfaces, and elastic-defect moving boundaries. Also, in order to correctly estimate the rate of energy dissipation, the thermodynamic conjugate forces are decomposed into energetic and dissipative components. The energetic components are derived by assuming a form for the Helmholtz free energy whereas the dissipative components are derived by assuming a form for the rate of energy dissipation. Moreover, the thermodynamic laws for the dissipative components are derived based on the maximum energy dissipation principle. Finally, it is shown through simulating plugging failure in ballistic penetration of high-strength steel targets by blunt projectiles that the length scale parameters in the nonlocal equations play the role of localization limiters allowing one to obtain meaningful values for the ballistic limit velocity (i.e. the minimum projectile impact velocity for complete perforation of the target) independent of the finite element mesh density. On the other hand, when classical (local) constitutive equations are used, the ballistic limit is highly mesh-dependent.
Stabilized Finite Element Methods for Incompressible Viscoelastic Fluids

Arif Masud
University of Illinois at Urbana-Champaign
3110 Newmark Civil Engineering Laboratory, MC-250,
205 North Mathews Avenue, Urbana, 61801-2352, US
Phone: 217-244-2832,

JaeHyuk Kwack
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

We present a new stabilized finite element method for modeling non-Newtonian viscoelastic flows of complex fluids described by the Oldroyd-B model. The weak forms of the momentum, continuity and constitutive equations are cast in the VMS framework that leads to a two-level description of the problem. The ensuing nonlinear stabilized form is presented and the consistent tangent is derived. Numerical convergence of the proposed method on uniform and distorted meshes that are composed of linear triangles, bilinear quadrilaterals, quadratic triangles and biquadratic quadrilaterals are presented. Numerical stability of the method at high Weissenberg numbers is investigated through the steady-state 4:1 planar contraction flow problem and numerical results are validated via comparison with published numerical results for the Oldroyd-B model.
On Unsteady Non-homogenous Flows of Incompressible Fluids

Mehrdad Massoudi
U. S. Department of Energy
National Energy Technology Laboratory (NETL), Pittsburgh, 15236, US
Phone: 412-386-4975, Email: MASSOUDI@NETL.DOE.GOV

Ashwin Vaidya
Montclair State University, Montclair, NJ

Abstract:

Researchers investigating flows of non-Newtonian fluids often use the power-law constitutive relation. Although the power-law model adequately fits the shear stress and the shear rate measurements for many non-Newtonian fluids, it cannot be used to accurately describe phenomena such as ‘die-swelling’ and ‘rod-climbing’ which are manifestations of the stresses that develop orthogonal to planes of shear in the flow of these complex fluids. In general non-Newtonian fluids differ from Newtonian fluids in at least two ways: (1) they exhibit normal stress effects, such as rod-climbing and die-swell; and (2) they exhibit shear-thinning or shear-thickening which is the decrease or increase in viscosity with increasing shear rate, respectively. Both of these phenomena introduce non-linearities into the equations.

The non-linear time-dependent response of complex fluids (such as drilling fluids, coal-water slurries, electro-rheological fluids, polymers) constitutes an important area of mathematical modeling of non-Newtonian fluids. For many practical engineering cases, where non-linear fluids such as paints, slurries, etc. are used, the shear viscosity can be a function of one or all of the following: Time; shear rate; concentration; temperature; pressure; electric field; magnetic field. Thus in general, \( \eta = \eta(t, \dot{\gamma}, \alpha, \theta, \Omega, p, E, B) \) where \( t \) is the time, \( \dot{\gamma} \) is some measure of the shear rate, \( \alpha \) the temperature, \( \Omega \) the concentration, \( p \) the pressure, \( E \) the electric field, and \( B \) the magnetic field. Of course, in certain materials or under certain conditions, the dependence of one or more of these can be ignored. In general, one can classify these fluids as non-homogenous fluids where the viscosity is given by an equation of the type.

In this presentation we will discuss a simple constitutive relation for a non-homogenous fluid and attempt to provide numerical solutions to the unsteady flow of such a fluid between two flat plates.
On the Flow of Maxwell Fluid with Relaxation Time and Viscosity Depending on Pressure

Satish Karra
Texas A&M University
200 Charles Haltom Avenu #7E, College Station, 77840, US
Phone: 925-963-5806, Email: satkarra@tamu.edu

Abstract:

The flow of a variant of the well known Maxwell fluid is studied wherein the material parameters (relaxation time and viscosity) are chosen to depend on pressure. Although several experiments suggest that the material parameters of a viscoelastic fluid can depend on pressure, especially for certain geomaterials and polymers, such a dependence is usually not considered in modeling. In this work, a simple boundary value problem which is a variant of the Stokes' problem is solved by assuming that the material parameters depend on pressure, and the results are compared to the classical Maxwell model.
Fluid Dynamics of the Deepwater Horizon Spill

Albert Kirwan
College of Earth, Ocean, and Environment, University of Delaware
Robinson Hall, University of Delaware, Newark, 19711, US
Phone: 302-831-2977, Email: adk@udel.edu

T. Özgökmen
University of Miami, Miami, FL

P. F. Fischer
Argonne National Laboratory, Waterfall Glen Preserve, IL

P. Hogan
Naval Research Laboratory, Stennis, MI

H. S. Huntley
University of Delaware, Newark, DI

B. L. Lipphardt, Jr.
University of Delaware, Newark, DI

Abstract:

Prediction of the movement of the Deepwater Horizon spill presents several fundamental challenges to fluid dynamicists. The spatial scales of the phenomenon span at least 8 orders of magnitude. The oil at the ocean surface behaves as a non-Newtonian fluid, whereas the underlying seawater is treated as a turbulent Navier Stokes fluid. The surface oil slick alters in unknown ways the surface stress boundary condition, dispersants affect the response of the predictive models to wind and current forcing, and the surface slick ages in a natural environment so that there is considerable change in its colligative properties. The fluid emanating from the leaks is a volatile mixture of oil and gas at extremely high temperatures and pressures. The pressure jump at the seabed and the cold subsurface waters causes considerable condensation of the gases as the plume rises 1600 meters through the water column. Modeling this is a difficult problem in multi-phase flow. At the same time the spill has provided a plethora of unique data to study in detail these processes and to assess spill model predictions. This is a preliminary report from a consortium of investigators from four institutions who have been studying this event. We compare simulations of the spill horizontal surface movements from several operational data assimilating general circulation models. Using Lagrangian analysis methods derived from dynamical systems theory we compare model predictions of slick movements with in situ data from drifting buoys and with sequential images of the slick. None of the models account for non-Newtonian behavior or for the multi-phase flow nature of the spill. Even though the models have comparable resolution and assimilate the same data they show surprisingly large differences in the spill area. Despite this, and the fact that the spill evolution is a Lagrangian problem while the models are Eulerian, they account reasonably well for many of the observations. In order to further our understanding of the processes taking place during the vertical rise of the plume, highly-resolved computations are carried using a non-hydrostatic spectral element model. This model does not contain multi-phase flows or
chemical reactions associated with oil-gas mixtures, but it is aimed at understanding the behavior of buoyant plumes interacting with sub-mesoscale oceanic flows. Results are presented quantifying the differences between surface and subsurface dispersion, and plume behavior after its source is shut off.
Dynamics and Rheology of Complex Fluids

ORGANIZERS:

David Saintillan, University of Illinois at Urbana-Champaign
Instability and Mixing in Driven and Active Suspensions

Michael Shelley
Courant Institute, New York University
NYU, 251 Mercer St, New York, 10012, US
Phone: 212-228-2901, Email: shelley@cims.nyu.edu

Invited Presentation

Abstract:

Fluids with suspended micro-structure -- complex fluids -- arise commonly in micro- and bio-fluidics, and have fascinating, ill-understood nonlinear behaviors that may prove useful for tasks such as microfluidic mixing and transport. Two examples from my own work involve transitions through hydrodynamic instability to flow states characterized by coherent structures and fluid mixing. The first arises in modeling studies of driven polymeric fluids at low Reynolds number. There a symmetry-breaking instability, related to the coil-stretch transition, occurs at finite Weissenberg number, that drives the system to multi-frequency oscillatory flows with with coherent vortices. We examine the mixing properties of these flows, and the effect of system scale. The second arises in modeling motile suspensions, such as bacterial baths, that show the emergence of large-scale dynamics in space and time. We show how the details of micro-swimmer actuation and geometry are inherited in the macroscopic dynamics of the "active" suspension. For the right kind of swimmer, say a "Pusher" like B. subtilis, these suspensions can show a form of low-Reynolds number turbulence that efficiently mixes fluid and which may also be useful for pumping and transport. We show how the onset of such dynamics is controlled by system size and swimmer concentration.
Modeling and Homogenization of Bacterial Suspensions

Leonid Berlyand
The Pennsylvania State University
McAllister Building, Department of Mathematics, University Park, 16802, US
Phone: 814 861 5502, Email: berlyand@math.psu.edu

Brian Haines
The Pennsylvania State University, State College, PA

Vitaliy Gyrya
The Pennsylvania State University, State College, PA

Igor Aranson
Argonne National Laboratory, Argonne, IL

Abstract:
We discuss recent results with B. Haines, I. Aranson, and D. Karpeev on the effective viscosity of dilute suspensions of swimming bacteria. In our first work, explicit formulas were obtained for the effective viscosity of such suspensions in a two dimensional model. These formulas includes the two terms from Einstein’s classical result for passive suspensions and a novel additional term due to self-propulsion. This term depends on geometric parameters (shape and concentration of bacteria) and the distribution of bacterial orientations. In subsequent work, analogous explicit formulas were obtained for a three dimensional model that includes the effect of tumbling (spontaneous bacterial reorientation), modeled by a stochastic torque. These results explained the mechanism of the reduction in the effective viscosity by an order of magnitude observed in experiments performed by our collaborator I. Aranson and his group. In particular, we show that there is a fundamental difference in the mechanisms of reduction in the effective viscosity for dilute suspensions in background flows with vorticity vs. ones without vorticity. In the latter case, tumbling is necessary to achieve the reduction, while in the former it is not. Next, we discuss non-dilute suspensions and show that interactions result in the reduction of the effective viscosity in flows with vorticity even in the absence of tumbling.

(joint work with V. Gyrya, K. Lipnikov, and I. Aronson).
Effective Shear Viscosity of Suspensions of Micro-Swimmers from Small to Moderate Concentrations

Vitaliy Gyrya
The Pennsylvania State University
10 Vairo blvd., Apt 5B, State College, 16803, US
Phone: 9738651226, Email: gyrya@math.psu.edu

Konstantin Lipnikov

Igor Aranson

Leonid Berlyand

Abstract:

Recently, there has been a number of experimental studies convincingly demonstrating that a suspension of self-propelled bacteria (microswimmers in general) may have an effective viscosity significantly smaller than the viscosity of the ambient fluid. This is in sharp contrast with suspensions of hard passive inclusions, whose presence always increases the viscosity.

We present a 2D model for a suspension of microswimmers in a fluid and analyze it analytically in the dilute regime (no swimmer-swimmer interactions) and numerically using a Mimetic Finite Difference discretization at moderate concentrations. Our analysis shows that in the dilute regime (in the absence of rotational diffusion) the effective shear viscosity is not affected by self-propulsion. But at the moderate concentrations (due to swimmer-swimmer interactions) the effective viscosity decreases roughly linearly as a function of the propulsion strength of the swimmers. These findings demonstrate that (i) a physically observable decrease of viscosity for a suspension of self-propelled microswimmers can be explained purely by hydrodynamic interactions, (ii) self-propulsion and interaction of swimmers are both essential to the reduction of the effective shear viscosity.
Dynamics of a Semi-flexible Polar Filament in Stokes Flow

Yuan-Nan Young
New Jersey Institute of Technology
519 Cullimore Hall, Department of Mathematical Sciences, NJIT, Newark, 07103, US
Phone: 9736427034, Email: yyoung@oak.njit.edu

Abstract:

In this work we examine the dynamics and transport of a polar filament driven by molecular polar proteins using a continuum slender-body model. The polar filament is immersed in a viscous fluid and the presence of the bottom wall is taken into account. Linear analysis on a straight polar filament indicates that the spatial gradient in the polar forcing, either due to spatial variation or the partial detachment from the motor proteins, is necessary for the buckling instability of the polar filament, which then deforms, undulates, and changes its direction of motion. The filament transport that results from buckling polar filaments is shown to be diffusive on scales much larger than the mean-free-path and the average duration between filament buckling events in the forcing landscape.
A Stokesian Viscoelastic Flow: Transition to Mixing and Oscillations

Becca Thomases
University of California, Davis
8060 Terrace Dr., El Cerrito, 94530, US
Phone: 510-406-2136, Email: thomases@math.ucdavis.edu

Michael Shelley
New York University, Courant Institute, New York, NY

Abstract:

To understand observations of low Reynolds number mixing and flow transitions in viscoelastic fluids, we study numerically the dynamics of the Oldroyd-B viscoelastic fluid model. The fluid is driven by a simple time-independent forcing that creates a cellular flow with extensional stagnation points. We find that at O(1) Weissenberg number these flows lose their slaving to the forcing geometry of the background force, become oscillatory with multiple frequencies, and show continual formation and destruction of small-scale vortices. This drives flow mixing. These new flow states are dominated by a single large vortex, which may be stationary or move persistently from cell to cell. Increasing the number of degrees of freedom by increasing the number of driving cells broadens the temporal frequency spectrum and yields richer dynamics with no persistent vortices and improved fluid mixing.
Dense Cellular Blood Flow in a Model Microvessel

Jonathan Freund
University of Illinois at Urbana-Champaign
1206 W. Green Street, Urbana, 61801, US
Phone: (217) 244-7729, Email: jbfreund@illinois.edu

Mara Orescanin
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Red blood cells in the smallest blood vessels appear to line up in orderly bullet-like shapes and flow down the center of the vessels. The low effective viscosity in capillary-scale tubes, and presumably in capillaries themselves, seem to occur near the largest vessel diameter for which the cells flow in this single-file configuration. For larger diameter tubes or vessels, the cells take on a disordered character, and the overall resistance to flow increases with increasing vessel size. We investigate flow near the onset of this relatively disordered behavior for a dense suspension (30 percent volume fraction cells) using an advanced simulation model of blood cells flowing in microvessels. A boundary integral formulation of Stokes flow is solved using Particle-Mesh-Ewald methods for computational efficiency. The red-cell membranes are modeled as neo-Hookean elastic shells and the hemoglobin solution in their interior is modeled as a Newtonian fluid. We consider both a cell-interior viscosity that matches that of the plasma suspending the cells and one that is five times larger, which is thought to be a more realistic model. The shell residual stresses are evaluated using spherical harmonic expansions. This spectral approach provides excellent accuracy and at the same time facilitates a de-aliasing procedure, which provides numerical stability without the addition of numerical dissipation. Simulations are shown to match experimental measurements of effective viscosity at the moderate-to-high shear rates reported in tubes of this size (11.3 micron diameter), irrespective of the cell-interior viscosity. There is a prominent cell-free layer near the vessel walls, which is well understood to be responsible for the relatively low resistance of blood-cell suspensions. In addition to these high flow rates, we also consider relatively slow flows, in which the cells are relatively stiff and thus deform little. At lower shear rates, the thickness of the cell-free layer decreases substantially. It seems that for mid-range shear rates, lubrication effects are responsible for thickening this layer. The results are remarkably insensitive to the cell-interior viscosity, which suggests that the tank treading motion, which is much discussed and easily observed in low-density sheared suspensions of cells, is unimportant in these small vessels. Quantitative metrics of tank treading are developed that confirm this. The viscosity-matched cells tank tread more that those with an elevated interior viscosity, but in all cases this treading rotation rate is a tiny fraction of what would be expected for, say, a small sphere rolled along the vessel wall by the flow.
Dynamics and Pattern Formation in Large-scale Suspensions of Polarizable Particles in Electric Fields

David Saintillan
MechSE, University of Illinois at Urbana-Champaign
1206 West Green St, 126 Mechanical Engineering Building, Urbana, 61801, US
Phone: 217-333-5118, Email: dstn@illinois.edu

David Saintillan
MechSE, University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

The ability to manipulate small particles at the micro- and nanoscale plays a central role in a wide range of technological applications, from self-assembly to sorting to biochemical analysis. To this end, electric fields offer a low-cost and efficient method of controlling particle motions. Yet, understanding and modeling the dynamics that result when many particles are present remains a challenge in many situations. In this work, we use theory and large-scale numerical simulations to analyze the dynamics in suspensions of polarizable particles undergoing dielectrophoresis (DEP) and induced-charge electrophoresis (ICEP). In suspensions undergoing DEP only, particle aggregates are predicted to appear in the form of long chains in the direction of the electric field, in agreement with previous studies. The rapid formation of these chains is then followed by a slow dynamic coarsening process, by which chains coalesce resulting in a mesoscopic pattern formation. When both DEP and ICEP occur, chaining altogether disappears and is replaced by transient particle pairings, which result in hydrodynamic particle diffusion and in a nonuniform microstructure with transient clusters surrounded by clarified regions, as demonstrated by particle occupancy statistics. We conclude by discussing applications of this study to the assembly of colloidal structures by electrophoretic deposition.
Drag, Diffusive Motion, and Mixing in Bubbly Fluids

Andrew Belmonte
Pritchard Labs, Penn State University
Dept of Mathematics, University Park, 16803, US
Phone: 814-865-2491, Email: andrew.belmonte@gmail.com

Michael Higley

Abstract:

The transient and steady state motion of a solid sphere falling through a fluid depends to a large degree on the constitutive properties of the fluid material itself - be it Newtonian, Stokes, viscoelastic, or something more complex. A field of rising bubbles provides a convenient way to slow down or even reverse particle sedimentation, and is utilized industrially. I will present an experimental and mathematical study of a single sphere descending through such bubbly fluids (Reynolds numbers around 1000) in a quasi-2D geometry. We observe two transitions: from falling to floating, and to a diffusive lateral motion. Scalar mixing is studied in the same system, and compared to the multi-sphere limit. A fluid Galton board model is presented, in which the sphere collides inelastically with a fixed distribution (ordered or disordered) of identical moving scatterers in an entrained fluid.
Targeted Enhanced Heat Transfer in Circular Tubes Using a Corona Jet

Reza Baghaei Lakeh
Southern Illinois University Edwardsville
Campus Box 1805, Department of Mechanical Engineering, School of Engineering, Edwardsville, 62025, US
Phone: 618-541-0029, Email: rbaghae@siue.edu

Majid Molki
Southern Illinois University, Edwardsville, Illinois

Abstract:

Natural convection heat transfer can be noticeably enhanced by the secondary flow generated by corona wind in tubes and ducts. A corona-induced secondary flow may be generated in circular tubes with no major changes in the geometry, or causing any noise or vibration. When a high electric potential is applied to an electrode located at the center of a tube, the gas neutral molecules are ionized. The corresponding transport of the charged particles under the effect of the electric field produces a dragging effect on the gas elements and forms a steady and strong electric body force. In this investigation, it is shown that the eccentric configuration of the corona electrode forms a local jet along the eccentricity direction, which impinges on the tube wall and improves the local heat transfer rate dramatically. Since the direction of the corona jet is determined by the eccentricity of the electrode, the jet may be oriented properly to target the hot spots for a more efficient and localized cooling of the electronic components. In this research, the influence of corona jet impingement on the local Nusselt number and heat transfer are investigated numerically and analytically. The heat transfer due to corona jet is compared with pure natural convection results to determine the level of enhancement.
Experimental Fluid Mechanics in Single and Multiphase Flows

ORGANIZERS:

Hui Hu, Iowa State University
Shankar Subramaniam, Iowa State University
A Combined Measurement Method of Temperature and Velocity using a Luminescent Lifetime

Satoshi Someya

The University of the Tokyo
Kankyo 221, 5-1-5 Kashiwanoha, Kashiwa, 277-8563, JP
Phone: +81-4-7136-5872, Email: some@k.u-tokyo.ac.jp

Invited Presentation

Abstract:

This study proposes a combined method for two-dimensional temperature and velocity measurement in liquid and gas flows using temperature sensitive particles (TSPs), a pulsed ultraviolet laser, and a non-intensified high-speed CMOS camera. TSPs respond to temperature changes in the flow and can also serve as tracers for the velocity field.

The luminescence from the TSPs was recorded at 40,000 frames per second as sequential images for a lifetime-based temperature analysis. These images were also used for the particle image velocimetry calculations. The temperature field was estimated using several images, based on the lifetime method.

The decay curves for various temperature conditions fit well to exponential functions, and from these the decay constants at each temperature were obtained. The proposed technique was applied to measure the temperature and velocity fields in natural convection driven by a Marangoni force and buoyancy in a rectangular tank. The accuracy of the temperature measurement of the proposed technique was ~0.35-0.40 Celsius degree.

In addition, the surface temperature inside an optical engine both with and without heating the intake gas was measured. The shot-to-shot standard deviation of the decay constant at uniform temperature conditions was 0.17-0.33%. And finally, we measured the temperature and the velocity distribution of gas flow in the optical engine. The engine was operated at 1500rpm, without combustion. The present method could measure a rapid temperature increase following the pressure increase without delay and the temperature changes due to the crank angle were successfully measured. The velocity distribution in the optical engine was also calculated successfully from the common images.

The proposed approach can be applied to the flow of any working fluid by selecting a suitable base-sphere or phosphor materials. The approach can be applied also to the combined measurement of oxygen concentration and velocity distribution by incorporating an oxygen-sensitive dye. Moreover, the TSPs method can be applied to a flow in a small scale channel with a microscope. In the presentation, the database for the sensor materials will be introduced and a few demonstrations of the combined measurement will be presented.
Population, Characteristics and Kinematics of Vortices in a Confined Rectangular Jet

Bo Kong
Iowa State University, 2025 Black Engr, Ames, 50010, US
Phone: 716-360-6600, Email: kongbo@iastate.edu

Michael G. Olsen
Iowa State University, Ames, IA

Rodney O. Fox
Iowa State University, Ames, IA

James C. Hill
Iowa State University, Ames, IA

Abstract:
Vortex behavior and characteristics in a confined rectangular jet were examined using vortex swirling strength as a defining characteristic. Experimental data were collected at $Re = 20K$ and $Re = 50K$. Swirling strength fields were calculated from velocity fields and then filtered. By identifying clusters of filtered swirling strength, vortex structures were identified. Instantaneous swirling strength field data indicate that the positively (counterclockwise) rotating vortices are dominant on the left side of the jet, and negatively (clockwise) rotating vortices are dominant on the right side. The characters of vortices, such as population density, average size and strength, deviation velocity, were calculated and analyzed, in both the cross-stream direction and the stream wise direction, using PIV data collected in simultaneous PIV/PLIF experiments. In the region close to the channel inlet, the population density, average size and strength all show high values on both side of the center stream. At further downstream locations the wake regions that initially form just downstream of the splitter plates disappear. As the flow develops further, the distribution of the vortices spreads throughout the channel. Stream wise population density profiles indicate the jet generates more dominant direction vortices after it enters the channel for some distance. The averaged size and strength of the vortices start to decrease after the flow enters the channel.

The signs of vortex deviation velocity indicate the vortices move from the high vortex population region to the low vortex population region, transferring low momentum to high velocity region and high momentum to the low velocity region. Tracing vortices using the high speed PIV experimental data also identified the developing trends of these characters. Both the mean tracked vortex strength and size decrease with increasing downstream distance overall. However the mean tracked vortex size increases before it starts to decrease in the area close to the jet inlet. At further downstream location, the vortex size and strength continue to slowly decrease. At the locations of the left peak of turbulent kinetic energy, two point spatial cross-correlation of swirling strength with velocity fluctuation and concentration fluctuation were calculated. All the correlation fields contain one positively correlated region and one negatively correlated region although the orientations of the correlation fields varied, due to the flow transitioning from wake to jet, to channel flow.
Swirling Strength Analysis of Vortex Characteristics In a Confined Rectangular Wake

Katrine Nilsen
Iowa State University
2025 Black Engr, Ames, 50010, US
Phone: 515-441-0955, Email: kmnilsen@iastate.edu

Bo Kong
Iowa State University, Ames, IA

Michael G. Olsen
Iowa State University, Ames, IA

Abstract:
Vortex behavior and characteristics in a confined rectangular wake were examined using vortex swirling strength as a defining characteristic. Experimental data were collected at Re = 37,500, based on channel hydraulic diameter and bulk average velocity. Swirling strength fields were calculated from velocity fields and then filtered. By identifying clusters of filtered swirling strength, vortex structures were identified. The characters of vortices, such as population density, average size and strength, deviation velocity, were calculated and analyzed, in both the cross-stream direction and the stream wise direction. 10,000 PIV velocity realizations at each of 6 different downstream locations were collected and used in this analysis. In the region close to the channel inlet, the population density, average size and strength all show high values in both wake regions. As the flow develops further, the distribution of the vortices spreads throughout the channel. The averaged size and strength of the vortices start to decrease after the flow enters the channel.

The signs of vortex deviation velocity indicate the vortices move from the high vortex population region to the low vortex population region, transferring low momentum to high velocity region and high momentum to the low velocity region. Tracing vortices using the high speed PIV experimental data also identified the developing trends of these characters. Both the mean tracked vortex strength and size decrease with increasing downstream distance overall. However the mean tracked vortex size increases before it starts to decrease in the area close to the jet inlet. At further downstream location, the vortex size and strength continue to slowly decrease. At the locations of the left peak of turbulent kinetic energy, two point spatial cross-correlation of swirling strength with velocity fluctuation and concentration fluctuation were calculated, with simultaneous PIV/PLIF experiment data. All the correlation fields contain one positively correlated region and one negatively correlated region, and the orientations and strength of the correlation fields varied with increasing downstream distance.
The Effect of Particle Concentration on the Pressure and Flow Rate in a Suspension

Ashwin Vaidya
Montclair State University
Department of Mathematical Sciences, 1 Normal Avenue, Montclair, 07058, US
Phone: 973-655-2139, Email: vaidyaa@mail.montclair.edu

Mehrdad Massoudi
National Energy Technology Lab, Pittsburgh, PA

Abstract:

In this presentation we will discuss our experimental results on some fundamental flow properties of suspensions. We consider a suspension of small spheres in a fluid which can be either Newtonian or viscoelastic. In particular, we examine the effect of concentration upon the flow rate of this system for various prescribed pressure heads. This also permits us to correlate the dependence of pressure with concentration which seems to have been ignored to a large extent in the existing literature.
Microfluidics and Nanofluidics

ORGANIZERS:

Hui Hu, Iowa State University
Shankar Subramaniam, Iowa State University
A Hybrid Simulation of Continuum and Molecular Dynamics

Guowi He
Institute of Mechanics, Chinese Academy of Sciences
LNM, Institute of Mechanics, Beijing, 100080, CN
Phone: 86-10-8254-3969，Email: hgw@lnm.imech.ac.cn

Invited Presentation

Abstract:

Micro- and nano-fluidics involve a broad range of scales from the atomic scales to the continuum ones. A full molecular dynamics simulation is affordable to simulate the fluid flows at the micro- and nano-scales. However, it is computationally prohibitive due to the limitation of computer memory and computation time. On the other hand, a full continuum description, such as the Navier-Stokes equation, is computationally available but unable to describe the fluid flows in the region where the continuum assumption breaks down. One of such problems is the superhydrophobics: the patterned roughness on a hydrophobic solid surface enhances its hydrophobics and yields a large slip velocity on the solid surfaces. The superhydrophobics property is particularly attractive, since it may provide an efficient method for mass transport and drag reduction in micro- and nano-channels. An appropriate approach to simulate the superhydrophobics is to use the molecular dynamics in one region where the continuum assumption breaks down and use the Navier-Stokes equations in another region where the continuum assumption holds true, and those two descriptions are coupled in the overlap region. The computation time in the hybrid method is expected to be much less than that in the full molecular dynamics simulation. The challenge is how to couple the Navier-Stokes equations with the molecular dynamics simulation. We have recently developed a dynamic approach to couple the Navier-Stokes equations with the molecular dynamic simulation, and use the dynamic coupling model to simulate the flows over superhydrophobic surfaces. The results obtained are in consistence with the experiments. The physical implications and numerical issues associated with the hybrid simulations are also discussed.
Abstract:

Microscale chemical reactors capable of operating in the turbulent flow regime, such as confined impinging jets reactors (CIJR), offer many advantages for rapid chemical processing at the microscale. One application where these reactors is used is flash nanoprecipitation, a method for producing functional nanoparticles. Because these reactors often operate in a flow regime just beyond transition to turbulence, modeling flows in these reactors can be problematic. With high-performance computational power becoming more affordable, large eddy simulation (LES) has become a viable option. However, validation of computational fluid dynamics models (CFD) like LES requires detailed and accurate experimental data, the availability of which has been very limited for turbulent microscale flows. In the present work, microscopic particle image velocimetry (microPIV) was employed on a planar CIJR to obtain instantaneous velocity fields for jet Reynolds numbers of 200, 600 and 1000, corresponding to the completely laminar, the transition from laminar to turbulent, and the fully turbulent regimes, respectively, in the reaction zone. For each Reynolds number, approximately 1500 instantaneous velocity fields realizations were collected to analyze the flow fields and calculate pointwise and spatial turbulence statistics. LES was then performed for the same Reynolds numbers on a grid having approximately 4.3 million hexahedral cells. The subgrid scales were modeled using the Smagorinsky-lily model. The simulations were performed using OpenFOAM (OF) on a high performance computing cluster. The time resolved simulated velocity fields were then used to compare the simulation with experimental results. When the mean velocity fields, Reynolds normal and shear stresses, and two dimensional turbulent kinetic energy were compared, good agreement was observed between the experimental results and the LES results. These results demonstrate the viability of using large eddy simulation as a tool for designing microscale reactors.
An Experimental Study of Pulsed Micro Flows Pertinent to Continuous Subcutaneous Insulin Infusion Therapy

Bin Wang
Iowa State University
321 S 5TH ST, #222, Ames, 50010, US
Phone: 5152319895, Email: binw@iastate.edu

Hui Hu
Iowa State University, Ames, Iowa

Ayodeji Demuren
Ayodeji Demuren, Norfolk, VA

Abstract:

An experimental study was conducted to investigate the transient behavior of the unsteady micro-flow driven by an insulin pump commonly used in continuous subcutaneous insulin infusion (CSII) therapy to elucidate the underlying physics for a better understanding of the microphysical process associated with the insulin delivery in CSII therapy. A microscopic Particle Image Velocimetry (PIV) system was used to provide detailed flow velocity field measurements inside a 300μm×300μm microchannel to characterize the transient behavior of the micro-flow upon the pulsed excitation of the insulin pump. It was found that the microflow inside the CSII tubing system is highly unsteady, which is much more interesting than a creeping flow that the nominal averaged flow velocity would suggest. The effects of air bubbles entrained inside the micro-sized CSII tubing system on the insulin delivery process were also assessed based on the detailed micro-PIV measurements. It was found that, in addition to reducing the total amount of the liquid fluid actually delivered by the insulin pump through the catheter of the infusion set, the air bubbles were also found to act as shock-absorbers to change the dynamic response of the micro-flow to the pulsed action of the insulin pump. While most solutions to insulin occlusion related problems are currently based on clinical trials, the new findings derived from the present study can be used to provide a better guidance for the troubleshooting of insulin occlusion in CSII therapy.
Microscale Fluid Flow Visualization in CIJR using Phenolphthalein

Yanxiang Shi
Iowa State University
2114 Sweeney Hall, Ames, 50011, US
Phone: 515-509-3542, Email: yanxiang@iastate.edu

Michael G. Olsen
Department of Mechanical Engineering, Iowa State University, Ames, IA

Rodney O. Fox
Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Abstract:

The process of producing nanoparticles via precipitation requires supersaturation due to rapid mixing effect at the smallest scale. This effect can be achieved in microscale reactors such as confined impinging jet reactor (CIJR) and multi-inlet vortex mixer (MIVM) at high Reynolds numbers where strong turbulence can be observed. With the help of computational fluid dynamics (CFD), "experimentless" design of such reactors can be possibly realized. Previously, the CFD model, DQMOM-IEM, developed by the Fox group at Iowa State University has been compared not only with the conversion of 2,2-dimethoxypropane (DMP) that was obtained experimentally by the Prud'homme group at Princeton University, but also with the microscale particle image velocimetry (μ-PIV) results. The model predicted both the conversion of DMP and the velocity field accurately.

In order to extend the validation and to get an intuitive understanding of the mixing, the pH indicator phenolphthalein, which gives a purple color at pH between 8 and 13 but is colorless if the pH is below 8, is employed to visualize the impinging jets. An acidic solution of pH=3 and an alkaline solution of pH=12 are prepared using a mixture of ethanol and deionized water. Both of them contain the same amount of phenolphthalein to eliminate the density difference between the two. Three jet Reynolds numbers, defined as the inlet Reynolds numbers, Rej = 600, Rej = 1000 and Rej = 1500, are employed. The mixing between the two streams and the flow fields are visualized and captured with a CCD camera. One essential component in the system is the xenon flash lamp, which has extremely short pulse duration, enabling freezing the flow pattern in a very short time. The results are then post-processed by using a threshold technique to obtain the time averaged mean, which is further utilized to validate the CFD models.
Fluid Issues in Renewable Energy Systems

ORGANIZERS:

Hui Hu, Iowa State University
Shankar Subramaniam, Iowa State University
Surface Roughness Effects on the Aerodynamic Performance of a Wind Turbine Airfoil

Yan Zhang
Iowa State University
Aerospace Engineering, Iowa State University, 2271 Howe Hall, Room 1200, Ames, 50011, US
Phone: 515-294-0094, Email: huhui@iastate.edu

Takafumi Igarashi
Iowa State University, Ames, Iowa

Hui Hu
Iowa State University, Ames, Iowa

Abstract:

Wind energy is one of the cleanest renewable power sources in the world today. The wind power capacity in the world is expected to expand with a 30% annual growth rate over the next decade. A total of 37.5 GW of wind power were added in 2009, bringing total worldwide wind energy installations up to 157.9 GW. With the expansion of wind power capacity, an increasing number of wind turbine installations have pushed their way into three distinct climatic zones, which include icy Nordic environments, humid regions that support large insect populations, and desert environments with sand-laden winds. Each of these environments can create significant operational issues for wind turbines. Inevitable leading edge contaminations due to insect debris, sand accumulation and ice accretion have been found to cause significant degradation of wind turbine performance in power output, particularly for the stall-regulated turbines.

While a number of previous studies have been conducted to investigate the effects of the surface roughness on the aerodynamic performance of wind turbine airfoils, the fundamental mechanism on how the surface roughness affect the development of boundary layers over the airfoils, to some extent, still remains unknown. In this study, a detailed experimental study was conducted to characterize the effects of the surface roughness on the aerodynamic performance of a wind turbine airfoil. In addition to mapping the surface pressure distribution around the airfoil with pressure sensors, a high-resolution PIV system was used to make detailed flow field measurements to quantify the effects of the surface roughness on the occurrence and behavior of laminar boundary layer separation, transition, and reattachment on the airfoil. The detailed flow field measurements were correlated with the surface pressure measurements to elucidate the underlying physics associated with the separation, transition, and reattachment processes of the laminar boundary layer over the airfoil. To the best knowledge of the authors, this is the first effort of its nature. The primary objective of the present study is to elucidate underlying physics to gain further insight into the fundamental mechanism on how the leading edge roughness affect the laminar flow separation, transition, and reattachment on wind turbine airfoils as well as the resultant aerodynamic performance. In addition, the quantitative surface pressure and flow field measurements will be used as the database for the validation of computational fluid dynamics (CFD) simulations of such complex flow phenomena for more effective and robust designs tailored for wind turbine blade protection from icing, dust and insect collision contamination.
Influence of Cylinder Aspect Ratio on the Mode Transition in the Wake behind a Heated Circular Cylinder

Yu Xie
Iowa State University
1095 Black, Ames, 50010, US
Phone: 515-294-7442, Email: yuxie@iastate.edu

Hui Hu
Iowa State University, Ames, Iowa

Baskar Ganapathysubramanian
Iowa State University, Ames, Iowa

Abstract:

The problem of flow past a heated cylinder has been investigated for several decades now. However, several aspects of the associated mechanisms of wake behavior still remain unexplored and have both fundamental as well as application based relevance. The study of the influence of heat input on the wake flow behind a cylinder provides key insights towards improving electronic devices packaging and cooling.

Both experimental and numerical studies reflect that heating of cylinder can significantly change vortex shedding characteristics. The present study investigates the influence of geometric factors on the wake behavior behind a heated cylinder. Stabilized finite element methods are applied to study how the cylinder aspect ratio (ar) influences the wake behind a heated circular cylinder. Accuracy of the numerical results is guaranteed by comparing results with experimental studies. Numerical and experimental results confirm that there exists a variety of flow transition behavior in the phase space of Richardson number (Ri) and aspect ratio (ar). Various factors -- including temperature dependent viscosity, aspect ratio, and end effects -- affecting the mode shifts are investigated. A phase portrait of the shedding behavior is constructed from the data. Two curves separate the different modes in the map of vortex shedding patterns in the near wake.
Comparison between Conventional and Ductwork Diffusers for Green Buildings: Experimental and Computational Studies

Anthony Fontanini
Iowa State University
2025 Black Engineering, Ames, 50011, US
Phone: (608)780-0025, Email: fontania@iastate.edu

M. Olsen
Iowa State University, Ames, IA

B. Ganapathysubramanian
Iowa State University, Ames, IA

Abstract:

Increasing energy standards for residential and commercial buildings (green buildings) demand an increase in efficiency of HVAC systems. Most efforts to improve efficiency are usually via improved design of compressors, condensers, evaporators, and fans. However, ductwork and diffuser designs have remained virtually unchanged. Conventional HVAC systems are comprised of sheet metal ductwork and diffusers. These systems can be heavy, have poor insulation without additional parts, exhibit large latency times and distribute air in localized positions within a room thus requiring multiple diffusers for homogeneous heating/cooling. Recent advances in fabric based ductwork use better insulating and lightweight materials to distribute the air in a more uniform manner, and use minimal parts to support these systems from the ceiling. These products have the potential to reduce the amount of electricity needed to run the heating and ventilation systems.

A comparison between fabric based ducting and conventional ducting is performed using a combined experimental and computational analysis strategy. A representative building-like enclosed structure was constructed with the two different ducting systems. The flow field variation and thermal transients were analyzed using particle imaging velocimetry (PIV) techniques. This data was used to validate a realistic three dimensional computational fluid dynamics model. The validated numerical framework was subsequently used to investigate thermal transients, and homogeneity of cooling/heating in both conventional ducting and fabric based ducting. These results allow for conclusions to be drawn about the efficiency of conventional and newer systems. These results also give insight to the problem for further optimization and the extrapolation of design decisions of these newer products.
Numerical Investigation of Aerodynamic Effects of Leading-edge Sinusoidal Tubercles on Airfoils at Low Mach Numbers

Qiaoyi Gui
Shenyang Aerospace University
Yuhong District Heishan Road 12-15-122, Shenyang, 110034, CN
Phone: 13324069579, Email: guiqiaoyi@yahoo.com.cn

Abstract:

A three-dimensional numerical investigation was performed to study the effect of tubercles on NACA 4412 and 0020 airfoils in freestream with speed of 10m/s and 15m/s. Tubercles are several regularly distributed blunt and round like bumps across the leading edges of humpback whale flippers which greatly enhance the whale’s dexterity. Wind tunnel tests of tubercles modified model humpback flippers have demonstrated that the tubercules can make significant fluid dynamic improvements, such as a staggering 32% reduction in drag, 8% improvement in lift, and a 40% increase in angle of attack over smooth flippers before stalling. Although the tubercles modified wind turbine and other kinds of blade are designed, the mechanism of tubercles on the airfoil performance are not well understood for the complexity of vortex flow on the airfoil surface. Chosing the number, size and location of tubercles and chord, span width as parameters, the airfoil structures are parametric designed with UGNX6 for the purpose of locating the highly performance sensitive parameters, and the relationship of these major parameters. Employing incompressible Navier-Stokes solver, and the realizable k-epsilon turbulence model, the flowfield around the airfoil was numerically predicted using CFX software package under unstructured grids. Sinusoidal tubercles with uniform sizes of 0.5%, 1.0%, 1.25%, 1.5%, 2.0%, and 3.0% of the airfoil chord, at tubercle numbers of 5, 10, 15 and evenly located were studied. Some computational results were compared with public available experimental results to testify the accuracy of the simulations. From the results, it can be found that the tubercles greatly increase the airfoil lift coefficient with only a slight increase in drag coefficient as the former study demonstrated. Comparing the results under different parameters, it also can be found that all the three parameters have a significant influence on the airfoil performance, and there exists a strong relationship between the size and the number by which we can conclude that the distance between the neighboring tubercle play a key role in it. Furthermore, the numerical solutions show the details of the flow structure at the airfoil surface and provide a possible explanation for the increased aerodynamic performance.
Mixing Time Estimation in a Double Jet Mixer of Hemispherical Bottom with Calcium Phosphate Solution as Working Fluid

Kalaichelvi Ponnusamy
National Institute of Technology,
Department of Chemical Engineering, Tiruchirappalli - 620 015, Tamilnadu, India
Phone: +91-431-2503113, Email: kalai@nitt.edu

P.Kalaichelvi
National Instituet of Technology, Tiruchirappalli, Tamilnadu

C. Shanawaskhan
National Instituet of Technology, Tiruchirappalli, Tamilnadu

N.Anantharaman
National Instituet of Technology, Tiruchirappalli, Tamilnadu

Abstract:

Mixing refers to the dispersion of one or more components, one throughout the other. Though it occurs in innumerable instances in process industry and is one of the most common in all process operations. Impellers are the conventional devices used for mixing purpose in industries. But they are very expensive for large storage tanks and underground tanks. Jet mixers have become alternative to impellers for over 50 years in the process industry. There are, however, some aspects of mixing that can be measured and that can be of help in planning and designing mixing operations. Many of the research articles have reported on the important parameters viz., jet configuration and orientations that affect the liquid - liquid mixing time. Recent advances on Computational Fluid Dynamics (CFD) have also attracted many researchers to work and analyze various mixing operations. In the present article, it was proposed to model and simulate the jet mixer using a general purpose CFD package, FLUENT 6.1. The jet mixer considered in the present study consists of a cylindrical tank of 0.36 m diameter and 0.36 m height with a hemispherical bottom having with two jets. The working fluid used in the present work is calcium phosphate solution (at 20.3% by mass of calcium phosphate and the rest water) and its specific gravity was 1.27. The simulated concentration profiles obtained from the concentration probes located at five different locations have been used estimating the mixing time. The estimated mixing time was also compared with the mixing time value estimated for other working fluids.
Multiphase Flow

ORGANIZERS:

Hui Hu, Iowa State University

Shankar Subramaniam, Iowa State University
Evolution of Random Roughness in Microchannel Materials and its Impact on Laminar Fluid Flow

Jing Ren
Iowa State University
0087 Black Engineering, Ames, 50011, US
Phone: 515-294-8020, Email: jren@iastate.edu

Baskar Ganapathysubramanian
Iowa State University, Ames, Iowa

Michael Olsen
Iowa State University, Ames, Iowa

Sriram Sundararajan
Iowa State University, Ames, Iowa

Abstract:

Roughness of channel surfaces is known to affect the fluid flow behavior in microscale fluidic devices. This has relevance particularly for applications involving non-Newtonian fluids, such as biomedical lab-on-chip devices. While several studies have investigated effects of relative large, deterministic structures on fluid flow, the effect of random roughness on micro fluid flow remains relatively unexplored. In this study random roughness was generated on glass surface by buffered HF etching and evolution of roughness parameters with etching time and orientation was studied. Specifically, amplitude parameter central line average (Ra) and spatial parameter autocorrelation length (ACL) were investigated. Statistical distribution of the surface roughness was also studied. Subsequently glass surfaces with different roughness parameters and PDMS were used to fabricate microchannels. Particle image velocimetry (PIV) was used to measure the flow velocities to assess the affect of random roughness. The affect of random roughness on velocity field in laminar flow are reported. The feasibility and implications of tailoring random roughness in microfluidic channels is discussed.
Three Dimensional Compressible Multi-Material Flows

Anil Kapahi
University of Iowa.
3131 Seamans Center for the Engineering Arts and Sciences, Iowa City, 52242, US
Phone: 319-400-0346, Email: anil-kapahi@uiowa.edu

John Mousel
University of Iowa, Iowa city, IA

Dr. Shivkumar Sambasivam
Los Alamos National Lab, Los Alamos, NM

Dr. HS udaykumar
University of Iowa, iowa city, IA

Abstract:
Shock Waves and Detonation waves have been topic of cutting edge research for decades. The interaction of these waves with multi materials can result in complex wave structures in two and three dimensions. Large-scale computations are required to simulate physical phenomena involving detonation and shock waves like supernova formation, explosions and hypervelocity impact and penetration. In this paper we describe the parallel implementation of fixed Cartesian grid flow solver with moving boundaries. A higher order conservation scheme such as ENO is used for calculating the numerical fluxes and level sets are used to define the objects immersed in flow field. A Riemann solver based Ghost fluid method (GFM) is used for interface treatment of embedded objects. This paper describes the methodology for parallelization with emphasis on strong shocks interacting with embedded interfaces (solid-fluid, solid-solid and fluid-fluid) in three-dimensional compressible flow framework. In order to accurately decouple the interface conditions and the associated impedance mismatch, a Riemann problem was constructed normal to the interface and the solution obtained from solving the Riemann problem were used to define the ghost states. In the case of embedded solid objects, a reflective boundary condition endowed with Riemann correction was employed to capture the interface conditions. The method developed was shown to be effective in solving a wide repertoire of problems involving shocks of varied magnitude interacting with the embedded object(s). The main idea of the parallel algorithm is to avoid storage of global information proportional to the size of the problem on a single processor. The algorithm is designed to execute on a distributed memory system. The inter processor communication is handled using MPI library. A domain decomposition software that creates balanced partitions is highly desirable for parallel algorithms. In the following setup, METIS a graph partitioning software is used for better load balancing. METIS uses the nodal connectivity as an input to generate partitions, which are optimally load balanced. It also minimizes the communication time by minimizing the total edge cuts. We have also addressed the problems related to handling (storage/retrieval) of global data, definition and construction of ghost layer, special treatment for moving boundaries and handling of GFM at processor boundaries. The numerical examples will be presented to demonstrate the capabilities of our work.
Visualization and Modeling of Flow Boiling of R-134a in Ribbed Minichannels

Venugopal Vengala
Cummins Inc. (Currently), Southern Illinois University Edwardsville (Research work)
2482 Thornybrook Dr, Columbus, 47203, US
Phone: 8124478751, Email: venugopal.vengala@cummins.com

Abstract:

The field of heat transfer is progressing with the high demand for improved designs of the compact heat exchangers. Over the last 50 years, a significant development has been made in the design of heat exchangers. There is an increasing demand for improved heat exchangers with high efficiency, reduced cost, and reduced size in the aerospace, refrigeration, and automotive industries. Minichannels have shown an increase in heat transfer compared to large diameter channels. They occupy a small volume and are suitable for use in compact heat exchangers. Extensive research is underway to study the thermal-hydraulic performance of minichannels. An experiment was carried out to investigate the characteristics of the evaporation heat transfer and pressure drop for R-134a flowing in a minichannel with transverse ribs. It was a compact and two-phase flow heat exchanger with high surface area to volume ratio and low inventory of working fluid. The dimensions of the flow cross-sectional area of the channel were 1 mm × 28.8 mm, resulting in a hydraulic diameter of 1.93 mm for the minichannel. The ribs provided a meandering path to the refrigerant flow, causing turbulence and intense mixing. These flow features were the key factors for heat transfer enhancement in this design. The variations of heat transfer coefficient and pressure drop with refrigerant flow rate, vapor quality and saturation temperature were studied. The wall super heat for all the data points was less than 2.75 C, indicating that the convection boiling is the dominant flow boiling mechanism. In addition, extensive high-speed photography was performed to visualize and to understand the flow patterns. Using the least-squares procedure, the experimental data were correlated. The correlation predicted the minichannel data to within +/-20%. The results indicated that the heat transfer coefficient was enhanced by a factor of 1.6 to 4.3 compared to smooth tubes.
Numerical Simulation of Gust Response for UAV Airfoil

Xiaoping Xu
Northwestern Polytechnical University
790 mail,127 youyi xilu, xi'an,shaanxi, xi'an, 710072, CN
Phone: 13619202033, Email: xuran.npu@163.com

zhou zhou

Abstract:

Gust response analysis plays a major role in aircraft structural design, as gust loads typically control the wing-design of large aircraft. Modern methods for dynamic gust analysis typically rely on panel-method aerodynamics. The current study aims at using the now-available CFD tools for dynamic gust response analysis.

The unsteady Euler equations were chosen to study the aerodynamic response of the airfoil to a step change in the angle of attack and One-minus-cosine gust. Since the aerodynamic quantity of interest in this study is the lift coefficient, the effect of viscous forces is expected to be unimportant. The gust to a step change in the angle of attack can be described in function, when airfoil encounter the gust area, an impulsive change of in the angle of attack can be got. And the gust velocity profile of One-minus-cosine gust can be shown as function.

The unsteady solvers are written to incorporate grid-velocity, which is used to calculate the gust response. The idea is to incorporate the step change in input as a step change in grid velocity over the entire flow field. The validation computations were performed for a NACA0006 airfoil for a step change in the angle of attack of rad. It shows the results comparing with computations in reference and the exact results of piston theory. The gust response of quasi "Global Hawk" airfoil for a step change in the angle of attack and the One-minus-cosine gust were simulated. From the result, it shows that the aerodynamic change is obvious in the gust progress. A grid-velocity method has been used to calculate the gust aerodynamic response of airfoil using CFD. It is shown in results that the calculated lift response of airfoil agrees well with both the exact theoretical value and calculated value in reference. Furthermore, according to the result of gust response of UAV airfoil, the aerodynamic change is obvious. And the work provides further guidance on designing gust alleviation system.
TRACK 4

Mechanics of Materials and Structures
Nanomechanics: Beyond Modulus and Hardness

ORGANIZERS:

Oden Warren, Hysitron Inc.
Quantitative Nanomechanical Testing in a TEM

Andrew Minor
U.C. Berkeley
One Cyclotron Road MS 72, Berkeley, 94720, US
Phone: 510 495-2749, Email: aminor@berkeley.edu

Invited Presentation

Abstract:

Recent progress in both in situ and ex situ small-scale mechanical testing methods has greatly improved our understanding of mechanical size effects in volumes from a few nanometers to a few microns. Besides the important results related to the effect of size on the strength of small structures, the ability to systematically measure the mechanical properties of small volumes through mechanical probing allows us to test samples that cannot easily be processed in bulk form, such as a specific grain boundary or a single crystal. In the case of individual nanostructures, the need to address the nanostructure in a direct manner is even more acute, and in situ transmission electron microscope (TEM) in many cases makes this possible.

This talk will describe our recent results from in situ compression and tensile testing of Cu to illuminate the origin of size-dependent yield strength behavior. In addition, comparing compression and tensile testing at small scales has led to some interesting observations regarding the evolution of flow strength during testing.

Lastly, by minimizing or even eliminating defects from FIB-prepared samples we have been able to experimentally achieve the ideal strength of Mo during in situ nanocompression testing. Achieving the theoretical strength of a material experimentally is hindered by the ability to create and mechanically test an absolutely defect-free material. Here we show that through annealing it is possible to employ the versatility of the FIB but recover a mechanically pristine limited volume. Starting with FIB-milled molybdenum pillars, we anneal them in situ in a TEM to produce a molybdenum pillar with a spherical cap. This geometry allows for the maximum stress to occur in the interior of the spherical cap and is ideally suited for experimentally achieving the ideal strength. During in situ compression testing in the TEM the annealed pillars show initial elastic loading followed by catastrophic failure at, or very near, the calculated theoretical strength of Mo.
Nano Adhesion and Indentation

Kenneth Liechti
University of Texas at Austin
210 East 24th Street WRW 110C, 1 University Station C0600, Austin, 78712, US
Phone: 512-471-4164, Email: kml@mail.utexas.edu

Abstract:

Adhesion and friction at small scales have become increasingly important with the advent of MEMS and NEMS devices. The characterization of surface adhesion is particularly challenging because of potential interactions between the measuring device and the quantity being measured. In classical tension testing, such interactions are well understood and avoided by conducting the experiments in displacement control. The situation is more complex when measuring adhesive interactions because there are situations where even displacement control will not always be able to avoid instabilities or snaps. That said, there are surprisingly few nano indentation devices that are capable of running even in displacement control.

One such device is the interfacial force microscope (IFM) invented by Houston at Sandia National Laboratories in the early 1990’s. This paper will review some of the interactions that have been examined with the IFM. Many of the early experiments were qualitative in the sense that interaction forces were compared and ranked. The remainder of the paper will focus on combining IFM data with molecular and continuum analyses to extract the mechanical and adhesive behavior of self-assembled monolayers on silicon and monolayers of ice-like water on mica.
Analysis of Dielectric Fracture Using Nanoindentation

Peter Woytowitz
Novellus Systems, Inc.
3970 N. 1st St., M/S 70D, San Jose, 95134, US
Phone: 408-771-4000, Email: sassan.roham@novellus.com

Sassan Roham
Novellus Systems, Inc., San Jose, CA

Dong Niu
Novellus Systems, Inc., Tualatin, OR

Haiying Fu
Novellus Systems, Inc., Tualatin, OR

Abstract:
In micro-electronic devices with feature sizes at 45nm and less, ultra-low dielectric constant (ULK) materials have been introduced into the semiconductor manufacturing process in order to improve device performance. ULK materials, however, present challenges associated with interfacial adhesion and cohesive fracture. Characterization of mechanical strength is critical to understanding ULK film behavior when it is integrated with other materials of differing thermal expansion coefficients. The thermal excursions of the semiconductor device drive thermal stresses which can eventually lead to device failures. Understanding the fracture characteristics also helps to drive deposition process development to ensure the integrated device can withstand downstream manufacturing processes such as chemical-mechanical planarization (CMP) and final packaging.

In this study the fracture strength of very thin films was determined using nano-indentation in conjunction with classical fracture mechanics formulas and fracture mechanics based finite element procedures. Nanoindentations were observed under SEM, which were loaded in a manner to induce cracks at the edge of the indents. Using the crack length obtained from SEM, modulus, hardness and peak indentation load from the nanoindenter machine and fracture toughness of the film were calculated using closed-form solutions to predict fracture toughness KIC and fracture energy, GIC. Detailed finite element analysis using different types of crack elements and finite element fracture mechanics formulations were also used to compute the same quantities. Comparisons between analytical and finite element predictions are presented, along with physically observed crack patterns and fracture. Conclusions regarding the applicability of the classical formulas for observed nanoindentation cracking versus the finite element based procedures are presented. While this work was performed using a particular ULK formulation, the methodology and conclusions concerning the classical formulation versus finite element based fracture mechanics are applicable to a wide range of nano materials. Therefore these methods and results will prove to be useful to a wide range of industries interested in integrating nano-materials into complex structures.
Atomistic Mechanisms of Cyclic Hardening of Metallic Glass under Nanoindentation

Chuang Deng
Massachusetts Institute of Technology
77 Massachusetts Ave, Cambridge, 02139, US
Phone: 6173243525, Email: chuangd@mit.edu

Christopher A. Schuh
Massachusetts Institute of Technology, Cambridge, MA

Abstract:

It is well documented that metallic glasses experience early failure under fatigue loading conditions. However, the fundamental physical mechanisms lead to fatigue failure in metallic glasses remain unclear, which must be well understood before metallic glasses can be seriously considered for structural applications despite their high yield strength and high hardness.

Nanoindentation is an experimental tool that has been widely used to investigate the shear banding events in metallic glasses. It has been reported that metallic glasses can be hardened by cyclic loading in the elastic range under nanoindentation. More specifically, the load required to trigger the first shear band in metallic glasses, which is known as the first "pop-in" event, can be significantly increased due to cyclic loading. This hardening effect is developed progressively over several cycles, and eventually saturates. Results from finite-element-method based shear transformation zone dynamics simulations indicate that confined microplasticity in local regions must be developed through significant structural change during the cycling.

The goal of this work is to use molecular dynamics simulations to investigate the possible structural change at atomistic scale that lead to both microplasticity and global hardening in metallic glasses during cyclic loading. In this research, nanoindentation of Cu-Zr metallic glasses that are quenched at dramatically different rates is simulated with an embedded-atom method potential. A virtual indenter of infinitely large modulus is used to impose cyclic load on each sample with various amplitudes at the elastic range. The structural changes in these samples due to cycling is studied in terms of free volume content, short-range chemical and geometrical ordering, and local shear strain field. The results from molecular dynamics simulations are in excellent agreement with that from both experiments and shear transformation zone dynamics simulations, which provide strong support for the hardening effect due to cyclic loading at elastic range. Moreover, microplasticity in confined regions beneath the nanoindenter is observed to develop progressively well before the first shear band is formed. This research together with experimental and finite-element analysis studies should be able to shed some light on understanding the fundamental mechanisms of early fatigue failure in metallic glasses.
Understanding Plastic Deformation in Si-SiC Nanocomposite Towers

Aaron R. Beaber
Department of Chemical Engineering and Materials Science, University of Minnesota
457 Amundson Hall, 421 Washington Ave. SE, Minneapolis, MN 55455, USA
Phone: 612-624-0515, Email: beaber@umn.edu

William W. Gerberich
Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

Abstract:

Unresolved issues with regard to dislocation nucleation, dislocation exhaustion, and work hardening of nanovolumes abound in the literature. Examples persist as to how much plasticity is related to phase transformations or dislocation nucleation. This is particularly evident during the compression of silicon, which has been shown to flow rather than fracture under high hydrostatic stresses. In the present work, a combination of nanoindentation and confocal Raman microscopy are used to probe the role of dislocation plasticity and phase transformations during fracture events in silicon at small length scales. First, TEM in situ indentations of single crystal Si nanospheres and Si(111) nanotowers are used to quantify a length scale dependence on the flow stress, fracture toughness, and critical pressure for metallization. These results are then used to explain toughening effects observed in Si-SiC core-shell composite nanotowers. Overall, these results demonstrate the importance of nanoscale confinement and localized stress in the design of mechanically robust nanocomposites.
Broadband Nanoindentation Spectroscopy

Don Stone
University of Wisconsin-Madison
Materials Science and Engineering, 1509 University Ave, Madison, 53706, US
Phone: 608-262-8791, Email: dsstone@wisc.edu

Joseph E. Jakes
Performance Enhanced Biopolymers, United States Forest Service, Forest Products Laboratory, Madison, WI

Abstract:
We have invented broadband nanoindentation creep (BNC) to measure viscoplastic properties across 4-6 decades of strain rate and broadband nanoindentation viscoelasticity (BNV) to measure viscoelastic properties across >8 decades of time scale. The measurements require an instrument with fast response that is nevertheless stable against thermal drift. Materials studied with BNC and BNV include poly methyl methacrylate (PMMA), polycarbonate (PC), polystyrene (PS) and molybdenum. BNC experiments generate hardness vs. strain rate. BNC data from polymers are all path-dependent (depending on initial rate of loading). BNC data from molybdenum are not path dependent (behavior does not depend on the initial rate of loading). By a simple formula that works for all materials studied, the hardness-strain rate data can be converted to flow stress vs. strain rate; and the converted data agree with literature compression data. Likewise, BNV data follow the trend of more conventional viscoelasticity measurements made using dynamic mechanical analysis (DMA) and broadband viscoelastic spectroscopy. However, the nanoindentation modulus values tend to be 10-25% higher than the more conventional modulus measurements. This effect might be due to hydrostatic pressure beneath the indenter. Collectively, these experiments suggest the possibility of using nanoindentation as a tool for quantitative mechanical spectroscopy. Not only can nanoindentation be used to probe the properties at microscopic length scales, but it also provides measurements that are nearly isothermal, even at very high strain rates.
Recent Technological Developments for Nanomechanical Testing

S.A. Syed Asif
Hysitron Inc.
10025 Valley View Road, Eden Prairie, 55344, US
Phone: 952-835-6366, Email: sasif@hysitron.com

Ryan C. Major
Hysitron Inc., Minneapolis, MN

Yunje Oh
Hysitron Inc., Minneapolis, MN

Oden L. Warren
Hysitron Inc., Minneapolis, MN

Abstract:

Structure-property correlation is an important step in the material design process and understanding the mechanical deformation of materials from macro to nanometer length scale is crucial to the design and development of materials for its intended applications. Many experimental techniques have been developed in the past to understand the mechanical response at micro/nanometer length scale. In the depth-sensing indentation technique, quantitative mechanical properties such as hardness and modulus can be routinely obtained from the load-displacement curves; however, the underlying physical mechanisms by which deformation proceeds are not always readily apparent. At shallow depths, the load-displacement curves often exhibit unusual features such as pop-in/pop-out load-displacement discontinuities which can be used to understand the fundamental deformation mechanisms but require additional characterization to uncover their source. Coupling depth-sensing nanoindentation to additional characterization techniques such as electron microscopy (TEM, SEM), electrical contact resistance measurements, etc., in an in-situ, quantitative manner, represents an attractive way of time correlating an unusual feature of a load-displacement curve to the corresponding change in the microstructure of the sample being tested. This talk will demonstrate this capability by highlighting results from in-situ nanomechanical testing of materials. Some new developments with respect to in-situ measurement techniques will be presented and the potential application for structure-property correlation will be discussed.
Importance of AFM Beam Dynamics for the Extraction of Viscoelastic Sample Properties

Philip Yuya
University of Nebraska-Lincoln
W317.2 Nebraska Hall, Lincoln, 68588-0526, US
Phone: 402-472-4046, Email: philip.yuya@huskers.unl.edu

Joseph A. Turner
University of Nebraska Lincoln, Lincoln, NE

Abstract:

In contact resonance force microscopy, a cantilever beam is used to detect forces between the tip and the sample. AFM-based characterization techniques rely on the dynamics of the AFM cantilever as it vibrates while in contact with the sample of interest. In this presentation, we highlight the importance of modeling the dynamics of a cantilever beam accurately for measurements involving viscoelastic samples. The dependence of the quality factor for the vibration modes on the sample properties is shown to have a complex combination of beam and sample properties as well as the applied static tip force. The quality factor cannot be used to infer the sample damping directly. The application of this model for finding the sample damping in terms of the measured quality factor of a beam in contact with a PMMA sample is used to demonstrate its value. The nonlinear relation between quality factor and sample damping is examined for several different factors, the most important of which is the applied tip load. We propose a method for mapping the viscoelastic properties of a sample surface in terms of storage and loss moduli from quality factor and resonance frequency information.
MEMS Transducers for Nanomechanical Characterization

Yunje Oh
Hysitron, Inc.
10025 Valley View Road, Eden Prairie, 55344, US
Phone: 952-835-6366, Email: joh@hysitron.com

S.A. Syed Asif
Hysitron, Inc., Eden Prairie, MN

Oden L. Warren
Hysitron, Inc., Eden Prairie, MN

Abstract:

Transducers used in nanomechanical testing have precision actuation and high resolution displacement sensing. As more nanomechanical testing applications need to measure lower force and smaller displacement with better stability and faster operation speed, further advances in transducer technology are highly demanding. MEMS has been identified as one of the promising technologies to make highly sensitive transducers for those challenging measurements and we have opened a new era in this transducer technology with new transducer development. The developed MEMS transducers have high bandwidth dynamic characteristics as well as low noise and high precision actuation. The advantages of those MEMS transducers for the applications in nanoindentation, nanoscratc and fast-scanning are tremendous since they have unprecedented high bandwidth actuations and controllability. Owing to its small scale, MEMS transducer also can be used in instruments allowing small space for transducer placement such as inside TEM holders.
Quantitatively Exploring the Mechanical Behavior of Materials from the Nanoscale

Zhiwei Shan
Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano) and Hysitron Applied Research Center in China (HARCC), State Key Laboratory for Mechanical Properties of Materials, Xi’an Jiaotong University, Xi’an, China
Phone: 952-201-9216, Email: zwshan@mail.xjtu.edu.cn

Invited Presentation

Abstract:

In this talk, I will review our recent progress in applying the unique in situ TEM nanomechanical apparatus developed by Hysitron Inc. on submicron-sized materials. It was found that prior to the compression tests, the <111> orientated single crystal nickel pillars fabricated through Focused Ion Beam (FIB) contained a high density of defects. However, quite unexpectedly, the dislocation density was observed to decrease dramatically during the deformation process and, in some cases, even resulted in a dislocation-free crystal. The phenomenon, which we termed as “mechanical annealing”, is the first direct observation of the dislocation starvation mechanism and sheds new light on the unusual mechanical properties associated with submicron- and nano-scale structures [1]. Most recently, by using a combination of micro-compression and in situ nano-compression experiments, we found that the stress required for deformation twinning increases drastically with decreasing sample size of a titanium alloy single crystal, until the sample size is reduced to one micrometre, below which the deformation twinning is entirely replaced by less correlated, ordinary dislocation plasticity. Accompanying the transition in deformation mechanism, the maximum flow stress of the submicrometre-sized pillars was observed to saturate at a value close to titanium’s ideal strength. We develop a ‘stimulated slip’ model to explain the strong size dependence of deformation twinning. The sample size in transition is relatively large and easily accessible in experiments, making our understanding of size dependence relevant for applications [2]. Despite of numerous research works carried out inside TEM, how the interactions between high voltage accelerated electrons and specimen atoms influence the physical properties of materials remains elusive, especially in a quantitative manner. We demonstrate that the mechanical properties of SiO₂ glass particles can be altered dramatically with the low-dose (<1.8×10⁻² A/cm²) e-beam illumination. Unlike their bulk counterpart which is known to be typical brittle material at room temperature, we found that submicron-sized SiO₂ glass particles can be compressed into a pancake shape plastically under e-beam illumination. We also report the first quantitative comparison of the mechanical responses of these particles without and with the e-beam illumination, revealing that the flow stress can change up to 4 times [3]. Because SiO₂ glass are widely used in today’s electronic and optical devices with their dimensions comparable to those we investigated, our finding are expected to have significant implications for the technical applications in both micro- or nano- electromechanical systems (MEMS or NEMS) [4].

References:

Acknowledgement:
The work at Xi’an Jiaotong University was supported by the National Outstanding Young Investigator Grant of China (50925104). The work at Hysitron was supported in part by U.S. Department of Energy SBIR grants (DE-FG02-04ER83979, DE-FG0-07ER84813) awarded to Hysitron, Inc., which does not constitute an endorsement by DOE of the views expressed in the article. The work related to NCEM, Lawrence Berkeley Laboratory was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
Abstract:

Due to their high thermal resistance and outstanding mechanical strength under elevated temperatures, Si-C-O polymer derived ceramics (PDCs) have wide applications in glow plug heaters, thermal barrier coatings, and wear protection coatings. The structure at nanometer and micron length scale is the predominant property determining feature in such materials. The focus of present investigation is on understanding the effect of length scale and temperature on indentation creep of polymer derived Si-C-O nano-composites dip-coated on Fe substrate. The effect of temperature and testing scale on elastic modulus, creep stress exponent and creep rate was investigated by nanometer and micron scale indentation creep tests at temperatures ranging from room temperature up to 500 oC. The results of nanoindentation and microindentation based elastic moduli measurements showed that the elastic modulus of the material system first decreases as a function of temperature up to 100 oC and then increases with further increase in temperature. Nano and micro-indentation creep tests examined the effect of testing peak load, and holding time on the creep rate and creep stress exponent. The creep rate of the material system at high temperatures was found to be one magnitude higher than that at room temperature, while the stress exponent was found to be more than two magnitudes higher than that at room temperature. At room temperature, the measured stress exponent decreased by one magnitude in the micro-scale tests compared with that in the nano-scale tests under similar testing conditions, while the creep rate increased by 1 to 3 times. The testing results show a strong temperature and scale dependence of the creep stress exponent and creep rate of the material, which is mainly caused by softening of the SiO2 matrix at high temperatures and the temperature and scale dependent movement of the SiC particles in this SiO2 matrix.
High Temperature Nanoindentation: Nanomechanics at Elevated Temperatures

Gaurav Mohanty
Iowa State University
3326 Hoover Hall, Iowa State University, Ames, 50014, US
Phone: 515-451-0105, Email: gauravm@iastate.edu

Krishna Rajan
Iowa State University, Ames, Iowa

Abstract:

While nanoindentation is a well established technique, its extension to high temperatures is a recent development. We present detailed experimental studies to assess the technical challenges associated with conducting such measurements at 500C and beyond. The instrumental, calibration and data correction issues will be discussed. Examples of studies on different materials are presented and the value of measuring high temperature property data in terms of extracting fundamental materials deformation characteristics at the nanoscale level is also presented.
Experimental and Model Developments of Interfacial Mechanical Integrity of Layered Stacks

Ben Burke
Iowa State University
Department of Aerospace Engineering, Ames IA 50011-2271, US
Phone: 515-294-3039, Email: bastaw@iastate.edu

Hui Wang
Iowa State University, Ames IA

Wei Hong
Iowa State University, Ames IA

Ashraf Bastawros
Iowa State University, Ames IA

Abstract:

A novel method is developed to measure the adhesion and cohesion energies for ultrathin films, with no specimen preparation. The technique utilizes combination of nanoindentation and nano-acoustic emission (AE) measurement techniques. The total fracture energy is acquired from the displacement excursion on the load-indentation depth curve. The fracture energy partition between the adhesive and cohesive mode is done via the measured AE energy ratio for each event. Preliminary measurements of adhesive and cohesive energies for Nitrogen-doped silicon carbide, SiC\textsubscript{x}N\textsubscript{y} has been carried out. Detailed Finite element analysis is carried out using cohesive elements/surfaces. The analysis is utilized to set the applicability limits of the proposed technique and overcome several of the measurements limitations.
Nonlinear Vibration of an Embedded Carbon Nanotube in a Polymer Matrix

Liying Jiang  
The University of Western Ontario  
Department of Mechanical and Materials Engineering, London, N5X 2Y7, CA  
Phone: (519) 661-2111, ext., 80422,   Email: lyjiang@eng.uwo.ca

M.H. Mahdavi  
The University of Western Ontario, London, N5X 2Y7, CA

L. Y. Jiang  
The University of Western Ontario, London, N5X 2Y7, CA

X. Sun  
The University of Western Ontario, London, N5X 2Y7, CA

Abstract:

Since the discovery of carbon nanotubes (CNTs), these novel materials have attracted considerable attentions from research community. CNTs are found to possess superior mechanical, electronic and thermal properties. These extraordinary physical properties make CNTs hold promise for potential applications as nanodevices and nanocomposites. For the application and design of these nanocomposites, it is essential to investigate the effect of polymer matrix on the vibrational behavior of the embedded CNTs. In the current work, the effect of the surrounding medium on the CNT is described by van der Waals (vdW) forces. The intrinsic nonlinearity of vdW forces will arouse the nonlinear vibration of CNTs. Thus, the resonant frequencies of CNT are deflection dependent. Using both Euler-Bernoulli and Timoshenko beam models, the relation between deflection amplitudes and resonant frequencies of CNT is derived through harmonic balance method according to different end conditions. It is found that the end conditions, cross-sectional dimension and length of the embedded CNT have a significant effect on the resonant frequencies. It is also found that the applicability and the accuracy of Euler-Bernoulli and Timoshenko beam models are influenced by the surrounding medium. For double-walled CNTs embedded in the polymer matrix, another source for nonlinear vibration comes from the nonlinear vdW interactions between tubes. This interlayer vdW forces results in both coaxial and non-coaxial vibrations of the CNTs. The vibration amplitude for the non-coaxial mode is more dependent on the frequency in contrast to the coaxial mode. It is also found that the surrounding matrix has a significant effect on resonant frequency of the coaxial mode, but not on the non-coaxial mode.
Abstract:

Although considerable progress has taken place in the area of carbon nanotube (CNT) junction synthesis, properties and applications, major obstacles still remain in controlled synthesis, posing significant limitations for the development of new CNT-based applications. Existing approaches for synthesizing CNT junctions do not produce CNT junctions with good controllability or favorable selectivity and yield. Here, we report a new approach for synthesizing CNT junctions, based on self-assembling process from two tailored graphene nanoribbons (GNRs). CNT junctions with two-, three- and four terminals, starting from GNRs either with perfect or irregular tailoring, are synthesized. The functionality of these self-assembled CNT junctions for nano-electronics is then confirmed using charge transport simulations. Based on state-of-the-art experimental capability, this approach with identified scalability down to atomic scale and screening-free selectivity is practically realizable and desirable for individually controlling both the chirality and shape of CNT junctions, thereby dramatically improving their effectiveness and further expanding their application repertoire.
An Elastica Model that Describes the Buckling of Cross-sections of Multi-walled Nanotubes

Pat Wilber
University of Akron
Department of Mathematics, University of Akron, Akron, 44325, US
Phone: 330 972 6994, Email: jw50@uakron.edu

James Leta
The Equity Engineering Group, Inc., Shaker Heights, OH

Abstract:

We model the cross-section of a multi-walled nanotube as a collection of rods. Each rod is modeled as an elastica with a circular reference configuration, and neighboring rods interact by van der Waals forces. We formulate a two-point boundary-value problem for a system of nonlinear ordinary differential equations that govern the deformation of the cross-section. We describe the buckling of the rods from their circular configurations as a function of the radii of the circles. Our results include a detailed description of the buckling loads. Also, we study post-buckling behavior both analytically and numerically.
Understanding the Influence of Strain on Quantum Transport in Graphene

Md Hossain
University of Illinois at Urbana-Champaign
1206 W Green St, MC 244, Urbana, 61801, US
Phone: 2173778474, Email: hossain2@illinois.edu

Harley T Johnson
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Low-dimensional systems such as graphene, graphene nanoribbons, carbon nanotubes, and quantum dots show remarkable promise for next generation electronic device applications. Nevertheless, owing to their nanoscale dimensions they are susceptible to undergo structural modifications and respond to thermal excitations or chemical interactions with dielectric surfaces, electrode contacts, or foreign atoms. An immediate technological concern of these nanoscale effects is the degradation or modulation of their outstanding material properties that can eventually impact their efficiency, reliability and performance in device applications. Here, using first-principles calculations it is revealed that graphene’s ballistic conductance which is defined by $G = G_0 T(E)$, where $G_0$ is the quantum of conductance and $T(E)$ is the total transmission at energy $E$, and expressed as a sum over the transmission probabilities of the conducting eigenchannels can be modulated by strain. In contrast to the assumption that graphene’s ballistic conductance is a constant, this research shows that strain alone can increase or decrease graphene’s ballistic conductance significantly.

Strain is unavoidable in graphene either suspended or supported on a dielectric substrate, such as SiO$_2$. In suspended graphene, strain is biaxial type and one-atom thick graphene is under tension along the transport direction. On the other hand, supported graphene can have hydrostatic strain arising from well-known structural corrugations. It is therefore crucial to identify the role of strain on transport properties in graphene. In a recent experiment, it is shown that local strain in graphene on a SiO$_2$ substrate can modify graphene’s conductance near the Fermi energy. The modification is attributed to a coupling of strain and phonon-mediated inelastic tunneling effects. However, conductance on the dielectric substrate is not ballistic and isolating the influence of strain is not possible. In this study, strain effects on ballistic conductance, an experimentally attainable transport property for suspended graphene, is studied using a combination of density functional theory and the Landauer-Buttiker formalism, and the results are presented in an article published recently [Appl. Phys. Lett. 96, 143118 (2010)]. It is demonstrated that, unlike in a CNT, regardless of the applied strain graphene’s conductance at the Fermi energy is 0.21$G_0$. Furthermore, for conducting electrons with energies higher or lower than the Fermi energy of the system tensile hydrostatic strain is found to increase conductance but compressive hydrostatic strain decreases conductance. For an 8% compressive hydrostatic strain conductance increases by as large as 30%. Surprisingly, for biaxial strain, if the energy of the conducting electrons is higher than the Fermi energy, conductance remain approximately unchanged, whereas conductance by electrons less than the Fermi energy decreases (increases) with compressive (tensile) strain along the transport direction. With technological advances, approaching ballistic values...
of electron conductance and harnessing the maximum possible conductance in graphene have now become possible. Thus the findings of this work would advance efforts in further enhancing superior transport characteristics in graphene.
Temperature and Strain Rate Sensitivity of Nanocrystalline Metals

Nikhil Karanjgaokar
Mechanical Science and Engg, University of Illinois at Urbana-Champaign
325 Talbot Lab, 104 S Wright St, Urbana, 61801, US
Phone: 2172333122, Email: nkaranj2@illinois.edu

Ioannis Chasiotis
Aerospace Engg., University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Nanocrystalline metal thin films are excellent materials for microelectromechanical Systems (MEMS) and microelectronics due to their outstanding electrical conductivity and high yield strength. However, our recent studies have shown that nanocrystalline FCC metal films are highly strain rate sensitive and their primary creep rates at room temperature are several orders of magnitude higher than the steady-state creep rates previously reported for meso- and micro-scale grain metals. This time dependent inelastic behavior is further accentuated at elevated temperatures: A comprehensive experimental investigation has been carried out to quantify for the first time the strain-rate dependent mechanical behavior of nanocrystalline Au thin films (grain size 64 nm) at strain rates in the broad range of 0.000001 - 10 /s and at temperatures between 25-110° C. Full-field strain measurements of uniformly heated sub-micron thick Au films were supported by microscale infrared temperature profiles for accurate and repeatable experiments. Contrary to expectations, relatively low temperatures (50 °C) resulted in marked shift in rate sensitivity and activation volumes providing strong evidence that nanocrystalline metals are significantly more temperature sensitive than their larger grain counterparts. This presentation will discuss these novel results and the interrelations between strain rate and temperature in nanocrystalline metals.
Theoretical and Computational Studies of Defects in Crystals and the Mechanical Properties of Solids

ORGANIZERS:

Scott Beckman, Iowa State University
The Influence of Chemical Substitution on the Mechanical Behavior of AlMgB\textsubscript{14} Studied by First Principles Methods

Liwen F. Wan
Iowa State University of Science and Technology
Department of Materials Science and Engineering, 2220 Hoover Hall, Ames, IA 50011, USA
Phone: 515-231-9455, Email: wliwen@iastate.edu

S. P. Beckman
Iowa State University of Science and Technology, Ames, IA

Abstract:

Due to their high hardness and chemical inertness the orthorhombic boron-riched borides have recently attracted the attention of engineers for possible uses as protective surface coatings, cutting tool edges, and as an abrasive medium. The measured hardness of AlMgB\textsubscript{14}, prepared by flux growth, is as large as 35 GPa, but the hardness of AlMgB\textsubscript{14} grown by mechanochemical synthesis is as large as 45 GPa. The principle difference between the two growth methods is the concentration of defects and impurities. The common substitutional impurities include Fe, vacancies, C, Ti, and intermetallic atoms. In particular the addition of TiB\textsubscript{2} is shown to significantly improve the mechanical performance. In this work the influence of impurity substitution on the bonding properties of AlMgB\textsubscript{14} is studied by ab initio methods. It is observed that the metal atoms are primarily electron donors and are not strongly bonded to the B covalent network. The substitution of impurities at the metal atom sites results in a rigid shift of the Fermi level within the electronic density of states. It is also observed that modifying the Fermi level, by changing the electron occupation number in the calculation, has a large impact on the volume of elastic parameters of the system. The connection between atomic substitution, the density of states, and the elastic response is investigated. In addition to studying atomic substitution at the metal sites, impurities in the B network are investigated. It is believed that C is the most likely element to substitute in the B\textsubscript{12} icosahedra. Although C can occupy any B site without destroying the crystalline structure, it is observed that the impurity atoms strongly prefer to occupy either the apex position in the icosahedra or the interstitial boron site that is located between the icosahedra. The influences of C on the elastic properties of AlMgB\textsubscript{14} are reported here.
Modeling Defect Chemistry for Scintillator Materials via Informatics

Chang Sun Kong
Iowa State University
Department of Materials Science and Engineering, 2220 Hoover Hall, Ames, IA 50011-2300, USA
Phone: 515-294-2670, Email: cskong@iastate.edu

Prasanna Balachandran
Iowa State University, Ames, IA

Scott Broderick
Iowa State University, Ames, IA

Krishna Rajan
Iowa State University, Ames, IA

Abstract:

Inorganic scintillators have the wide ranging applications as a high energy, ionizing radiation detector in scientific, medical, industrial and many other fields. Prompted by the highly diverse and specific needs on novel scintillator materials, the extensive efforts have been continued in this field by means of both experimental and computational methods. At present, the two-fold objective of the scintillation materials research, i.e. the improvement of existing scintillators and the development of completely new scintillation materials, is being guided by much larger knowledge/data bases accumulated over the past several decades.

The performance of a scintillator is highly influenced by varying degrees of multiple conditions of the selected materials. Finding the materials criteria to attain the target performance becomes therefore a crucial part of the development of novel scintillation materials. The scintillation efficiency of a material is known to be largely determined by the presence and formation of defects, and can be improved via co-doping. However, co-doping presents a multi-dimensional problem by considering the charge and ionic radii of co-dopant, ionic radii of impurity, and ionic radii of host lattice, beyond the identification of defect mechanisms. Beginning with the existing studies measuring defect mechanisms, we apply informatics to fully assess the multi-dimensional parameters with scintillation efficiency to optimize the lattice and co-dopant selection. In addition to the scintillation efficiency, the mechanical strength of solid phase scintillators is a key requirement along with other optical performances and chemical resistance for the practical applications. Using statistical learning and data mining methods, we investigate the effects of atomic point defects on the mechanical stability of the inorganic scintillator materials.

Using these new informatics based approaches, we have predicted defect mechanisms, as well as the relationships between the defective crystal structure at the atomic length scale and macroscopic mechanical tolerance of scintillator crystals. This work thus provides a template for optimizing the performance of scintillator materials.
Abstract:

Static multiscale and atomistic simulations aim to obtain an equilibrium configuration (local energy minimum) of a body composed of discrete atoms subject to applied loads and/or displacements. Often a system of "proportional loading" is considered and the evolution of the body's equilibrium configuration is determined in an incremental fashion as the scalar "loading parameter" is varied. At each step, a minimization procedure, such as the conjugate gradient method, is employed using the previous relaxed configuration as an initial guess.

A practical problem with such simulations is that due to the highly nonlinear nature of such problems, many equilibrium configurations should be expected -- especially at instabilities that lead to defect nucleation. Unfortunately, the simulation procedure described above provides only one of the possible equilibrium evolutions. Even more troubling is the fact that this one equilibrium evolution will, generally, depend on the numerical energy minimization method employed and the particular values used for its parameters.

This work takes a different approach to the exploration of the equilibrium behavior of atomistic and multiscale systems. It performs a Branch-Following and Bifurcation (BFB) investigation in order to map out a large number of equilibrium configurations over a wide range of the problem's loading parameter. Once a reasonably complete picture of the system's possible behaviors is in hand, it is then possible to interpret these results to draw conclusions about the most likely behavior of the system.

To illustrate this novel application of BFB methods to atomistic multiscale problems, some representative problems will be presented including the results for a small "simple" atomic column subjected to axially compressive displacements will be presented. The set of possible equilibrium states found is much more complex than first expected and is a vivid illustration of the complex behavior these systems are capable of. These results will be described as well as some suggestions for "new" simulation/interpretation procedures.
Density-functional-theory Results for the Vacancies and Self-Interstitials in GaAs

Alan Wright
Sandia National Laboratories
Albuquerque, NM 87185-1415, USA
Email: afwrig@sandia.gov

N. A. Modine
Sandia National Laboratories, Albuquerque, NM

Invited Presentation

Abstract:

Density-functional-theory calculations have been performed for the vacancies and self-interstitials of GaAs in order to advance understanding of gain degradation and recovery in GaAs-based heterojunction bipolar transistors (HBT’s) exposed to high-energy neutron irradiation. A survey was first performed, using moderate levels of precision in 216-atom cells, to identify the charge states, stable configurations, and migration pathways of the vacancies and self-interstitials. Additional calculations were then performed to resolve cell size dependences in results for the As interstitial, which was found to have the lowest diffusion activation energies among these defects and thereby will be most likely to contribute to gain recovery in HBT’s. The additional calculations employed 216-, 512-, and 1000-atom cells and a fit of their formation energies to the Makov-Payne formula to obtain formation energies at infinite cell size where spurious cell-to-cell electrostatic interactions are zero. Results will be presented pertaining to defect charge states, structures, diffusion paths, activation energies, and levels in the gap.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration under Contract DE-AC04-94AL85000.
Coarse-Graining Atomistic Dynamics of Dislocations: from the Atomic to the Mesoscopic

Liming Xiong
University of Florida
Department of Mechanical and Aerospace Engineering, 2901 SW 13th ST 325, Gainesville, FL 32608, USA
Phone: 352-871-4014, Email: lmxiong@ufl.edu

Youping Chen
University of Florida, Gainesville, FL

Abstract:
This paper presents a new methodology for coarse-grained atomistic simulation of dislocation dynamics. The methodology combines an atomistic formulation of balance equations and a modified finite element method with rhombohedra-shaped 3D solid elements. With significantly less degrees of freedom than that of a fully atomistic model and without additional constitutive rules to govern dislocation activities, this new coarse-graining (CG) method is shown to be able to reproduce key phenomena of dislocation dynamics, including dislocation nucleation and motions, formation of stacking faults and Lomer-Cottrell locks, and splitting of stacking faults, all comparable with atomic-level molecular dynamics simulations. Using a uniform coarse mesh, the CG method is then applied to simulate a submicron-sized copper thin film without introduction of initial dislocations in the specimen. The results show that the CG simulation has captured the nucleation and migrations of large amount of dislocations, formations of multiple stacking fault ribbons, and the occurrence of complex dislocation activities such as dislocation annihilations and dislocation cutting and passing through the stacking faults. The distinctions of this method from existing coarse-graining or multiscale methods and its potential applications and limitations are also discussed.
Dislocation Glide Mediated Plasticity in Carbon Nanotubes

Elif Ertekin
Massachusetts Institute of Technology
Department of Materials Science, 77 Massachusetts Avenue, Rm 13-4080, Cambridge, MA 02139, USA
Phone: 510-847-7073, Email: elif1@mit.edu

Shuo Chen
University of California, Berkeley, Berkeley, CA

D. C. Chrzan
University of California, Berkeley, Berkeley, CA

Abstract:
The types of mechanical behaviors exhibited by carbon nanotubes are rich, from ultra high tensile strengths to abilities to withstand large torsional strains to ductile and brittle fracture to superplastic elongation at high temperatures. The carbon nanotube, with its special geometry and topology, gives us a unique opportunity to explore defect-mediated deformation in two-dimensional surfaces embedded in three-dimensional space. Defects known as Stone-Wales defects are the two-dimensional analog to deformation-mediating dislocations in conventional bulk materials, and have long been implicated in the plasticity of carbon nanotubes. In this talk, a continuum based topological elasticity theory that can accurately predict the energies of Stone-Wales defects in carbon nanostructures will be discussed. In this theory, no a priori assumptions about the analytical form of the dislocation strain fields are made, and boundary conditions and defect-defect interactions are explicitly considered. The formalism reproduces trends in defect energetics obtained in atomistic simulations remarkably well, and demonstrates the necessity of considering long-ranged effects to accurately describe defect energetics in graphene-based systems.

Then, a new Monte Carlo formalism for describing large-scale deformation of nanotubes will be introduced. In this formalism, deformation is described as a sequence of bond rotations within the graphene lattice consisting of dislocation formation, propagation, and annihilation. Within this formalism, a new type of defect that may facilitate plastic deformation in carbon nanotubes is identified. This defect is composed of a linear array of Stone-Wales defects -- in effect, a dislocation whose strain fields are screened by other dislocation dipoles -- that wanders through the nanotube as the nanotube is plastically deformed under high stress conditions. The existence of this defect, which is called a dislocation worm, is attributed to a competition between dislocation core energy, the screened (or unscreened) dislocation strain fields, and the buckling of the graphene membrane that takes place to accommodate the large strain fields. Thus, the lengths of the dislocation worms propagating through the nanotube exhibit a dependence on the applied stress and the nanotube radius. In graphene and large radii nanotubes, in which isolated dislocations have large strain fields and small accommodation by buckling, the worm length is much larger. For nanotubes with sufficiently small radii, buckling allows for the reduction in the energy of an isolated dislocation, and hence the associated worm length is smaller. A transition from worm-mediated deformation to conventional isolated dislocation glide-mediated deformation is predicted based on this analysis. The results of kinetic Monte Carlo
simulations will also be discussed, demonstrating that even when the effects of temperature and bond rotation energy barriers are considered, the dislocation worms are observed to play a role in nanotube deformation. Finally, the influence of these defects on the predicted mechanical properties of carbon nanostructures will also be considered.
The Structural Complexity of the 90° Partial Dislocation Cores in Diamond Cubic Semiconducting Crystals

Peter J. Huffman  
Iowa State University  
Department of Materials Science and Engineering, 2220 Hoover Hall, Ames, IA 50010, USA  
Email: phuffman@iastate.edu

D. C. Chrzan  
University of California, Berkeley, CA

S. P. Beckman  
Iowa State University, Ames, IA

Abstract:

Modern electronics are rapidly shrinking. As the smallest transistor gates approach 20nm, crystallographic defects become increasingly important to device performance. Dislocations in semiconductors are not well understood. In spite of extensive effort toward predicting their presence and behavior, their small size makes them difficult to observe even with the most advanced microscopy techniques available. The directionality and covalent character of the bonding also makes their behavior more difficult to predict. Elasticity theory does not adequately describe the impact that dislocations have on the electronic and optical properties of semiconductors, in part due to the difficulty in predicting long-range interactions and strain fields caused by the dislocations. Because of this, it is necessary to understand the atomic bonding in the core of the dislocation. There are two proposed ground state structures for the 90° partial dislocation core in diamond cubic crystals, the so-called single and double period structures. It is predicted that the energy difference of these phases is small, and it is likely that the two will coexist along the same dislocation line. In addition to the ground state structures, there exists a plethora of structural point excitations including kinks and phase interfaces. While it is desirable to apply high-precision quantum mechanical techniques to investigate the evolution of the dislocation core structure at finite temperature, such calculations introduces unnecessary complexity and computational cost. Instead, a simple statistical mechanical model is constructed and used to investigate the thermal dependency of the core structure. Using this method the essential physical interactions are captured within a scalable Monte Carlo framework. The bonding and excitation interactions can be parameterized from atomic scale calculations or experimental measurements. Using this model, the temperature dependent structure and phase interactions along the dislocation line are predicted. It is found that the double period reconstruction is stable at low temperatures, but an amorphous reconstruction is energetically favorable at higher temperatures. For a small energetic advantage the double period phase becomes substantially more stable than the single period phase, whereas a much larger energetic advantage is required for the single period phase to become stable.
Dislocation Cores in Elastically Anisotropic Materials

D. C. Chrzan
University of California at Berkeley
Department of Materials Science and Engineering, 318 Hearst Memorial Mining Building, Berkeley, CA 94720, USA
Phone: (510) 643-1624, Email: dcchrzan@berkeley.edu

M. P. Sherburne
University of California, Berkeley, CA

Y. Hamlumyuang
University of California, Berkeley, CA

T. Li
George Washington University, Washington, DC

J. W. Morris
University of California, Berkeley, CA

Abstract:

The core structures of dislocations in elastically anisotropic materials are considered. The dislocation core radius is defined to be that radius for which continuum linear elasticity theory predicts that the dislocation stress field exceeds the ideal strength of the material. For screw dislocations in elastically isotropic materials, this definition yields a dislocation core radius equal to $b$, the magnitude of the Burgers vector. However, for elastically anisotropic materials, the dislocation core radius can be much larger. In the case of strongly elastically anisotropic materials, such as the Ti-Nb based alloys known as Gum Metals, the core radii are expected to be very large -- so large that the core radii for adjacent dislocations overlap. The atomic scale structures of dislocation cores in such materials are studied using first principles electronic structure based methods. The predicted atomic scale structures are reminiscent of the “nanodisturbances” observed in Gum Metals. The implications for the mechanical properties of such materials are discussed. This research is supported by the US National Science Foundation under Grant No. DMR-0706554. Computations were conducted using the resources at the National Energy Research Supercomputer Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
Limits to Poisson's Ratio in Isotropic Materials

Peter Mott
US Naval Research Laboratory
Code 6120, Washington, DC 20375, USA
Phone: 202-767-1720, Email: peter.mott@nrl.navy.mil

C. Michael Roland
US Naval Research Laboratory, Washington, DC

Abstract:

A long-standing question is why Poisson’s ratio, \( \nu \), nearly always exceeds 0.2 for isotropic materials, whereas the limits from linear elasticity are from -1 to 1/2. We show that the roots of quadratic relations from linear elasticity divide \( \nu \) into three possible ranges: \(-1 < \nu \leq 0\), \(0 \leq \nu \leq 1/5\), and \(1/5 < \nu < 1/2\). Since elastic properties are unique there can be only one valid set of roots, which must be \(1/5 \leq \nu < 1/2\) for consistency with the behavior of real materials. Materials with Poisson’s ratio outside of this range are rare, and tend to be either very hard (e.g., diamond, beryllium) or porous (e.g., auxetic foams); such substances have more complex behavior than can be described by classical elasticity. Thus, classical elasticity is inapplicable whenever \( \nu < 1/5 \), and the use of the equations from linear elasticity for such materials is inappropriate.
Strain Rate Effects in Low Impedance Materials

ORGANIZERS:

Eric Brown, Los Alamos National Laboratory
Phillip Rae, Los Alamos National Laboratory
Dynamic Tensile Characterization of Foam Materials

Bo Song  
Sandia National Laboratories  
7011 East Avenue, Livermore, 94551, US  
Phone: 925-294-2699, Email: bsong@sandia.gov

Helena Jin  
Sandia National Laboratories, Livermore, CA

Wei Yang Lu  
Sandia National Laboratories, Livermore, CA

Abstract:

Due to their superior performance of impact energy absorption, foam materials have been used in many packaging and transportation applications to protect the inside electronic devices from external impact. The mechanical properties of the foam materials are desired to be understood under different loading conditions particularly at high rates of loading. Compared to extensive investigation under high-rate compression, dynamic tensile experiments on the foam materials have been less touched due to experimental difficulties. In this study, we employed the newly developed Kolsky tension bar at Sandia California to explore dynamic tensile testing of the foam materials. Remedies including employing laser displacement measurement, digital image correlation, and highly sensitive transducers have been implemented to the Kolsky tension bar technique. These remedies validate the testing conditions in the Kolsky tension bar experiments. Dynamic tensile stress-strain curves at various strain rates are obtained. Strain rate effects on the tensile response are also investigated.

ACKNOWLEDGEMENTS
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.
Abstract:

Dynamic-Tensile-Extrusion (Dyn-Ten-Ext) experiments have been utilized to probe the dynamic tensile responses of polytetrafluoroethylene (PTFE) and polychlorotrifluoroethylene (PCTFE). These fluoropolymers exhibit more irregular deformation and stochastic-based damage and failure mechanisms than the stable plastic elongation and shear instabilities observed in metals. The technique elucidates a number of tensile mechanisms that are consistent with quasi-static, SHPB, and Taylor Impact results. Similar to the observed ductile-to-brittle transition for Taylor Impact loading, PCTFE failure occurs at a peak velocity greater than for PTFE. However, for the Dyn-Ten-Ext PCTFE exhibits even greater resistance to failure due to the tensile stress-state. While PTFE generates a large number of small fragments when extruded through the die, PCTFE draws out a smaller number of larger particles that dynamically evolve during the extrusion process through a combination of local necking mechanisms and bulk relaxation. Under Dyn-Ten-Ext loading, the propensity of PTFE to fail along normal planes is observed without indication of any localization, while the PCTFE clearly forms necks during the initial extrusion process that continue to evolve.
Impulsive Pressurization of Neuronal Cells

Matthew Nienaber
University of Nebraska-Lincoln
Department of Engineering Mechanics, 317.4 Nebraska Hall, Lincoln, 68588-0526, US
Phone: 402-472-0953, Email: mattn@huskers.unl.edu

J. S. Lee
Department of Engineering Mechanics University of Nebraska Lincoln, Lincoln, NE

R. Feng
Department of Engineering Mechanics University of Nebraska Lincoln, Lincoln, NE

J. Y. Lim
Department of Engineering Mechanics University of Nebraska Lincoln, Lincoln, NE

Abstract:

Blast-induced traumatic brain injury (bTBI) has become one of the leading injuries of the U.S. soldiers involved in the current military operations. One possible mechanism for bTBI is blast-induced overpressure, or high stress impulse in the brain. To study the functions of the neuronal cells exposed to the pressure impulses relevant to the blast loading generated by improvised explosive devices, we have developed a new compressional Kolsky bar experiment. The technique uses pre-stalled elastic strain energy in the input bar to produce a trapezoidal stress pulse that can be varied in length and intensity based on the apparatus’s configuration. The impulsive loads up to 1.0-ms duration can then be applied to an in vitro neuronal cell sample contained in a cylindrical pressurization chamber. The pressurized neuronal cell sample is then studied with microscopy for morphology and assays for assessing gene expression specific to apoptosis and neuronal cell markers and in comparison with the control sample. Results will be presented for pressurization levels of 0.5, 1.0, and 2.0 MPa. Issues regarding dynamic loading and measurement at very low stress levels, test chamber seal, variable pulse duration, and effective prevention of reloading will also be discussed in detail.
Wave Profile Shaping for Shock-Tube-Simulated Blast Testing

Nicholas Kleinschmit  
University of Nebraska-Lincoln  
941 Roanoke Ct. Apt 10, Lincoln, 68510, US  
Phone: 402 841-2833, Email: n_kleinschmit@yahoo.com

Aaron Douglas Holmberg  
University of Nebraska Lincoln, Lincoln, NE

Ruqiang Feng  
University of Nebraska Lincoln, Lincoln, NE

Abstract:

Blast-induced traumatic brain injury (bTBI) caused by exposure to detonation of improvised explosive device (IED) has become one of the leading injuries of the U.S. soldiers in recent military operations. Well-controlled laboratory experiments that can simulate the IED-induced blast loading are critically important for bTBI-related studies, especially those aimed at determining the pathological mechanisms leading to bTBI. To address this need, we have explored the use of shock tube for simulating the typical open-field blast loading, which has a wave profile similar to that of a Friedlander wave. A specially designed shock tube has been constructed at the University of Nebraska-Lincoln. Preliminary experiments have been carried out. Designs and measurements will be presented to demonstrate how to shape the air shock wave profile in the shock tube to the desired blast loading at a particular location, how to minimize the unwanted secondary shock, and how to prevent excessive magnitude of the negative (vacuum) pulse, which is crucial for preserving the specimen in blast testing of animal modes.
Shock-Tube-Simulated Blast Wave Propagation and Interactions with Solid Structures

Aaron Holmberg
University of Nebraska-Lincoln
5055 Francis St, Lincoln, 68504, US
Phone: 402 326-8888, Email: holmbergaaron@hotmail.com

Nicholas N. Kleinschmit
University of Nebraska Lincoln, Lincoln, NE

Ruqiang Feng
University of Nebraska Lincoln, Lincoln, NE

Youn Do Ha & Florin Bobaru
University of Nebraska Lincoln, Lincoln, NE

Abstract:

In recent U.S. military conflict an increased number of soldiers have been returning with mild traumatic brain injuries (mTBI) caused by exposure to improvised explosive devices (IED). Experimental techniques for simulating blast wave loading and testing head protection systems in laboratory setting are crucially important for mTBI-related studies. As part of a trauma mechanics research project sponsored by Army Research Office, we have recently developed a shock tube apparatus designed specifically for simulating blast loading caused by IEDs. The characteristics of the blast-like air shock wave generated by the apparatus have been studied experimentally and computationally in terms of its wave front planarity, its wave profile variation with propagation distance, and its interactions with elastic solid structures of various configurations. Experimental measurements will be presented along with the results of numerical simulations performed using the arbitrary Eulerian-Lagrangian coupling method available in the ABAQUS finite element code. Issues related to the proper use of piezoelectric sensors for diagnostics of the propagation of shock-tube-simulated blast wave will also be discussed in detail.
Size Scale Effects in Micro/Nano Structured Materials and Composites

ORGANIZERS:

Rashid K. Abu Al-Rub, Texas A&M University
Non-local Models for Dynamic Fracture and Damage in Brittle Materials with Peridynamics

Florin Bobaru
University of Nebraska - Lincoln
Department of Engineering Mechanics, W317 Nebraska Hall, Lincoln, 68588-0526, US
Phone: 402-472-9490, Email: yha4@unl.edu

Abstract:

Experimental observations indicate that dynamic fracture in brittle materials is a complex phenomenon influenced strongly by stress wave interactions. Crack branching takes place when a certain stress intensity magnitude and distribution are reached around the crack tip. The problem of modeling the behavior of brittle cracks running dynamically has been under study for many decades, and yet the problem has remained largely unsolved. Here we present results on dynamic brittle fracture using peridynamics, in particular the dynamic crack branching problem. Peridynamics is an extension of the classical continuum theory well suited for modeling of problems where discontinuities (such as cracks) initiate, propagate, and interact dynamically. The departure from the classical approach is conceptually significant, and the benefits from this departure are yet to be fully explored. In peridynamics, material points are thought to interact through long-range forces. This fundamental modification of the classical continuum model results in a mathematically-sound formulation well suited for modeling, for example, fracture in a much simplified way. As a result, in peridynamics cracks are part of the solution, not part of the problem. The peridynamic analysis can capture a wide range of behaviors of dynamic brittle fracture phenomena, including cascade crack branching, microcracking, secondary cracking (at ~90 degree angles from primary cracks), etc. Also, we present models and simulations with peridynamics that show crack propagation speeds at branching, for cracks running dynamically in brittle materials, in the range of those measured in the experiments. In theoretical models, the predicted velocity for when crack branching should happen is much higher than the actual values observed in experiments. No explanation for this discrepancy has been offered so far. Through numerical investigations with the developed peridynamic model, we comment on the influence of stress waves on slowing down the crack or changing the direction of the crack path. The numerical results compare favorably with the experimental results.
Atomistic and Continuum Understanding of the Particle Clustering and Particle Size Effect on the Room and High Temperature Strength of SiCN Nanocomposites

Vikas Tomar
Purdue University-West Lafayette
3205 ARMS, 701 W Stadium Avenue, West Lafayette, 47907, US
Phone: 3172943251, Email: tomar@purdue.edu

Abstract:

Silicon Carbide (SiC)-Silicon Nitride (Si3N4) nanocomposites are future important high temperature materials. Factors that could affect the mechanical strength of such nanocomposites include nanodomains size, grain boundary (GB) thickness and strength, thickness of domain boundaries, sizes of SiC particle etc. This work presents our recent findings that analyze the effect of morphological variations in second phase SiC particle placement and GB strength on the room temperature fracture strength of SiC-Si3N4 nanocomposites using continuum analyses based on a mesoscale (~50 nm) cohesive finite element method (CFEM) and using molecular dynamics (MD) based analyses at nanoscale (~15 nm). CFEM and MD analyses have revealed that high strength and relatively small sized SiC particles act as stress concentration sites in Si3N4 matrix leading to inter-granular Si3N4 matrix cracking as a dominant failure mode. However, the particle’s presence does not have a significant effect on the mechanical strength of bicrystalline or nanocrystalline Si3N4 phase matrices. The strength of the structures showed an uncharacteristic correlation between the GB thickness and temperature. The strength showed decrease with increase in temperature for structures with thick GBs. However, for structures with no appreciable GB thickness, due to the particle clustering and increase in SiC-Si3N4 interfacial strength with temperature, the strength improved with increase in temperature. Overall, analyses confirm that the temperature dependent strengthening in both the nanocomposite material systems is a function of GB thickness, particle clustering, grain size, and temperature.
Dislocation Dynamics Simulations of Plasticity at Small Scales

Caizhi Zhou
Iowa State University
3159 Gilman Hall, Ames, 50011, US
Phone: 515-294-9984, Email: zhou@iastate.edu

Richard LeSar
Iowa State University, Ames, IA

Abstract:
In the past few decades, small-scale metallic structures have been widely utilized in microelectronic circuits, optical and magnetic storage media, micro-electro-mechanical systems (MEMS) and so on, owing to their excellent mechanical, chemical, or electrical properties. Recently, size-dependent deformation properties of single crystals have attracted much attention in the materials science community, in part because they are closely related to the reliability of such structures in technical applications. The objective of our study is to identify what critical events (i.e., dislocation multiplication, storage, nucleation and reactions etc.) determine the deformation response at small scales and how these change from bulk behavior as the system decreases in sizes and improve our current knowledge of bulk plasticity with the knowledge gained from the direct observations of small-scale plasticity. Discrete dislocation dynamics simulations in three dimensions have been used to examine the role of dislocation multiplication and mobility on the plasticity in small samples under uniaxial compression. To account for the effects of the free surfaces a boundary element method, with a superposition technique, was employed. Cross-slip motion of the dislocation was also included, and found to be critical to the modeling of the dislocation behavior. To compare directly with recent experiments on micropillars, simulation samples at small volumes were created by cutting them from bulk three-dimensional simulations, leading to a range of initial dislocation structures. Comparison of the simulation results and the experiments are excellent, finding essentially identical behavior. Examining details of the dislocation mechanism illuminates many features unique to small samples and point directly to the importance of both the surfaces forces and cross-slip in understanding small-scale plasticity. Dislocation sources can be formed by cross-slip in confined volumes and have shorter residence lifetime in smaller samples under the influence of attractive image forces and confined geometries. The general single-arm source model can not only reasonably predict the increase of yield strength with sample sizes decreasing, but also the statistical variation of the strength at small scales. With the decrease of sample sizes and initial dislocation density, starvation hardening and nucleation of surface dislocations will dominate plastic deformation process at post-yielding region, while the extra strength increase with the strain in larger samples is mainly due to the exhaustion hardening caused by dislocation reactions.
Physical Interpretation and Experimental Identification of the Length Scale Parameter in Gradient Plasticity

Rashid Abu Al-Rub
Texas A&M University
3136 TAMU, 710 B CE/TTI Building, College Station, 77843, US
Phone: 9798626603, Email: rabualrub@civil.tamu.edu

Abstract:

Recently, there has been a great interest in formulating and applying gradient and nonlocal plasticity theories in order to bridge the gap between material length scales. The theory overcomes many of the limitations of classical (local) plasticity theory in predicting size scales effects at the macro to nano length scales due to the incorporation of a material length scale parameter. However, one of the biggest issues in applying the nonlocal gradient plasticity theory to engineering problems is the physical interpretation and experimental identification of the material length scale parameter. Therefore, in this study, this issue is discussed thoroughly based on dislocation mechanics and micro/nano-indentation testing. In micro- and nano-indentation tests for evaluating strength and stiffness properties of engineering materials, a commonly observed phenomenon is the dependence of material properties on the indent size, also known as, indentation size effect (ISE). In this study, a micro-mechanical based model is developed based on dislocation mechanics for predicting ISE from conical or pyramidal (Berkovich and Vickers) indenters, and is compared with the most widely used Nix-Gao model. The key idea proposed here while deriving the model is a nonlinear coupling between the geometrically necessary dislocations (GNDs) and the statistically stored dislocations (SSDs) that eventually allows it to simultaneously predict ISE from both micro- and nano-indentations tests on a wide range of metallic materials while the Nix-Gao model fails to do so. A fundamental difference between the formulation of the present ISE model and that of Nix-Gao model is in the assumed coupling between the densities of SSDs and GNDs in the Taylor’s hardening law for metals such 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. The current study also presents a method for identifying the length scale parameter from micro- and nano-indentation experiments and also correlates it with the spacing between dislocations and thus gives a physical interpretation of the material intrinsic length scale. Moreover, based on many micro- and nano-indentation experimental data for many metals, it is shown that this length scale parameter is not fixed but evolves with deformation and microstructural features.
Thermodynamic-based Higher-order Gradient Plasticity Captures Size and Interfacial Effects at the Micron and Submicron Scales

Masoud Darabi
Texas A&M University, Zachry Department of the Civil Engineering, Texas A&M University, College Station
Phone: 979-739-7504, Email: masouddrb@neo.tamu.edu

Rashid K. Abu Al Rub
Texas A&M University, College Station, Texas

Abstract:
It is well-known by now that the classical (local) plasticity theories cannot be used successfully in predicting the experimentally observed size-effect (i.e. smaller is stronger) at micron and submicron length scales. Therefore, in the past decade there has been a significant interest by the mechanics community in formulating higher-order gradient plasticity based on laws of thermodynamics. Most of these theories have been shown to completely or partially solve the problem of strain localization and/or size-dependent problems at the micron and submicron length scales. However, at very small scales with high ratio of the surface-to-volume, the free and bounded interfaces play a significant role in size-dependent yield strength in materials. For these cases, a lower-order gradient plasticity theory could not predict any boundary layer effect, which makes them unsuitable for modeling interfacial effects in thin films, particle-matrix interfacial effects in nanocomposites, and nonuniform and scale-dependent response of micropillars under uniform stressing. Moreover, very few of the gradient plasticity theories correctly estimate the rate of energy dissipation due to local and nonlocal effects. The correct estimation of rate of energy dissipation requires the decomposition of thermodynamic conjugate forces into energetic and dissipative components as it is shown in the pioneering works of Shizawa and Zbib [1] and Gurtin [2].

A thermodynamic based higher-order gradient plasticity theory that enforces microscopic boundary conditions at interfaces and free surfaces and decomposes all thermodynamic conjugate forces into energetic and dissipative components is presented in this work. The elastic strain tensor, the effective plastic strain, and its gradient are assumed as the state variables. It is shown that interfacial effects have a profound impact on the scale-dependent yield strength and strain hardening of micro/nano-systems even under uniform stressing. Energetic components of the thermodynamic conjugate forces are related to the Helmholtz free energy and dissipative components of the thermodynamic conjugate forces are related to the rate of energy dissipation. Moreover, a procedure based on maximum energy dissipation principle is proposed for deriving the dissipative components directly from the rate of energy dissipation. A systematic way for derivation of different local/nonlocal plasticity/viscoplasticity yield surfaces is also proposed. Finally, the model capabilities in capturing size and interfacial hardening effects in metal matrix composites, interfacial effects on the yield strength of thin metal films on substrates, and nonuniform size-dependent deformation of micropillars under uniform stressing are illustrated through several examples.

References:
Tensile Ductility and Plasticity Mechanisms in Nanocrystalline Metals

Ryan Ott
Ames Laboratory (USDOE)
106 Metals Development, Iowa State University, Ames, 50014, US
Phone: 515 294 3616, Email: rtott@ameslab.gov

Morris Wang
Lawrence Livermore National Laboratory, Livermore, CA

Matthew Besser
Ames Laboratory (USDOE), Ames, IA

Matthew Kramer
Ames Laboratory (USDOE), Ames, IA

Abstract:

Nanocrystalline (nc) metals (grain sizes less than 100 nm) can exhibit exceptional mechanical properties including high-yield strengths, however, they also typically exhibit very limited tensile ductility. An exception to this behavior is nc-Co, which displays both large work hardening and tensile ductility prior to failure. Therefore, understanding the plasticity mechanisms that control the mechanical behavior of ductile nc metals such as Co is critical for achieving enhanced plasticity in nanostructured metals and alloys. Previous molecular dynamics simulations have suggested that plastic deformation in nc-Co is characterized by an hcp-fcc phase transformation, while bulk mechanical tests have suggested a possible mechanical twinning mechanism. Despite previous experimental and simulation studies, the plasticity mechanisms responsible for the large tensile ductility in nc-Co have not been clearly identified. We have examined the deformation behavior of both ductile nc-Co and nc-Ni, which shows limited tensile ductility, using in situ high-energy X-ray diffraction (XRD). The changes in the lattice strain and the peak intensities were measured in real-time for the two metals subject to cycled loading at different strain rates. From these experiments we do not see any evidence of a strain-induced phase transformation in the nc-Co. Instead, we find that the lattice strain exhibits a large deviation from linearity at the onset of macroscopic yielding. Moreover, we see distinct changes in the crystal orientations during plastic flow. The texture changes in the nc-Co correspond to &lt110&gt;(102) mechanical twinning during plastic deformation. Transmission electron microscopy analysis of the nc-Co samples after deformation confirms that a large amount of planar defects are present in the nano-grains. In contrast, the nc-Ni shows no significant texture changes during deformation and the lattice strain exhibits minimal deviation from linearity, which suggest that twinning is not the operative plasticity mechanism. The effects of the different plasticity mechanisms on the tensile ductility of the two metals are discussed.
Size Effects on the Nanoindentation of Ni Nanowires using Molecular Dynamics

Virginie Dupont  
Los Alamos National Laboratory  
PO BOX 1663, MS B268, Los Alamos, 87544, US  
Phone: 505-665-5905, Email: vdupont@lanl.gov

Frederic Sansoz  
The University of Vermont, Burlington, VT

Abstract:

There has been a recent scientific interest in one-dimensional metal nanowires because of their potential use in nanotechnologies. Experimental evidence shows a strong influence of the sample dimension on the mechanical properties of metals at nanometer scale. The relevant studied length scale has a strong influence on the results of mechanical tests such as hardness, ductility, strength. In macroscopic samples, the relevant length scale is often the grain size, which is much smaller than the sample size, but as the sample size is reduced, the relevant length scale becomes the diameter or volume of the sample, and the material strength significantly increases as the length scale decreases. A micro-plasticity mechanism based on dislocation starvation has been proposed, which has been confirmed experimentally on nanopillars of diameters larger than 150 nm. Atomistic simulations have already been used to gain fundamental insight into the dislocation activity during metal nanopillar compression, but little has been done on the radial nanoindentation of metal nanowires. We used Molecular Dynamics simulations to study crystal plasticity and size effects in sub- 100 nm nanowires deformed by spherical indentation. This work focused on &lt111&gt-oriented defect-free single crystals, as well as nanocrystalline Nickel (Ni) nanowires. The indentation of thin films was also comparatively studied to characterize the influence of free surfaces in the emission and absorption of lattice dislocations in single crystal Ni. In single crystals, the nanoindentation response for both thin films and nanowires in the elastic regime was found to obey a Hertzian behavior. The mean value of Young's modulus for all samples for single crystals showed that the sample size had no noticeable effect on the elastic properties of the nanowires during nanoindentation. No significant change at the onset of plasticity (contact pressure and deformation mechanisms at yield point) were observed between the samples. In the plastic regime, the hardness of Ni nanowires was found to be size-dependent, such that the nanowire became softer as the wire diameter decreased. In contrast, no significant size effect of hardness was revealed in thin films as a function of the film thickness. In nanocrystalline samples, grain boundary sliding dominates the plastic deformation, and free surfaces are no longer significant due to the accommodation of deformation by grain boundaries.
A New Nonlocal Shell Model for Axisymmetric Wave Propagation in Carbon Nanotubes

Yang Yang
City University of Hong Kong
Department of Building and Construction, City University of Hong Kong, Hong Kong, 000000, CN
Phone: 852-27887646, Email: yanyang6@student.cityu.edu.hk

Abstract:

By the first time that employed nonlocal elasticity continuum model to study mechanics behaviors of carbon nanotubes (CNTs) in 2003, various works are published about this research field. However, most of this job predicted suspicious results when compare with other approaches such as molecular dynamic simulation (MD), couple stress models and strain gradient models. The main reason leads to this paradoxical conclusion is the equilibrium equations and boundary conditions based on classical elasticity theory is employed directly without any correction, even though the mechanics quantities such as bending moment and axial force are in nonlocal form. Thus the nonlocal models based on classical elasticity theory are only called as partial nonlocal models.

In our work, a new nonlocal elasticity model is developed for axisymmetric wave propagation in CNTs which modeled as cylindrical shells. The nonlocal constitutive relations in cylindrical coordinate system are applied. New relations for nonlocal stress with higher-order strain gradients and the complete nonlocal strain energy are derived. Subsequently, new governing equations of motion are established from the variation principle. Comparing to other partial nonlocal approaches which directly replaced the nonlocal quantities into the classical equilibrium conditions or the governing equation of motion, the new nonlocal model here predicts stiffness-increased, rather than reduced stiffness, dispersion relation for axisymmetrical wave propagation in CNTs. Among the various models including partial nonlocal beam and cylindrical shell models, the solutions predicted here are in excellent agreement with the molecular dynamics simulation solutions especially for high wavenumber. Furthermore, the influences of nanoscale and other geometric parameters of CNTs on the phase velocity have also been investigated. The rationality of prediction using this new nonlocal is further confirmed.

As a summary, the enhancement of stiffness due to the presence of nanoscale, which has been confirmed by other numerical and experimental methods previously, is also predicted by the new nonlocal stress model here while the previous partial nonlocal stress models predict otherwise.
Quantitative Tensile Testing at the Nanoscale

Matthew Kramer
Materials Sciences and Engineering, Ames Laboratory
USDOE, 225 Wilhelm Hall, Ames Laboratory, Ames, 50011, US
Phone: 515 294 0276, Email: mjkramer@ameslab.gov

Ying Zhang
Materials Sciences and Engineering, Ames Laboratory, Ames, Iowa

Joong Mok Park
Materials Sciences and Engineering, Ames Laboratory, Ames I, Iowa

Zhiwei Shan
Hysitron, Inc, Minneapolis, MN

Julia Deneen Nowak
Hysitron, Inc, Minneapolis, MN

Oden L. Warren
Hysitron, Inc, Minneapolis, MN

Abstract:
Conventional transmission electron microscopy (TEM) tensile holders provide only constant displacement rate. Sample geometry is such that only a small portion of the sample is thin enough for electron imaging. In situ deformation studies, using this type of holder, is qualitative at best. To obtain quantitative nanomechanical properties, the sample geometry, load-frame and associated control electronics must be designed specifically for this purpose. Using the advanced control electronics and nano-indenteter transducer, Hysitron has modified their pico-indenteter to perform load/displacement control of electron transparent samples in tension. These innovations also include a unique design to eliminate initial load transients, active damping of the load or displacement control and a removable sample holder for ease of sample preparation. Ames Laboratory has developed techniques to fabricate nanowires (~ 150 x 50 nm up to 10’s of μm in length) from a wide variety of transition metals and &lt 70 nm thick single crystal films of Cu. We are now capable of testing polygrained wires of Al, Ti, Cu and Au under both constant load and constant strain rate. Using a focused ion beam we will be able to extract thin single grain foils with orientations which will be both favorable and unfavorable to slip in fcc Cu. Together with high speed imaging in the TEM, we will be able to study the dynamics of the deformation mechanism in both nanoscale polygrained materials and slip systems in single crystals. Key science questions for nanograined materials are 1) what is the role of grain size in grain boundary sliding and 2) how is this affected by loading rate? Doing these studies in the TEM, we can also track the orientations of the various grains to see if certain grain boundaries are stiffer than others. Key science questions for single grain samples are 1) what are the relative length scales necessary for dislocations motion, 2) what is the effect of grain size in strengthening alloys and 3) do the defect mechanisms change as the cross section is reduced to < 20 nm? Results of our preliminary studies will be presented.
Effect of Surface Roughness and Functionalization on the Shear Strength of Individual Carbon Nanofiber-Epoxy Interface

TANIL OZKAN
University of Illinois, Urbana-Champaign
104 S. Wright St. Talbot Building MC-236, Aerospace Engineering, Urbana, 61801, US
Phone: 217-333-3122, Email: tozkan2@illinois.edu

QI CHEN
University of Illinois, Urbana-Champaign, IL

IOANNIS CHASIOTIS
University of Illinois, Urbana-Champaign, IL

Abstract:

Modeling and optimization of nanostructured composites have been hindered by the lack of interfacial properties at the level of individual nanoconstituents. Novel nanoscale fiber pull-out experiments, supported by MEMS mechanical testing platforms, provided for the first time the interfacial shear strength (IFSS) of individual carbon nanofibers (250 nm average diameter) embedded in an epoxy matrix. The as-grown carbon nanofibers with 5 nm surface roughness and turbostratic annulus exhibited high IFSS, averaging 110 +/- 25 MPa, which is significantly larger than that of non-functionalized (15-28 MPa) and functionalized (40-65 MPa) microscale carbon fibers. Contrary to expectations, the IFSS of high temperature heat treated and graphitized carbon nanofibers was drastically reduced to 66 +/- 10 MPa, while the nanofiber surface roughness was also reduced to 1-2 nm. Thus, it is evident that this minute nanofiber surface roughness is a major factor controlling the IFSS along with the chemical composition and morphological aspects of the nanofiber-polymer matrix interface. The reduction in IFSS because of reduced surface roughness accommodated through the graphitic conversion of the previously turbostratic nanofiber annulus was restored by oxidative functionalization of the nanofiber surface resulting in IFSS values of 190 +/- 14 MPa, indeed much higher than current achievable values with conventional micron sized carbon fibers. All the aforementioned measurements were independent of the nanofiber embedded length and diameter, which provides confidence in the reported numerical values. These local IFSS measurements from individual nanofibers represent the first direct explanation of the improved global composite fracture toughness reported before in the literature. The findings of this experimental investigation, which emphasized the critical role of surface roughness and chemical functionalization in IFSS, underline the importance of scale-specific interfacial experiments and assert that linear extrapolations of macroscale interfacial measurements to the nanoscale are not valid for polymer nanocomposite design and mechanical modeling purposes.
Determination of Nano-scale Mechanical Properties near Hybrid Fiber Interfaces in Polymer Systems

Charles Wood
Northwestern University
2145 Sheridan Rd, Mechanical Engineering, Evanston, 60208, US
Phone: 352-262-2841, Email: cwood@u.northwestern.edu

L. Catherine Brinson
Northwestern University, Evanston, IL

Abstract:

Hybrid composites involve a designed incorporation of nanoparticles into a traditional composite to improve matrix properties in areas prone to failure, e.g. interlaminar areas. Hybrid fibers, where carbon nanotubes are incorporated directly attached to traditional aligned fibers, provides a unique approach to strengthen specific areas of weakness by controlling the placement of nanoparticles in the matrix. Incorporation of designed nanoparticle phases in hybrid composites demands understanding polymer property changes near interfaces, due to the enormous surface area of nanoparticles exposed to polymer in the matrix. Near attractive interfaces, mobility of the polymer chains is restricted due to geometric and chemical interactions. The regime of altered polymer properties, the ‘interphase’, extends in a graded fashion deep into the matrix due to the macromolecular nature of polymers. While previous studies have shown clear effects on thermomechanical properties of polymers near interfaces in thin films, direct mechanical investigation of the interphase has been limited. Nanoindentation provides a unique technique to probe structures at small length scales to obtain properties such as hardness and elastic modulus associated with surface interactions. In these hybrid composite systems, coupled use of finite element (FE) models with experimental data is critical to assess the complex structures associated with the nanotube coated fibers; where surfaces of interest can be located underneath free surfaces and/or complicated by neighboring surfaces. In this study, nanoindentation techniques are employed to directly measure interphase properties in an epoxy(Epon 828/NMA)/hybrid fiber system. Two types of hybrid fibers were studied, carbon and glass parent fibers, with carbon nanotubes (CNTs) grown radially on the surface of the parent fiber. Nanoindentation was employed to probe discrete areas to quantify interphase gradients due to the incorporation of CNT growth. The nanoindentation experiments are accompanied by numerical analysis and fiber pull-out studies to assess the strength enhancements, and their resulting dimensions, due to the incorporation of CNTs.
An Analysis of the Effects of Surface Elasticity on an Elastic Solid Incorporating a Crack (Mode-I & II): Complete Solution

Chun IL Kim
University of Alberta
Department of Mechanical Engineering, 4-9 Mechanical Engineering Building, Edmonton, T6G 2G8, CA
Phone: 1.780.492.5635, Email: cikim@ualberta.ca

C Q. Ru
University of Alberta, Edmonton, Alberta

Abstract:

The analysis of stresses in the general region of a crack tip is of fundamental importance in the understanding of failure and in the general deformation analysis of engineering materials. In macroscopic models, the stresses at the crack tip are found to be infinite reflecting the fact that the crack front is usually taken to be perfectly sharp. In fact, an infinitely sharp crack in a continuum is a mathematical abstraction since, in reality, most crack tips are, in fact, blunt, with a radius of convergence of the order compatible with the nanoscale. This suggests that a more accurate analysis of the region in the vicinity of a crack tip can be achieved at the nanoscale. In the context of a continuum model this means the incorporation of surface effects into the model of deformation.

In the presentation, we consider plane deformations of a linearly elastic solid in the case where either a mode-I or mode-II crack is present but, perhaps more significantly, when surface effects are included in the mechanics of the crack faces. The surface effects lead to a more accurate description of deformation and are incorporated using the continuum based surface/interface model of Gurtin and Murdoch. We obtain a complete semi-analytic solution valid throughout the entire domain of interest (including at the crack tips) via two series of coupled Cauchy singular integro-differential equations which are solved numerically using an adapted collocation method. It is shown that, among various other interesting phenomena, when the solid incorporates a traction-free crack face and is subjected to uniform far-field stresses (tension and in-plane shear), the surface effects result in the elastic response and corresponding stress fields being size-dependent. In particular, we note that, in contrast to classical linear elastic fracture mechanics, our model predicts that the stresses at the (sharp) crack tip remains finite. At the end, we also briefly discuss the analogous situations, yet more complicate in nature, plane interface crack problems under the influences of surface effects.
Temperature and Strain Rate Sensitivity Effects in Nanocrystalline Metal Films

Nikhil Karanjgaokar
Mechanical Science and Engg, University of Illinois at Urbana-Champaign
325 Talbot Lab, 104 S Wright St, Urbana, 61801, US
Phone: 2172333122, Email: nkaranj2@illinois.edu

Chung Seog Oh
School of Mechanical Engineering, Kumoh National Institute of Technology, Gumi, S. Korea,

Ioannis Chasiotis
Aerospace Engg, University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Nanocrystalline metal thin films are excellent materials for microelectromechanical Systems (MEMS) and microelectronics due to their outstanding electrical conductivity and high yield strength. However, our recent studies have shown that nanocrystalline FCC metal films are highly strain rate sensitive and their primary creep rates at room temperature are several orders of magnitude higher than the steady-state creep rates previously reported for meso- and micro-scale grain metals. This time dependent inelastic behavior is further accentuated at elevated temperatures: A comprehensive experimental investigation has been carried out to quantify for the first time the strain-rate dependent mechanical behavior of nanocrystalline Au thin films (grain size 64 nm) at strain rates in the broad range of 0.000001 - 10 /s and at temperatures between 25-110° C. Full-field strain measurements of uniformly heated sub-micron thick Au films were supported by microscale infrared temperature profiles for accurate and repeatable experiments. Contrary to expectations, relatively low temperatures (50 °C) resulted in marked shift in rate sensitivity and activation volumes providing strong evidence that nanocrystalline metals are significantly more temperature sensitive than their larger grain counterparts. This presentation will discuss these novel results and the interrelations between strain rate and temperature in nanocrystalline metals.
A SEM Image-based Finite Element Approach on the Viscoelastic Behaviors of Rubber-carbon Black Composites

Hua Deng
Northwestern University
Department of Mechanical Engineering, 2145 Sheridan Road, Evanston, 60208-3111, US
Phone: 5173752505, Email: hua-deng@northwestern.edu

Yu Liu
Northwestern University, Evanston, II

Cate Brinson
Northwestern University, Evanston, IL

Abstract:
A finite element modeling approach based on SEM images is presented. The geometry of our FE model is obtained by discretization of 2D binary images, which are directly retrieved from the SEM images of rubber-carbon black composites. These binary images, wherein carbon black particles are represented by black pixels and the polymer matrix by white ones, are then used as the geometries in the finite element model. One through six layers of grey pixels are manually added surrounding the carbon black pixels into the image, to represent the interphase region. Each pixel (either matrix, carbon blacks, or interphase) is treated as a 4 noded plane stress quadrilateral element in this 2D plain stress ABAQUS model. The frequency domain response of the polymer matrix was measured by DMA tests at a reference temperature of -50 C. This mastercurve constructed by using the Time-Temperature-Superposition was then fit by a 28-term Prony Series and imported into the material property of matrix in this model. The carbon black particles are regarded as isotropic elastic. In this work, the Young's modulus of the carbon black is chosen as 100 GPa and the Poisson's ratio is assumed to be 0.4. While the properties of the interphase are still under investigation, it is assumed here that the frequency response curve of the interphase region is related to that of the bulk polymer matrix simply by a 2 decades shift in the frequency domain.

Simulation results based on the abovementioned 2D SEM image based ABAQUS model are then compared with the DMA data of rubber-carbon black composites in both frequency and temperature domains. While the real interphase properties are still unknown, the simulation results indicate that assuming interphase properties shifted 1.5 decades (toward lower frequencies) from the matrix master curve, and modeling the interphase region by ONE layer of pixels (~ 15-25 nm), provide the best fit between the simulated curves and the experimental curves for this particular rubber-carbon black composite.
Experimental Observations of the Failure Mechanisms in a Bulk Metallic Glass Composite

Hui Wang
Iowa State University
0241 Howe Hall, Ames, 50010, US
Phone: 5152317668, Email: hhwang@iastate.edu

Ashraf Bastawros
Iowa STate University, Ames, IA

Bulent Biner
Iowa State University, Ames, IA

Abstract:

The deformation and damage evolution behavior of a Ni-based bulk metallic glass composite reinforced with elongated brass phase is studied under cylindrical indentation. The estimated fracture toughness values based on the energy dissipation and the in-situ observation during the loading reveal the details of the damage evolution and toughening mechanisms in this composite system. The experimental results showed that the enhanced toughness of the BMG composite is plausibly an outcome of crack bridging mechanisms by the ductile brass phase, rather than a diffused array of nucleated shear bands in the hard BMG and arrest by the ductile reinforcing phase.
Phase Transformations and Mechanochemistry

ORGANIZERS:

Valery Levitas, Iowa State University
The Pogorelov’s Geometric Theory of Shells and Phase Transformations in Solids

Michael Grinfeld
The US Army Research Laboratory
US Army Research Laboratory, Aberdeen Proving Ground, 21005-5066, US
Phone: 410-278-7030, Email: mgreenfield@arl.army.mil

Invited Presentation

Abstract:

The Modified Pogorelov’s Geometric Theory of Shells and Phase Transformations in Solids
Soft shells are widespread in biomechanics [1]. Those shells are characterized by weak resistance to bending and extremely high deformations. Different techniques of analysis of shells can be applied to bio-shells. One of the attractive theories for biomechanical applications is the geometrical shell theory suggested by the famous Ukrainian geometer Pogorelov in 1960s [1-3]. In this talk we demonstrate that the Pogorelov’s theory have some common features with the theory of phase transformations in solids.

Pogorelov’s theory of shells is based on his famous theorem: Continuous isomers of a sphere include motions as a rigid whole and segmental reflection. Driven by this theorem, Pogorelov supposed that the shell’s median surface in the post-buckling configurations can be approximated by a smooth surface, which is close to the isometric transformation of the median surface of the undeformed shell. The main strength of this theory is associated with its relative simplicity in dealing with the post-buckling behavior.

We modify the Pogorelov’s theory in several respects but preserve his main idea: the full energy is the sum of the elastic energy of the smooth sub-surfaces and the rib energy of the separating contour. In particular, we explicitly take into account the membrane energy of the shell. Following the techniques presented in the author’s variant of the theory of phase transformations [4] we explore the problem of equilibrium and stability of the post-buckling configurations. Then, we make comparison with the Pogorelov’s original theory and discuss applications to biomechanics of soft tissue.

References
Modeling and Simulation of Strain-induced Phase Transformations in Rotational Diamond Anvil Cell under Compression and Torsion

Oleg Zarechnyy
Iowa State University, Department of Aerospace Engineering, Ames, 50011, US
Phone: (806)224-7412, Email: olegzar@iastate.edu

Valery Levitas
Iowa State University, Departments of Mechanical Engineering, Aerospace Engineering, and Material Science and Engineering, Ames, IA

Abstract:

Strain-induced phase transformations under high pressure differ significantly from the pressure-induced phase transformations under hydrostatic conditions. A model and finite-element approach to strain-induced phase transformations under compression and torsion of a sample in rotational diamond anvil cell are developed. Results are obtained for three ratios of yield strengths of low-pressure and high-pressure phases. Effect of addition of a torsion on phase transformation process is studied and compared with results for phase transformation under compression only. A very nontrivial, nonlinear interaction between strongly heterogeneous stress and plastic strain tensor fields and phase transformation kinetics is revealed, quantified, and analyzed. Various experimental effects are reproduced, including plateau at pressure distribution at the diffuse interface, a pressure self-multiplication effect, simultaneous occurrence of direct and reverse transformations, and irregular stress distribution for transformation to a weaker phase. The obtained results change the fundamental understanding of strain-induced phase transformation in terms of interpretation of experimental measurements and the extracting of information on material processes from sample behavior. Intense radial plastic flow moves the high-pressure phase into the low-pressure region, which may lead to misinterpretation of measurements and to drawing wrong conclusions. Various interpretations based on a simplified equilibrium equation (for example, about zero yield strength of phase mixture and hydrostatic conditions during transformation) appears to be wrong because of inapplicability of this equation for cases with large gradients of phase concentration and yield strength. For phase transformation to a stronger phase, pressure at the diffuse interface corresponds to the characteristic pressures in the kinetic equation, which allows us to determine them experimentally. For phase transformation to a weaker phase, this is not true, and analysis of experiments is much less robust. In fact, for this case torsion does not promote phase transformation, and the statement that plastic straining reduces phase transformation pressure (while generally correct) was not experimentally justified. The approach developed represents a tool for designing experiments for different purposes and for controlling phase transformations, and it opens unexpected ways to extract material information by combining simulation and experiment.

Molecular Simulations of Nucleation in Tetrahedral Solids

Tianshu Li
Department of Civil and Environmental Engineering, George Washington University, Washington, 20052, US
Phone: 510-918-2001, Email: tianshuli@gmail.com

Davide Donadio
Max Planck Institute for Polymer Research, Mainz, Germany

Giulia Galli
Department of Chemistry and Department of Physics, University of California, Davis, Davis, CA

Abstract:

The early stages of crystallization of tetrahedral systems remain largely unknown, due to experimental limitations in spatial and temporal resolutions. By employing advanced sampling techniques, we provide atomistic details of nucleation process, including the atomic structure of critical nuclei and nucleation dynamics, of supercooled liquid silicon [1, 2] and water. Defect structure, e.g., stacking fault, is shown to develop prior to the formation of critical nucleus. The defect density and the density of crystalline polymorphs in tetrahedral solid are shown to depend on nucleation temperature. A comparison between simulation results and those of classical nucleation theory shows that the free energy of the liquid solid interface $\gamma_{ls}$ inferred from our computations differ significantly from that obtained for bulk liquid solid interfaces. However our results further showed that the $\gamma_{ls}$ obtained at the microscopic level at one nucleation temperature can be indeed used as an effective parameter to predict nucleation rates at another temperature, within classical nucleation theory.

Nanovoid Nucleation Inside Elastoplastic Material:
Sublimation Versus Fracture

Nataliya Altukhova
Iowa State University, Department of Aerospace Engineering, Ames, 50011, US
Phone: 806-224-7722, Email: nataliya.s.altukhova@ttu.edu

Valery Levitas
Iowa State University, Departments of Mechanical Engineering, Aerospace Engineering, and Material Science and Engineering, Ames, IA

Abstract:

Thermodynamic and kinetic approaches for sublimation inside elastoplastic material are developed for large strains. Various conceptual problems related to the effect of irreversible plastic deformation and dissipation, path-dependence of appearance of a critical nucleus, and presence of large strains are considered for a spherical bubble. Four transformation paths are studied: nucleation via homogeneous transformation in the nucleus of fixed mass, nucleation via continuous interface propagation, sublimation inside elastoplastic material via intermediate (virtual) melting, and nanovoid nucleation as a fracture process inside elastoplastic material. For all four paths, the expressions for the thermodynamic driving forces and activation energies are derived. The activation energy is equal to the minus driving force for appearance of a nucleus maximized with respect to nucleus mass and minimized over the nucleus shape, transformation path, and position. This definition corresponds to the principle of the minimum of transformation time and transforms to the traditional one in the limit of elastic materials. Virtual melting represents the appearance of subcritical liquid drop that immediately transforms to gas bubble. The radius of the critical gas nucleus differs from the classical one because elastic energy of melt is size-dependent due to surface tension. Arrhenius-type kinetic equation for nucleation time and kinetic nucleation criterion are formulated. The variety of mechanisms and transformation paths are revealed in different pressure ranges. For small stresses, elastic deformation of a sphere takes place and the results for both paths coincide. For large stresses nucleus size is equal to the minimum radius for which one still can distinguish between solid and gas. For the intermediate stresses, radius of the critical nucleus maximizes the activation energy. However, such a homogeneously transformed nucleus cannot grow. It is necessary to slightly increase temperature or tensile pressure (to a value well below that for nucleation via interface propagation) to cause growth. Below some critical temperature, while the nucleus cannot grow because of solid-gas transformation, it expands like a balloon due to loss of mechanical stability. To our knowledge, this is the only known example of transformation of a subcritical nucleus into a supercritical one due to mechanical instability. Thermodynamics and kinetic of evaporation is considered as well. It is demonstrated that a nanovoid nucleation as a fracture is kinetically favorable below equilibrium melting temperature and (for high surface energy) below kinetic melting temperature.

Melt-Dispersion Mechanism of Reaction of Aluminum Nano- and Micron Scale Particles

Valery Levitas

Iowa State University
Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, 2028 Black Engineering Building, Ames, 50011, US
Phone: (515) 294-9691, Email: vlevitas@iastate.edu

Abstract:

Aluminum nano- and micron scale particles are widely used in various energetic and material synthesis applications, including thermites, thermobaric and reactive materials, and synthesis of biomaterials. A new and unexpected mechanochemical mechanism for fast reaction of Al nanoparticles covered by a thin oxide shell during fast heating is proposed and justified theoretically and experimentally. For nanoparticles, the volume change due to melting of Al induces pressures of 1-2 GPa and causes spallation of the oxide shell. A subsequent unloading wave creates significant tensile pressures resulting in dispersion of small liquid Al clusters, reaction of which is not limited by diffusion (in contrast to traditional mechanisms). All processes (heating, melting, nanomechanics of stress development, fracture of the oxide shell, wave propagation, and cavitation) are treated analytically and numerically. FEM with the COMSOL code is employed to solve phase field equations. Physical parameters controlling this process are determined by our analysis. A number of experimental results confirm predictions based on the melt-dispersion mechanism. Methods to improve efficiency of energetic nanoparticles, as well as to promote the melt-dispersion mechanism for micron particles have been suggested. Our ultimate goal is to design and synthesize an optimal micron Al core-strong shell particle that transforms in situ (in flame) into multiple nanoscale bare particles that react like the best nanoscale particles. Cost of micron particles is 30-50 times smaller than nanoparticles, and they do not have safety and environmental issues.

References:
Molecular Dynamics Study of Thermal and Mechanical Behavior of Aluminum Core/alumina Shell Nanoparticles under Conditions of Rapid Heating

Chengping Wu
Department of Materials Science and Engineering, University of Virginia
395 McCormick Road, P.O. Box 400745, Charlottesville, VA 22904-4745, US
Phone: 4343277529, Email: cw5xj@virginia.edu

Leonid V. Zhigilei
Department of Materials Science and Engineering, University of Virginia
395 McCormick Road, P.O. Box 400745, Charlottesville, VA 22904-4745, US

Abstract:

Aluminum nanoparticles are finding an increasing use in the design of energetic materials due to their enhanced reactivity compared to larger micron-sized particles. The high burning rates of the nanoparticles observed in experiments cannot be explained by the diffusive oxidation mechanism and have lead to the suggestions of alternative mechanisms, such as the mechanochemical or melt-dispersion mechanism [1]. In this study, molecular dynamics simulations are used to investigate the thermal and mechanical response of Al core/alumina shell nanoparticles to a rapid heating. The simulations are performed for nanoparticles with a radius of about 5 nm and different shell thicknesses. The results of the simulations reveal several stages in the thermo-mechanical evolution of the Al/Alumina nanoparticles subjected to the rapid heating. At the initial stage of the heating process, the expansion and melting of the Al core creates large tensile stresses in the alumina shell which remains solid and undergoes an elastic deformation. As the compressive pressure in the melted core confined by the shell increases up to about 4 GPa, the shell starts to deform plastically and partially relaxes the high compressive pressure in the core. Finally, the plastic deformation leads to a localized thinning and eventual disruption of the shell, causing the ejection/jetting of the Al melt. The ejection velocities of the liquid Al are found to be very high, in the range from 200 to 500 m/s, providing a hint for explaining the high rates of the nanoparticle reaction with surrounding oxidizers. The physical picture emerging from the MD simulations is consistent with the results of time-resolved spectroscopy measurements reported for 100 ps laser heating of energetic materials containing Al nanoparticles [2]. It is also in a good semi-quantitative agreement of the results of the theoretical analysis given in Ref. [1], with a notable difference being the prediction of the localized jet-like ejection of the melt rather than the spallation of the oxide shell discussed in Ref. [1]. The jet-like ejection of the melted Al results in increased ejection velocities and may have implications for the kinetics of the oxidation process. The observation of the substantial elastic deformation followed by plastic thinning of the alumina shell is consistent with the results obtained by in-situ heating of Al/alumina nanoparticles in a transmission electron microscope [3].

Phase Field Modeling of Melting of Aluminum Nanoparticles

Kamran Samani
Department of Mechanical Engineering, Iowa State University, Ames, Iowa, 50014, US
Phone: 515 520 2093, Email: samani@iastate.edu

Valery I. Levitas
Iowa State University
Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, 2028 Black Engineering Building, Ames, 50011, US

Abstract:
Surface pre-melting and melting of nanoparticles are fundamental problems, which are currently under intense study. For aluminum nanoparticles, this study also has applied aspects. Aluminum nanoparticles represent important class of nanoenergetic materials that are used in rocket propellant mixtures and other energetic applications. They possess significantly enhanced burning rate and reduced ignition delay time. Aluminum nanoparticles usually have a several nanometers thick oxide layer. According to the recently developed melt-dispersion mechanism of reaction of Al nanoparticles, one of the processes that determines the reactivity of Al nanoparticles is melting of Al and stress development in Al core-shell system due to volume increase during melting. Melt nucleation, melting temperature and rate of melting at high heating rates ($10^8$ K/s and above) determine mechanics of deformation and fracture of alumina shell, which are important for the melt-dispersion mechanism.

We expanded a phase field approach for the pre-melting (surface melting) and melting of nanoparticles by introducing correct expression for surface tension at the solid-melt interface and correct description of variation of surface energy of the external surface. New definition of surface tension yields results that are consistent with sharp interface approach, in contrast to previous theories. Suggested description of variation of surface energy eliminates drawbacks of known approaches to surface melting.

Coupled phase field and mechanical equations are solved using finite element method and COMSOL code. Melting, without and with mechanics, is considered. Calculated results for the thickness of the molten layer versus temperature and melting temperature versus particle size are in good correspondence with experiments. Surprisingly, for the particles with radius from 2 to 5 nm, melting temperatures are even in better agreement with experiments than the molecular dynamics results. For heating rates greater than $10^{13}$K/s, homogeneous nucleation competes with interface propagation. It is also found that classical expression for the interface velocity based on sharp-interface equation is well reproduced in our calculations even for temperatures for which solid is completely unstable and for particle radii exceeding interface width, which is approximately 4 nm. For spherical particle, interface energy is independent of interface radius down to 4 nm. Classical relationship for pressure jump across the interface is confirmed for $r > 5$nm and neglected internal stresses. The effect of alumina shell is also considered. Alumina shell increases melting time and melting temperature considerably. Large hoop stresses and strain rates developed in the shell can yield spallation of the shell.
Effect of Surface Tension and Energy on Multi-variant Phase Transformations Based on Phase Field Approach

Mahdi Javanbakht
Iowa State University Department of Mechanical Engineering, Ames, 50011-2161, US
Phone: 515-2948020, Email: mahdj@iastate.edu

Valery I. Levitas
Iowa State University
Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, 2028 Black Engineering Building, Ames, 50011, US

Abstract:

Phase-field or Ginzburg-Landau modeling represents a unique approach for simulation of various aspects of stress-induced multi-variant martensitic phase transformations, especially at nanoscale. However, despite the significant progress in the field, a lot of fundamental physics is missing in the phase field equations. In the present work, the Ginzburg-Landau theory for multivariant martensitic phase transformations is advanced in three directions [1]:

First, a potential is developed that introduces a thermodynamically consistent expression for surface tension, which is consistent with a sharp interface limit. Nontrivial point is that, even for negligible small strains we have to use a large strain formulation.

Second, a mixed term in gradient energy is introduced by considering the product of gradients of different order parameters corresponding to different martensitic phases. This allows us to control the energy of martensite-martensite interface. The resultant Ginzburg-Landau equations become coupled through Laplacians, in addition to traditional coupling.

Third, a noncontradictory expression for variable surface energy is suggested. The main drawback of previous works is that the product phase always has a surface structure toward the alternative phase, even when this phase is completely unstable. This also leads to unphysical regions in the phase diagram. Here, we derive the expression that does not possess the above problem, generalize it for multi-variant phase transformations, and study surface-induced pre-transformation and barrierless nucleation of multiple martensitic variants.

Combining all the above advancements, the coupled system of time-dependent Ginzburg-Landau equations for all order parameters, the continuum of mechanical equations, and the boundary conditions are formulated. The finite element method approach, algorithm, and subroutines are developed using COMSOL code. Model problems of surface-induced pre-transformation, barrierless multivariant nucleation, and nanostructure evolution in a nanosize sample are solved, and the effect of the above contributions is elucidated. Also, the obtained results represent a much more detailed and precise model for coherent solid-solid interface than current phenomenological models.

Oxidation and Hole Formation in Aluminum Nanoparticle

Hamed Attariani
Iowa State University
Departments of Mechanical Engineering, Ames, 50010, USA
Phone: 515-290-7874, Email: hamed82@iastate.edu

Valery I. Levitas
Iowa State University
Departments of Mechanical Engineering, Aerospace Engineering and Material Science and Engineering, 2028 Black Engineering Building, Ames, 50011, USA

Abstract:

This work is concerned with modeling of thermo-mechanochemical processes that occur in aluminum nanoparticles covered by oxide shell during heating. This study is important for understanding and optimization of synthesis and application of Al nanoparticles, in particular pre-stressed nanoparticles and nanoparticles with holes. Aluminum nanoparticles have a broad range of application as nanoenergetic material. They are being considered for overlapping technologies such as: materials synthesis application, explosive additives, and propellant rate modifiers; MEMS energy sources, as well as thermites, nanobarics, and reactive materials for ordnance applications. In manufacturing process or during oxidation, solid nanoparticle may change its structure to hollow sphere due to the Kirkendall effect. The difference in diffusion of metal and oxide layer causes the migration of atoms from core to shell, which leads to supersaturation of vacancy in the core and nanovoid nucleation. Additionally, aluminum reacts with oxygen and form the growing oxide layer. Coupled system of equations for diffusion of Al, oxygen, and vacancies, oxidation reaction and elasticity theory is formulated and solved using finite element method and COMSOL code. Conditions for void nucleation and growth are determined depending on particle’s parameters. Depending on the achieved level of supersaturation, void can disappear, grow or first shrink and then grow. Thermodynamically consistent volumetric reaction kinetics with finite reaction rate is used. Reaction occurs inside of alumina shell where diffused Al and oxygen meet. Diffusion is coupled to mechanics through diffusion expansion (for atoms) and contraction (for vacancies), contribution of the stress gradient into diffusion equation, and through pressure-dependence of equilibrium vacancy concentration and diffusion coefficient. Surface energy of all interfaces (hole, Al-alumina, and alumina-oxygen) is taken into account. Reaction is coupled to mechanics through misfit (reaction) strain, change in properties and pressure-dependence of reaction kinetics. Expression for misfit strain is determined. Misfit strain creates large stresses, which lead to expansion of the reaction zone. Various diffusion and oxidation scenarios are investigated.
A bi-crystal Aggregate Model of Martensitic Phase Transformations in Shape-Memory Alloy Polycrystals

Henryk Petryk
Institute of Fundamental Technological Research (IPPT PAN)
Pawinskiego 5B, Warsaw, 02-106, PL
Phone: +48 228269834, Email: hpetryk@ippt.gov.pl

Invited Presentation

Abstract:

A multi-scale model of stress-induced martensitic phase transformation and martensite variant reorientation in shape memory alloy (SMA) polycrystals is developed. The model provides a link between crystallographic lattice transformations on the lowest scale and the macroscopic stress-strain relationship at the polycrystal level. In between, several intermediate scales are considered, going through internally twinned martensite, rank-two laminates of austenite and martensite, laminated sub-domains within grains containing multiple variants of martensite, and interaction between grains in a polycrystalline aggregate. In comparison to typical mean-field approaches, a distinctive feature of the proposed model (Stupkiewicz and Petryk, Int. J. Mech. Sci, 2010) is to include neighboring-grain interaction in a simple manner by introducing an additional intermediate bi-crystal level into the sequential averaging scheme for SMA. All constitutive relationships are defined by specifying the respective free energy and dissipation functions. At the level of a single grain, the rate-independent dissipation function is used that incorporates the dissipation due to forward and reverse austenite-to-martensite transformation as well as reorientation of martensite variants. The global response of the model is simulated numerically by minimizing the total incremental energy supply. That minimization rule has been found to provide a convenient and effective way of implementing the rate-independent thermodynamic criteria of phase transformation and martensite variant rearrangement.

Specific examples are calculated for a NiTi SMA polycrystal for proportional and non-proportional loading paths. It is shown that the introduction of an intermediate bi-crystal level leads to a considerable reduction of the gap between the stress-strain curves calculated using the most straightforward, constant-strain (Taylor) and constant-stress averaging schemes. The Taylor averaging scheme applied to bi-crystals may thus provide results of comparable accuracy to computationally more complex approaches based on the finite element modeling. By comparison with experimental data taken from the literature, it is demonstrated that certain qualitative and quantitative details of the stress-strain response along combined tension-torsion paths can be well reproduced. Finally, by introducing interfacial energy on three different scales (Petryk at al, J. Mech. Phys. Solids, 2010) the model is extended to describe grain-size effects. A numerical example of a size-dependent hysteresis associated with the forward and reverse stress-induced martensitic phase transformation in a NiTi SMA polycrystal is presented.
Isomorphic Phase Transformation of Cerium Under Shock Loading Using Molecular Dynamics

Virginie Dupont
Los Alamos National Laboratory
PO BOX 1663, MS B268, Los Alamos, 87544, US
Phone: 505-665-5905, Email: vdupont@lanl.gov

Timothy C. Germann
Los Alamos National Laboratory, Los Alamos, NM

Shao Ping Chen
Los Alamos National Laboratory, Los Alamos, NM

Abstract:

Cerium (Ce) has an atypical phase diagram, presenting a large number of unusual structures, a minimum in the melting curve, an isomorphic phase transition between two FCC structures alpha and gamma, and a critical point around the point 550 K and 1.9 GPa. The isomorphic phase transition is believed to be caused by the transfer of valence electrons from the 4f state to the 5d state and induces a volume collapse of ~16%. There is an interest in developing multiphase equations of state, and Ce, with its complex phase diagram at low pressure, is a good material to start with. The isomorphic phase transition has been shown to occur at the same critical pressures under static and dynamic loading, so that shock loading is often used to study the transformation. Moreover, shock loading time scales are well within range of molecular dynamics (MD) simulations. We present an Embedded Atom Method (EAM) potential for Ce and its use in shock loading via MD simulations. The samples studied are single crystalline and defect-free. We study two different shock loading directions (<001> and <111>) as well as different initial temperatures (10K and 300K). The velocity profiles of the shocked samples show a split wave structure typical of a phase transition. Two waves are observed, an elastic precursor followed by a plastic wave. The plastic wave causes the expected phase transition. Comparisons to experiments on Ce and MD simulations on Cesium (Cs) indicate that three waves could be observed, one elastic precursor, a first shock compression wave in the gamma phase, and finally the phase transition wave from gamma to alpha. Also, an influence of the initial orientation or a lattice re-orientation is not observed in our simulations. The choice of an EAM potential is believed to be the source of the discrepancy, and future simulations shall use a different potential of the form used for the Cs simulations.
Multifunctional Composite Materials

ORGANIZERS:

Michael Kessler, Iowa State University
Structural Composite Capacitors, Supercapacitors, and Batteries

Eric Wetzel
U.S. Army Research Laboratory, RDRL-WMM-A, Aberdeen Proving Ground, 21005, US
Phone: 410-306-0851, Email: ewetzel@arl.army.mil

James Snyder
U.S. Army Research Laboratory, Aberdeen Proving Ground, MD

Danny O'Brien
U.S. Army Research Laboratory, Aberdeen Proving Ground, MD

Abstract:

Many U.S. Army applications require storage and release of electrical energy, necessitating the use of energy storage devices such as batteries and capacitors. Due to weight and volume concerns, there exists a need to reduce the mass and volume burdens created by these devices. One approach to utilizing these systems more efficiently is to engineer multifunctional devices that, in addition to storing and releasing energy, can also be used to carry structural loads. This presentation will review ARL's work on engineering structural batteries, supercapacitors, and capacitors. All of these devices leverage materials and fabrication techniques used in conventional fiber-reinforced polymer matrix composite materials.

Structural capacitors are fabricated by interleaving thin metallized papers and polymer films between structural dielectrics composed of continuous glass fiber-reinforced epoxy. High dielectric energy density is achieved by minimizing voids and inclusions in the dielectric, ensuring complete cure, and maintaining consistent electrode spacing. These structural capacitors are able to achieve energy densities above 0.1 J/g while maintaining mechanical properties comparable to structural composites.

Structural supercapacitors are fabricated using a salt-loaded polymer electrolyte with continuous carbon fiber electrodes. Homopolymer, copolymer, nanocomposite, and gel electrolytes have been studied to achieve an appropriate balance of mechanical and electrolytic properties. Techniques to increase the capacitive surface area of the carbon fiber electrodes, while maintaining good mechanical properties, are under evaluation. Separators are placed between electrode layers to prevent electrical shorting while permitting ion transport. Selecting efficient separator materials that provide robust electrical isolation while permitting mechanical bonding and load transfer is a critical challenge.

Structural batteries utilize structural electrolytes and separators similar to the structural supercapacitors. In contrast to the supercapacitors, the anodes of the structural batteries can effectively utilize unmodified carbon fiber fabrics. Structural cathode materials under development include thin-film coated metal meshes, screens, and foils. Engineering the morphological details at the interfaces of the current collector, active cathode material, and electrolyte remains a topic of continued study.

The talk will also include a general discussion on multifunctional design, and performance metrics that can be used to engineer mass-saving and volume-saving multifunctional materials.
Electrified Carbon Fiber Polymer Matrix Composites: Multi-Field Coupling Problem

Olesya Zhupanska
University of Iowa, Department of Mechanical & Industrial Engineering, 2416A Seamans Center, Iowa City
Phone: 319-335-5678, Email: ozhupans@engineering.uiowa.edu

Abstract:
Future technological advancements will demand materials with multifunctional capabilities that are expected to provide at least one additional function to their primary function or adapt their performance in response to changes in the operating environment. Composite materials lend themselves naturally to the concept of multifunctionality, which may be achieved through interaction of mechanical, electromagnetic, thermal, and other fields. The purpose of this study is investigation of electrical properties of carbon fiber polymer matrix composites and their influence on the impact behavior of electrified composites.

This works builds upon studies of Telitchev et al. (2008a, 2008b) and Sierakowski et al. (2008) who studied the impact response of electrified carbon fiber polymer matrix composites and show that impact resistance of composites can be improved by subjecting them to electrical load at the moment of impact. Moreover, it was demonstrated that the duration of the electric current application and current-induced heating play an important role in the impact behavior of electrified composites: in contrast to a short-term current application that improves the impact response of the tested composite plates, a prolonged application of an electric current appeared to have a detrimental effect on the composites.

In order to develop better understanding of the relationship between an electric current, Joule heating, and mechanical behavior of carbon fiber polymer matrix composites, a new fully instrumented experimental setup has been developed. This setup enables one to measure electric field characteristics (amperage, voltage, resistance) and temperature at the surface of the electrified composites samples in real time. The experimental procedure ensured a low contact resistance between the composite and electrodes, high uniformity in the density of the applied electric current, and low resistance heating. An extensive experimental study on the electrical characterization of carbon fiber polymer composites of different composition, ply sequence, thickness, etc. was performed. The effect of the resistance heating was carefully analyzed through experimental analysis as well as the finite element modeling. Lastly, a series of low velocity impact tests on electrified carbon fiber polymer matrix composites was performed. The interplay of the electric current, thermal changes, and impact load in the response of the electrified composites will be discussed.

References:
Polymer-Ceramic Formulations for Dielectric Applications

Eduard A. Stefanescu
Iowa State University
2220 Hoover Hall, Ames, 50011, US
Phone: 225-772-1064, Email: eduards@iastate.edu

Diana Gottschalk, Xiaoli Tan, Zhiqun Lin, Nicola Bowler, Michael R. Kessler
Iowa State University, Ames, IA

Abstract:

Polymer composites obtained through the addition of ceramic powders to polymeric matrices, make them good dielectric candidates for capacitors with a broad spectrum of applications. If such capacitors are designed with structural characteristics, the spectrum of applications can be further expanded. Poly(methyl methacrylate), PMMA, is a high-strength, amorphous polymer, possessing very good dimensional stability and excellent outdoor wearing properties. CaCu3Ti4O12, CCTO, is a cubic perovskite-related material that has been shown to exhibit a near-room-temperature effective permittivity of approximately 10,000. Additionally, montmorillonite (MMT) is a well-known filler, very often utilized for its exceptional ability to exfoliate and disperse within polymer matrixes such as PMMA. Using a thermally-initiated, in-situ, radical polymerization, a series of PMMA-CCTO-MMT ternary systems have been prepared with various CCTO loadings, and the resultant dielectric and thermal behaviors have been tested. The initiator utilized in this work, benzoyl peroxide (BPO), was added in concentrations that insured monomer-to-initiator molar ratios of 1 : 2*10^-3 in all systems. While CCTO filler was added to improve the dielectric behavior of the systems, MMT was added for its thickening ability that helped disperse and suspend the CCTO particles. Preliminary results suggest that a gradual increase of the CCTO amounts in the composites leads to a steady improvement (increase) of the dielectric constant, â. While maintaining dissipation factors (tan â) smaller than 3%, the â of the best-performing PMMA-CCTO-MMT sample was almost 4 times larger than that of the unfilled PMMA sample. Regarding the thermal characteristics of composites, the addition of MMT alone was observed to decrease the glass transition temperature, Tg, of PMMA from 122 °C to approximately 112 °C. Further addition of CCTO to the PMMA-MMT samples did not lead to any further variation of Tg in the resultant composites. Notably, Tg of PMMA in the resultant materials is high enough to allow the composites to retain their structural integrity from below room temperature to about 90 °C. Further mechanical investigations will be conducted to determine the suitability of such systems for designing structural capacitors that have the ability to carry load while storing energy.
Thermal and Mechanical Properties of Bisphenol E Cyanate Ester Matrix Composites Embedded with Nano- and Micro-scale Fillers for Multifunctional High Energy Density Capacitor Applications

J. Eliseo De Leon
Iowa State University
Materials Science & Engineering Department, 2200 Hoover Hall, Ames, 50011, US
Phone: 509-592-0202, Email: jdeleon@iastate.edu

Eduard A. Stefanescu
Iowa State University, Ames, IA

Xiaoli Tan
Iowa State University, Ames, IA

Michael R. Kessler
Iowa State University, Ames, IA

Abstract:
The aim of this investigation is to characterize the thermal and mechanical properties of nanocomposite materials consisting of a thermoset matrix, bisphenol E cyanate ester resin, bis(4-cyanatophenyl)-1,1-ethane (BECY), embedded with nano- and micro-scale fillers. The fillers under investigation include COOH functionalized multi-walled carbon nanotubes (MWCNT), barium titanate (BaTiO3) with surface modifying epoxy-silane groups, and ionic, exfoliated clays at the nano- and/or micro-scales. BECY exhibits excellent thermo-mechanical properties, such as high glass transition temperature (Tg), and excellent strength and toughness. As such, our objective is to provide proof-of-concept that composites containing the above constituents can provide industrial-grade structural components, and simultaneously serve as charge storage devices.

To date, we have identified a dielectric composite containing 2.6 wt% CNT, 40 wt% BaTiO3 and 10 wt% nanoclay capable of yielding a dielectric constant, \( e \), of c.a. 30, with nominal tan delta below 0.1 over a broad range of frequencies. Current efforts are focusing on optimizing the mechanical strength, toughness and Tg variations in the candidate dielectric composites. Dynamical mechanical analyses (DMA) and mechanical tensile strength experiments are planned to ascertain the improvement of the composite’s Young’s modulus, and toughness respectively. Preliminary data show a drop in the Tg when all three fillers are present. Further investigations on the interactions between each individual filler and BECy matrix have been conducted in order to determine which of the constituents most dramatically affects Tg. Under the premise that our composite retains high Tg, we foresee that this composite will be useful in high temperature applications.

We predict that the results of this study will aid in the development of discrete passive components (i.e. multifunctional capacitors) that may serve not only as charge storage devices but also load bearing structural components. Such light multifunctional composites may lead to significant weight savings in aerospace vehicle design, and other advanced, innovative applications.
High Energy X-ray Diffraction Measurements: Uncertainty Analysis

John Edmiston
University of California Berkeley
Phone: 5104954665, Email: jedmiston@berkeley.edu

David Steigmann
University of California Berkeley, Berkeley, CA

George Johnson
University of California Berkeley, Berkeley, CA

Nathan Barton
Lawrence Livermore Nat'l Lab, Livermore, CA

Abstract:

In this presentation, we discuss a rapidly improving experimental method for probing material structure using high energy (~80 keV), synchrotron x-ray diffraction measurements. As background, the primary quantitative outputs of these experiments are the strain and orientation tensors which describe the local crystal lattice, as well as the center of mass of the diffracting grain. The experimental technique quickly captures strain, orientation, and center of mass information simultaneously for up to several hundred grains, depending on the quality and nature of the polycrystalline sample. Additionally, recent improvements in hardware and software capabilities at the beamline at Sector 1 at the Advanced Photon Source, Argonne National Lab, have made making diffraction measurements with in situ loading a continually improving proposition. Overall these advances in the experimental method have greatly improved the quality of data attainable from studies of fundamental topics such as crystal plasticity and phase transformation.

Beyond a general description of the experimental method the presentation is focused on understanding the precision with which one can state the lattice strain, orientation, and center of mass position of a given grain during such an in situ test. Conventional methods of quantifying the uncertainty associated with a particular measurement prescribe simply repeating observations and performing basic statistical analysis on the resulting distribution of data. However irreversible processes occurring during large strain in situ tests, such as plastic deformation, make repeated measurements of the same crystal state impossible. Therefore using conventional methods to state the uncertainty associated with the lattice state are unavailable for these tests.

We present a method for quantifying the uncertainty associated with x-ray diffraction measurements of lattice stretch and orientation based on data from a single measurement using finite strain kinematics. We implement a hierarchical framework in which uncertainty in the locations of diffraction peaks is communicated into lattice stretch and rotation tensors, and center of mass position through a weighted least squares formulation. This classical method is generally applicable to many studies, but specific results pertain to monochromatic x-ray diffraction experiments.
Carbon Nanotube Buckypaper Material: An Important Platform for Developing Multifunctional Composites

Richard Liang
Department of Industrial and Manufacturing Engineering, High-Performance Materials Institute (HPMI)
Florida State University
2525 Pottsdamer Street, Tallahassee, FL 32310, US
Phone: 850-645-8998,   Email: liang@eng.fsu.edu

Ben Wang
Florida State University

Chuck Zhang
Florida State University

Abstract:
Carbon nanotubes (CNTs) have a great potential for developing high-performance multifunctional composites due to their exceptional mechanical, thermal and electrical properties. In this research, we explored and demonstrated the effectiveness of utilizing CNT buckypaper, a thin film (10-20 microns) of preformed CNT network, to achieve high CNT concentration and alignment for multifunctional composite applications. We successfully demonstrated that we can achieve up to 80% degree of alignment and 60 wt.% loading of CNTs in buckypaper composites, which leads to substantial improvement of mechanical and electrical properties. The resultant composites possess the mechanical properties higher than the state-of-the-art unidirectional carbon fiber composites and electrical conductivity is more than 5,000 S/cm along the alignment direction. High electrical conductive buckypaper is also a promising candidate for EMI shielding application. We studied the mechanism and effectiveness of using different buckypapers (SWNT, MWNT and carbon nanofiber or CNF) and their composites for EMI shielding application. A model was also developed to explore different EMI shielding mechanisms in buckypaper composites. The results show that microwave reflection is the governing mechanism. Utilizing high conductive buckypaper and unique multiple reflection mechanism is effective to improve the EMI shielding performance. We also demonstrate that buckypaper is a good candidate material for developing lightweight and low power consumption actuator and morphing structures. Lightweight all-solid-state buckypaper composite actuators developed in this research were a bimorph configuration with a high conductive solid electrolyte layer sandwiched by two buckypaper electrode layers. The effects of driving voltages and frequencies were studied. The nanotube buckypaper composite actuators demonstrated consistent responses to electrical stimulation frequencies up to 40 Hz. We realized significant performance improvements by using long MWNT buckypapers and lithium ion doped SWNT buckypapers as electrode layers. The resultant actuators can achieve more than 20 mm displacements, which is about 10 times greater than untreated buckypaper composite actuators. Ionic doped SWNT buckypaper actuators are especially promising because they consume 70% less power to perform the same amount of actuation compared to other buckypaper actuators.
Relating Molecular Self-Assembly to Mechanical Strength in Nanocomposite Hydrogels

Gudrun Schmidt
Purdue University
Biomedical Engineering, 206 S. Martin Jischke Drive, West Lafayette, 47907, US
Phone: 7654961427, Email: gudrun@purdue.edu

Patrick Schexnailder
Purdue University

Akhilesh Gaharwar
Purdue University

Chia Jung Wu
Purdue University

Abstract:
Understanding the chemistry and physics of self-assembly processes in nanocomposite hydrogels is critically important for the rational design and fabrication of high performance materials. Work presented here investigates molecular interactions leading to the self-assembly and mechanical strength of nanocomposite hydrogels. These hydrogels are made from polyethylene oxide, (PEO) and Laponite nanoparticles, (Na+0.7[(Mg5.5Li0.3)Si8O20(OH)4]-0.7) that cross-link the PEO by ionic interactions and hydrogen bonding. Physically cross-linked nanocomposite hydrogels based on Laponite and PEO have been extensively studied as model systems for investigating polymer nanoparticle interactions and responses to shear flow. Laponite nanoplatelets which are synthetic silicate poly-ions act as reversible cross-linkers to PEO because the polymer readily adsorbs onto the nanoparticle surfaces. Despite much effort to understand molecular interactions in physically cross-linked hydrogels, little is known about covalent cross-linked hydrogels made from Laponite and PEO’s.

We use PEO-dimethacrylate polymerization to stabilize the microstructures that self-assemble within a PEO-Laponite nanocomposite hydrogel. The cross-linking chemistry of end functionalized PEO is well known as this polymer can be easily optimized for specific biotechnological applications. Using covalent cross-linking chemistry, mechanical deformation, imaging and scattering techniques, the molecular interaction parameters that are responsible for self-assembly and mechanical strength are investigated. Small Angle Neutron Scattering and Ultra-SANS can be used to investigate the shear induced molecular interactions and nanometer structural responses of Laponite cross-linked PEO hydrogels. Overall evaluation of data obtained from these scattering experiments gives us some information on how molecular interactions between PEO polymer chains and Laponite nanoparticles (on a nanometer length scale) influence the formation of large-scale structures (inhomogeneities, layers) that are detected on micrometer length scales. Ultimately this approach allows determining how interactions such as hydrogen bonding, ionic and covalent bonds influence the organization of microstructures and how self-assembly can be used to understand mechanical properties.
Effective Parameters of Bucky Gel Morphing Nanocomposites
Dynamic Behavior

Ali Ghamsari
Louisiana State University
101 ERAD Bldg, Louisiana State University, Baton Rouge, 70803, US
Phone: 225-803-8063, Email: akadkh2@tigers.lsu.edu

Tige Brown
Southern University, Baton Rouge, LA

Eyassu Woldesenbet
Louisiana State University, Baton Rouge, LA

Abstract:
In the last decade, a great effort has been made to fabricate electrically triggered morphing composites which can operate in dry condition without any need for electrolyte solution. Bucky gel, which is a gelatinous mixture of carbon nanotubes and ionic liquid at room temperature, was first successfully employed in a soft actuator in 2005. This three-layered composite is a bimorph actuator which can be driven by just a few voltages at varying frequencies and long durations. There are currently no publications in the literature on the dynamic mechanical behavior of Bucky gel actuator. Here, the effect of different material and geometrical parameters (thickness, layer combinations, carbon nanotube fraction) on the storage modulus, glass transition temperature and the hardness of the actuator are investigated by the means of DMA and Nanoindentation. Different types of carbon nanotubes (pristine single-walled, pristine multi-walled, functionalized single-walled, and functionalized multi-walled) are employed in fabrication of the nanocomposites to examine their influence on dynamic mechanical response. Finally, the possibility of replacing the ionic liquid with another type of solvent with improved properties and more diversity is investigated.
The Deformation of Magentoreheological Elastomers Coupled with Their Magnetic Properties

Zelalem Aga
Iowa State University, 2025 Black Engineering Blg, Ames, 50011, US
Phone: 515-294-1423, Email: zaaga@iastate.edu

LeAnn Faidley
Iowa State University, Ames, IA

Wei Hong
Iowa State University, Ames, IA

Abstract:
Magnetoreheological elastomers (MREs) are composite materials made up of ferromagnetic particles suspended in a polymer matrix that are capable of changing their mechanical properties in response to an externally applied magnetic field. These field-induced changes in properties are attributed to the magnetic interaction between the ferromagnetic particles as well as the accompanying elastomeric response of the polymer matrix, which results in magneto-elastic effects. One of the magneto-elastic effects is the change in dimension or shape of the material due to the applied magnetic field i.e., magnetostriction. Experimental evidence shows that the magnetostriction of MREs is comparable to (or in some cases greater than) other common giant magnetostrictive alloys such as Terfenol-D. MREs can also change their stiffness when exposed to magnetic fields as a result of the same magneto-elastic effect. Variable stiffness bushings, engine mounts, and releasable attachments used in the automotive industry; tunable vibration absorbers of various types and noise control devices are some of the applications for MREs that have been proposed using the field induced change in stiffness. Applications utilizing the magnetostrictive property of MRE are fewer; however, it is believed that they can be used for actuators and sensors.

In this study, the magnetostricticiton of MREs is analyzed using micromagnetics and elasticity theory. In order to reach equilibrium, the energy increase in MREs due to an applied magnetic field reduces due to magnetization vector rotation of the single domain particles accompanied by the relaxation of the system through elastic deformation of the host matrix. For magnetization evolution we use the Landau-Lifshitz equation of micromagnetics. The energies for this magnetization evolution consists of: (a) local demagnetizing energy which accounts for the dipole-dipole interaction of the particles; (b) magnetic anisotropy energy which defines the initial easy direction of magnetization and takes into account the crystal symmetry of the particles; (c) exchange interaction energy which accounts for the inhomogeneous magnetization direction of different particles; and (d) Zeeman energy which accounts for the interaction of the magnetization of the particles with the external field. The magnetic and elastic deformation is coupled through the interface boundary condition between the polymer and iron particles. The equilibrium magnetostriction is determined from energy minimization with respect to strain. It is noteworthy that the equilibrium of MRE with respect to magnetization precedes the elastic equilibrium as the magnetization due to electron spins in the iron particles is faster than the slow relative motion and deformation of the polymer.
Influence of Surface Roughness and Functionalization on Shear Strength of Individual Carbon Nanofiber-Epoxy Interfaces

TANIL OZKAN
University of Illinois, Urbana-Champaign
104 S. Wright St. Talbot Building MC-236, Aerospace Engineering, Urbana, 61801, US
Phone: 217-333-3122, Email: tozkan2@illinois.edu

IOANNIS CHASIOTIS
University of Illinois, Urbana-Champaign, IL

Abstract:

Modeling and optimization of nanostructured composites have been hindered by the lack of interfacial properties at the level of individual nanoconstituents. Novel nanoscale fiber pull-out experiments, supported by MEMS mechanical testing platforms, provided for the first time the interfacial shear strength (IFSS) of individual carbon nanofibers (250 nm average diameter) embedded in an epoxy matrix. The as-grown carbon nanofibers with 5 nm surface roughness and turbostratic annulus exhibited high IFSS, averaging 110 +/- 25 MPa, which is significantly larger than that of non-functionalized (15-28 MPa) and functionalized (40-65 MPa) microscale carbon fibers. Contrary to expectations, the IFSS of high temperature heat treated and graphitized carbon nanofibers was drastically reduced to 66 +/- 10 MPa, while the nanofiber surface roughness was also reduced to 1-2 nm. Thus, it is evident that this minute nanofiber surface roughness is a major factor controlling the IFSS along with the chemical composition and morphological aspects of the nanofiber-polymer matrix interface. The reduction in IFSS because of reduced surface roughness accommodated through the graphitic conversion of the previously turbostratic nanofiber annulus was restored by oxidative functionalization of the nanofiber surface resulting in IFSS values of 190 +/- 14 MPa, indeed much higher than current achievable values with conventional micron sized carbon fibers. All the aforementioned measurements were independent of the nanofiber embedded length and diameter, which provides confidence in the reported numerical values. These local IFSS measurements from individual nanofibers represent the first direct explanation of the improved global composite fracture toughness reported before in the literature. The findings of this experimental investigation, which emphasized the critical role of surface roughness and chemical functionalization in IFSS, underline the importance of scale-specific interfacial experiments and assert that linear extrapolations of macroscale interfacial measurements to the nanoscale are not valid for polymer nanocomposite design and mechanical modeling purposes.
Three-Dimensional Microvascular Fiber-Reinforced Composites

Scott White
University of Illinois at Urbana-Champaign
306 Talbot Lab, 104 S. Wright St., Urbana, 61801, US
Phone: 217-333-1077, Email: swhite@illinois.edu

Aaron Esser-Kahn, Piyush Thakre, Hefei Dong, Jason Patrick, Nancy R. Sottos, Jeff Moore
University of Illinois, Urbana, IL

Abstract:

Microvascular systems are essential to a broad range of technological applications, including biotechnology, microelectronics, sensors, chemical reactors, and autonomic materials. Several approaches have emerged for fabricating three-dimensional (3D) microvascular systems including lithographic techniques, laser micromachining, and various two-dimensional methods extended to 3D. Recently, sacrificial sugar fibers have been used to create 3D microvascular networks. We have previously reported a method for the fabrication of 3D microvascular networks utilizing fugitive inks that allowed the fabrication of interconnected micro-channels1 and demonstrated their use in the construction of self-healing coatings and materials2,3. All of these methods have their advantages, but none can be integrated into large-scale fiber composite materials. Here we show a simple method for the creation of structural composite materials containing microvascular networks via interweaving of a sacrificial fiber. The polymeric fiber is extracted during a post-cure procedure at high temperature. Sacrificial fibers are chemically treated prior to integration into the composite perform with a catalyst that activates depolymerization of the fiber into a gaseous monomer at elevated temperature. These fibers are woven directly into glass and carbon fiber composites and after evacuation leave behind networks of interconnected empty channels that can be filled with fluid. Microvascular composites formed with sacrificial fibers should facilitate the thermal management in composites, enable more sophisticated self-healing materials, and provide a test-bed for new self-healing chemistries.

References:
Microvascular Networks for Thermal Acceleration of Self-Healing

Christopher Hansen
University of Illinois at Urbana-Champaign
1304 W Green St, 216 MSEB, Urbana, 61801, US
Phone: 217.244.4527, Email: chansen3@illinois.edu

Scott R. White
University of Illinois at Urbana Champaign, Urbana, IL

Nancy R. Sottos
University of Illinois at Urbana Champaign, Urbana, IL

Jennifer A. Lewis
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Self-healing materials are a new approach to materials designed to restore a physical property after degradation. The first generation of self-healing polymeric materials (White et al) were based on an embedded microcapsule design, whereby microcapsules of dicyclopentadiene (DCPD) monomer would be released upon fracture and wick by capillary action into contact with Grubbs catalyst. The resulting polymerization leads to an impressive recovery of mechanical properties, yet are limited to a single heal cycle due to depletion of healing components. The next generation of self-healing materials pursues the goal of multiple healing cycles by integrating complex three-dimensional microvascular networks into structural composites via direct-write assembly. This generation of self-healing materials contained the same DCPD-Grubbs catalyst system and displayed up to 7 consecutive heal cycles, above which the catalyst was locally depleted (Toohey et al).

To extend this further, these self-healing architectures are now modified through a combination of dual and vertical ink writing to create interpenetrating microvascular networks. In this case, these two independent networks are filled with liquid epoxy resin and epoxy hardener, respectively. These reactive fluids remain sequestered in their respective microvasculature until crack(s) form in a brittle coating layer. At this point, both liquid resin and hardener flow into and mix in the crack plane where they undergo polymerize to restore mechanical properties. Importantly, we find that neither healing agent is preferentially depleted, enabling up to 30 consecutive cycles (and beyond) of mechanical property recovery.

We now extend this technique by introducing a third interpenetrating network devoted to thermal control of the composite. This additional network permits circulation of a constant-temperature fluid that locally heats the composite in regions of mechanical damage. Increased temperature is shown to accelerate polymerization kinetics of the epoxy healing system by over an order of magnitude. As a fully integrated system, the microvasculature promises to efficiently deliver healing fluids to damaged coatings and thermally heat the mixed fluids to significantly decrease the time required to recover mechanical properties.
Damage Recovery In Composites With Transverse Microcracking

Piyush Thakre
Beckman Institute of Advanced Science and Technology, UIUC
405 N Mathews Ave Suite 3324, Urbana, 61801, US
Phone: 9797390172, Email: pthakre@illinois.edu

Martin Blouet
Visiting Student Intern from Universite, de la Rochelle, France, Urbana, IL

Nancy R. Sottos
Beckman Institute for Advanced Science and Technology, Department of Materials Science and Engineering, University of Illinois at Urbana Champaign, Urbana, IL

Scott R. White
Beckman Institute for Advanced Science and Technology, Department of Aerospace Engineering, University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

There has been remarkable progress in self-healing polymers; however, the ability to autonomically heal damage in fiber-reinforced polymer composites continues to present challenges. We propose to develop glass fiber reinforced composites with the ability to recover damage in the form of transverse cracks in thermoset matrix composites. Self-healing matrix consists of microcapsules containing a healing agent, which is released in the event of matrix cracking. The size scale of the crack damage determines the necessary size and concentration of capsules for effective healing.

We first evaluate healing in a composite in which microcracking is induced in a confined interlaminar zone between two surrounding (stiff) layers. A matrix rich interphase region consisting of self-healing microcapsules is introduced between two outer skins made out of glass fiber reinforced polymer (GFRP) composite plates. Transverse cracking in the matrix rich interphase region is achieved through tension testing of rectangular coupons. Controlled progressive damage is achieved through varying stress levels that are a fraction of the ultimate tensile strength of such composites. We propose a new experimental protocol using X-ray tomography to investigate the change in crack density with stiffness reduction due to progressive damage. Apart from providing 3-D distribution of cracks, X-ray tomography can also give information about different size scales involved in the transverse cracking. Recovery of damage at intermediate stress levels is determined from the stress-strain response of self-healed specimens along with change in crack density post self-healing.
Self-Healing High Temperature Cured Epoxy

Henghua Jin
University of Illinois at Urbana Champaign
405 North Mathews Avenue, Urbana, 61801, US
Phone: 2177222124, Email: jin6@illinois.edu

Chris Mangun,
CU Aerospace, Urbana, IL

Dylan S. Stradley, Nancy R. Sottos, Scott R. White
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

A dual-microcapsule self-healing system has been developed for use in high temperature cured epoxy. One capsules contain a modified aliphatic amine (EPIKURE 3274) while the second capsule contains a diluted epoxy monomer (EPON® 815C). The reactive amine microcapsules are prepared by vacuum infiltration of EPIKURE 3274 into hollow polymeric microcapsules. Epoxy microcapsules are prepared by an in situ polymerization method [1]. Both types of capsules were incorporated into an epoxy matrix (EPON® 828/DETA) at various concentrations.

Fracture of the epoxy matrix ruptures both types of capsules releasing their respective core materials into the crack plane. Upon the mixing of both healing agents, polymerization occurs at room temperature without any external intervention.

Recovery of mode-I fracture toughness was measured using tapered-double-cantilever-beam (TDCB) specimens [2] that were post cured at 121°C for 1h followed by 177°C for 2.5h. Specimens were allowed to heal for 48 h at room temperature following the virgin fracture test. The effect of capsule concentration on healing efficiency and the stability of this self-healing system within a high temperature cured epoxy are presented.

References:
Fracture Behavior of Mechanophore-Linked Glassy Polymers

Asha-Dee Celestine
University of Illinois at Urbana-Champaign
306 Talbot Laboratory, MC-236, 104 South Wright Street, Urbana, 61801, US
Phone: 202-641-8802, Email: celesti1@illinois.edu

Brett Beiermann, Douglas Davis, J. S. Moore, N. R. Sottos, S. R. White
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

A new class of mechanoresponsive polymers has been developed by incorporating force sensitive molecules called mechanophores into glassy polymers. In these materials, mechanical energy induces a chemical reaction of the mechanophore [1, 2]. Applications for such polymers include monitoring and assessing damage and initiating self-healing reactions. In this study, we explore the mechanical behavior of the glassy polymer poly(methyl methacrylate) (PMMA), which contains a spiropyran (SP) mechanophore. Upon the application of force, the central spiro carbon-oxygen bond ruptures, and this is accompanied by a vivid color change and an increase in fluorescence. Both linear and cross-linked PMMA were tested.

Linear SP-PMMA was synthesized by an ATRP process using the SP mechanophore as a bis-initiator resulting in a single SP in the center of each polymer chain. Cross-linked SP-PMMA (1 mole% cross-link density) was prepared by free radical polymerization with the SP mechanophore acting as a cross-linker. Fracture and mechanical test specimens were obtained by compression molding and in-situ polymerization.

Storage and loss moduli and tan delta of both the linear and cross-linked material were determined through Dynamic Mechanical Analysis (DMA). The fracture behavior of the mechanophore-linked polymers was examined by Double Cleavage Drilled Compression (DCDC) testing of rectangular specimens measuring 25 mm x 8 mm x 2 mm with hole radii of 2 mm. The DCDC test facilitates stable crack growth and provides a method for determining the fracture toughness of the linear and cross-linked SP-PMMA in addition to the stress required to activate the SP at the crack tip. The effects of loading rate, SP concentration, and cross-link density on fracture properties and mechanophore activation were also investigated.

References:
A High Temperature Cured Structural Self-Sealing Composite

Jericho Moll
Department of Materials Science and Engineering, University of Illinois
1304 W Green St, Materials Science and Engineering, Urbana, 61801, US
Phone: 217-898-9319, Email: jmoll2@illinois.edu

Prof. Nancy Sottos
Department of Materials Science and Engineering, University of Illinois, Urbana Champaign, IL

Prof. Scott White
Department of Aerospace Engineering, University of Illinois, Urbana Champaign, IL

Abstract:

Fiber reinforced composite tanks provide a promising method of storage for liquid oxygen and hydrogen 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 monomer and wax protected Grubbs catalyst into an epoxy matrix has shown the ability to self-heal micron scale crack damage in low Tg 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. In the past, the incorporation of this healing chemistry into a fiber reinforced epoxy composite has provided the necessary functionality for autonomic sealing of crack damage subject to modest pressures [4]. Currently, a new two capsule sealing chemistry comprised of silanol terminated poly(dimethyl siloxane) plus a crosslinking agent and a tin catalyst, shown to be stable to 150 °C, can be used to self-seal a composite with a Tg of 130 °C. In this work, sealing of mechanical damage is assessed through the use of a pressure cell apparatus to detect nitrogen flow through the thickness direction of a damaged composite.

References:
Self-Healing of Impact Damage in 3D Woven Composites

Amit Patel
University of Illinois
MSEB, 1304 W. Green St., Urbana, 61801, US
Phone: 217-714-1331, Email: ajpatel4@illinois.edu

Nancy R. Sottos
Dept. of Materials Science and Engineering, University of Illinois, Urbana, IL

Eric D. Wetzel
Materials Division, US Army Research Lab, Aberdeen Proving Ground, MD

Scott R. White
Department of Aerospace Engineering, Urbana, IL

Abstract:

Fiber-reinforced composite laminates with polymeric matrices are extensively used in many structural applications. However, 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 investigated for the repair of impact-induced damage. Previously, autonomic self-healing of 2D woven S2 glass composites containing a microencapsulated dicyclopentadiene and 1st generation Grubbs catalyst healing system was demonstrated using compression-after-impact (CAI) tests [1]. CAI testing revealed that residual compressive strength (RCS) was fully recovered up to a threshold impact energy which was 84% higher for self-healing systems. RCS decreased with increasing incident impact energy, a result attributed to the increase in damage volume.

In this work the same self-healing system is incorporated into 3D woven S2 glass composites. These materials may exhibit decreased damage volume compared to 2D woven composites due to z-tow bridging of delaminations, thus making them more amenable systems for incorporation of self-healing functionality. To investigate the effect of z-tows on damage separation, damage analysis of impact damage in 3D and 2D woven panels was conducted using a semi-automated crack analysis program to measure relevant damage properties. In addition, a processing technique has been developed to incorporate microcapsules into 3D woven composites by pre-impregnation of 3D woven fabric prior to vacuum-assisted resin infusion.

References
Autonomic Structural Cooling via Adaptive Microvascular Networks

Brian Kozola
University of Illinois at Urbana-Champaign
306 Talbot Laboratory, MC-236, 104 South Wright Street, Urbana, 61801, US
Phone: 217-819-1248, Email: bkozola2@illinois.edu

Scott R. White
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Adaptive microvascular cooling networks combine the efficiency of micro-scale convective heat transfer with autonomically triggered thermal response to manage temperatures in structural materials. Embedded vascular networks exploit the unique thermal advantages of the microscale where the heat transfer coefficient is inversely proportional to the channel diameter. The system autonomic response is biologically inspired where localized cells sense increased thermal loads and adapt accordingly by activating more thermally efficient cooling mechanisms such as disperse capillary flow and evaporative surface cooling.

This study develops and tests a new autonomic microvascular system to actively cool a surface over a broad temperature range. We utilize direct-write assembly to fabricate highly complex, branching networks embedded directly into a structural epoxy matrix. The network architecture utilizes a hierarchical design with channel diameters varying from 600 micron arteries branching down to 200 micron capillaries and ultimately to 5-20 micron pores. Thermally activated internal valves utilizing a coefficient of thermal expansion (CTE) mismatch were fabricated using polydimethylsiloxane (PDMS) and integrated into the network arteries. The valves activate at elevated temperature (80-90 C) and control the local balance between low pressure drop flow through arteries and enhanced heat transfer through disperse capillary networks. Additionally, 5-20 micron diameter surface pores were created via sacrificial fiber mats linking the underlying network to the surface. The pores allow capillary fluid flow to the surface resulting in evaporative cooling and enhanced thermal dissipation.

Experiments were performed utilizing three specimen types: a control specimen with no embedded network, a vascular network with no embedded valves, and an active specimen with an adaptive vascular network. The system performance was evaluated by monitoring fluid and surface temperatures and system pressure drop as the substrate temperature is varied from 25 to 130 C.
Design of Microvascular Materials in Actively-Cooled High-Temperature Composites

Soheil Soghrati
University of Illinois at Urbana-Champaign, 504 E. White st, Apartment 35, Champaign, 61820, US
Phone: 217-819-8815, Email: ssoghra2@illinois.edu

Alejandro M. Aragon, Philippe H. Geubelle, Scott R. White

Abstract:
The design of microvascular channels for active cooling of 3D woven composites involves multiple modeling and manufacturing challenges. One of the biggest obstacles for incorporating the microchannels in woven and 3D composites is the evacuation of the sacrificial fibers used to generate the embedded network. The approach adopted in this work involves pre-treating PLA (Poly-Lactic Acid) fibers with a Sn-based catalyst to facilitate the degradation of the sacrificial fiber and thereby the generation of the embedded microchannels. Among the key challenges is the elimination of the plugs which prevent the complete evacuation of the sacrificial fibers, and the need to achieve the degradation of the PLA fibers without affecting the properties of the composite.

To support the development of these new materials, a modeling effort is conducted at both macro- and meso-scales. At the macro-scale, i.e., at the scale of the composite part, the microchannels are modeled as line segments that serve as heat sinks in the (homogenized) composite part. The solution of the associated thermal problem is obtained using a generalized finite element solver that provides the added flexibility of adopting a finite element discretization that does not conform to the geometry of the embedded network [1]. To optimize the topology of the embedded network, we use a shape optimization scheme inspired by a multi-objective and multi-constraint genetic algorithm. Competing objective functions including void volume fraction, maximum temperature and network flow efficiency are considered in the optimization study, yielding a complex optimal Pareto front from which a set of optimal network geometries is extracted [2]. These geometries then serve as inspiration for a simpler and more efficient shape optimization strategy, for which the network geometry is captured through a small set of design variables. At the meso-scale, the impact of the microchannels on the thermal field in a periodic unit cell of the microvascular composite is investigated by explicitly modeling the thermal solution in the microchannels, and the heterogeneous nature of the fiber tows and matrix. Due to the small size of the microchannels (typically between 100 and 500 microns in diameter) and the relatively small mass flow rates, Poiseuille flow conditions are assumed.

References
Pressurized Vascular Systems for Healing Fatigue and Quasi-Static Fracture Damage

Andrew Hamilton
University of Illinois at Urbana Champaign
Beckman Institute, 405 N. Mathews Ave., Urbana, 61801, US
Phone: 217-417-9865, Email: ahamilt3@illinois.edu

Scott R White
University of Illinois at Urbana Champaign, Urbana, IL

Nancy R Sottos
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Synthetic materials with micron-sized vascular features mimic the ability of biological materials to distribute and transport fluid throughout the material volume. These synthetic vascularized materials are utilized to autonomously heal crack damage in coatings, at sites of interfacial delaminations, and within the vascular material itself. In most cases, capillary forces drive the flow of the liquid healing agents into the crack plane where they react to form an adhesive bond across the crack faces. Some of the most effective healing agents for these applications consist of two liquid-phase components (i.e. a resin and hardener) that must be well-mixed, ideally at a specific ratio, in the crack plane for complete polymerization and optimal healing. With capillary forces driving fluid flow, there is little opportunity to influence the mixing of the fluids the relative amount of fluid released. Pressurizing the healing agents within the vascular network provides an opportunity to facilitate mixing by pumping them in a manner that maximizes the contact between the two fluids thereby reducing the diffusional distances. It also enables the delivery of a larger amount of healing agents to a more substantial damage volume. Using pressurized vascular systems, we achieve consistently higher recovery of fracture toughness over a greater number of cycles of damage and healing as compared with samples where capillary forces drive the flow of healing agents. Furthermore, we assess the ability of these materials to impede fatigue crack growth and are able to significantly extend the fatigue life of the material as compared with control samples with no vascular system.
Toughening of Bisphenol E Cyanate Ester

Xia Sheng
Iowa State University
Department of Materials Science and Engineering, 2220 Hoover Hall, Ames, 50014, US
Phone: 1-515-231-9660, Email: xsheng@iastate.edu

Michael R. Kessler
Department of Materials Science and Engineering, Iowa State University, Ames, IA

Abstract:

Cyanate esters are widely used in applications ranging from aerospace to microelectronics because of their excellent thermomechanical properties. Bisphenol E cyanate ester (BECy) is a unique cyanate ester monomer with a very low viscosity at room temperature and very high glass transition temperature after it is fully cured. This combination of low viscosity and high temperature stability differs from other high-temperature thermosetting polymers, which begin as highly viscous or solid monomers at room temperature. In our group, BECy was successfully used as the matrix for fabricating multifunctional high-temperature composites, such as composites with controllable thermal expansion and flexible piezoelectric composites for NDE (nondestructive evaluation) applications. However, the highly cross-linked BECy thermoset is brittle, and it is necessary to improve its toughness for some applications. Traditionally, phenols and mono-functional cyanate esters have been co-polymerized with bi-functional cyanate esters to toughen the resulting networks. Additional novel cyanate ester monomers have been reported, which, when cured, result in thermosets with enhanced toughness. However, the synthesis of custom cyanate ester monomers often requires the very toxic bromine cyanide, making the synthesis of novel monomers dangerous and difficult. In this study, a commercial available polymer, poly(ethylene glycol) diglycidyl ether (PEGDE), was copolymerized with BECy monomer. Since the PEGDE contains soft ethylene glycol segments in its backbone, the resulting thermoset was expected to have improved toughness and elongation. Moreover, inorganic and/or organic fillers have been applied to physically modify the properties of the cyanate esters. When chopped Kevlar fibers were introduced to the BECy, the toughness and other mechanical properties of the composites were improved significantly. In addition to characterizing the mechanical properties of the two systems (BECy/PEGDE and BECy/Kevlar), oscillatory rheology, dynamic mechanical analysis (DMA), and thermogravimetry were used to evaluate the gel time, viscoelastic behavior, and thermal stability, respectively. The optimized compositions and cure conditions may expand the applications of BECy to a broader range of advanced composites and manufacturing processes.
Photovoltaic Waveguide Polymer Composite

Fareed Dawan
Southern University and A&M College
367 P.B.S. Pinchback Engineering Bldg., Southern University and A&M College, Baton Rouge, 70813, US
Phone: 225-771-4701, Email: fareeddawan@engr.subr.edu

Treva T. Brown
NextGenC^3 Composites CREST Center, Louisiana State University, Baton Rouge, Louisiana

Yoonyoung Jin
NextGenC^3 Composites CREST Center, Southern University and A&M College, Baton Rouge, Louisiana

Eyassu Wolidesenbet
NextGenC^3 Composites CREST Center, Southern University and A&M College, Baton Rouge, Louisiana

Abstract:

Photovoltaic materials and devices have attracted heightened interest in recent years due to both increased energy demands and noticeable adverse climate change (global warming) largely due to the use of fossil fuels [1]. The Utilization of green energy sources such as solar cell devices would, amongst many other impacts, reduce the carbon emissions footprint. Balancing conversion efficiency with manufacturing costs has led to the development of flexible dye-sensitized solar cells (DSSCs), such as the Graetzel cell which utilizes the photovoltaic response of titanium dioxide [2]. Increasing efficiency and flexibility of DSSCs is critical in determining the commercial potential of these relatively inexpensive yet versatile devices.

Presented in this research is the fabrication of a flexible photovoltaic waveguide polymer composite. The photovoltaic material used is a dye-sensitized titanium dioxide (TiO2) wire. Anodization of the wire is first performed to form titanium nanotubes. The formation of titanium nanotubes using anodization of titanium foil has been recently shown to greatly increase the efficiency of TiO2 based DSSCs over the use of TiO2 nanoparticles [3]. This is because the growth of the nanotubes can be controlled providing an increase in the surface area and light absorption enhancement of the photoactive material. Solar cell modules typically suffer from loss of efficiency due to wavelength selectivity of the top electrode material, recombination of electron-hole pairs, and inefficient electron transfer into the bottom electrode [4]. In order to reduce these losses, the wire is embedded into a highly refractive-indexed polymer waveguide trapping and sending the light down the length of the wire. In this fashion, the design resembles that of an optical fiber in which the titanium nanotube enhanced TiO2 wire serves as the core, and the polymer composite serves as the cladding.

We investigate different anodization parameters along with dye-sensitizers, various wire lengths, various polymer composites and cell design configurations to determine the optimum parameters for increased conversion efficiency. The performance is also investigated under different atmospheric and environmental conditions. Furthermore, we explore the advantages of bundling the wire composites and reducing the design into the microscale using microfabrication techniques and how the PV OF wire composites can be utilized as an embedded power source for a multitude of applications from advanced aircraft and vehicular structures to on-board powering of microelectromechanical systems.
References
Effect of Silane Coupling Agent on Interfacial Properties of Glass Fiber Reinforced Bio-renewable Resin

Hongyu Cui
Iowa State University
Department of Materials Science and Engineering
2220 Hoover Hall, Iowa State University, Ames, 50010, US
Phone: 515-203-1874, Email: cuihy@iastate.edu

Michael R. Kessler
Department of Materials Science and Engineering, Iowa State University, Ames, IA

Abstract:
In recent years, bio-renewable resins have received significant attention as alternatives to petroleum-based materials due to their low cost, adequate mechanical properties, and superior environmental impact. Bio-polymers derived from soybean oil, corn oil, linseed oil, fish oil and castor oil have been reported over the last decades using a variety of polymerization methods, such as free radical, cationic, and ring-opening metathesis polymerization (ROMP). Bio-renewable-resins have also been used to make composite materials with glass fibers, carbon nano-tubes, nanoclays, and natural fibers.

In this research, bio-based resin was prepared by the ROMP of a modified linseed oil and dicyclopentadiene (DCPD). Based on previous studies, composites from these bio-based resins and glass fibers had relatively low modulus values compared with theoretical models due to poor adhesion between the glass fiber and the polymer matrix. To overcome this problem, a unique norbornenyl functionalized silane coupling agent is used to modify the glass surface so that it is more compatible with the bio-based resin. X-ray photoelectron spectroscopy (XPS), which can measure elemental concentrations on the fiber surface, confirmed that the norbornyl silane was effectively grafted onto the glass surface. Composite panels, made with silane-treated glass fabric and non-treated fabric, were manufactured by hand layup, and their thermomechanical properties were analyzed using dynamic mechanical analysis (DMA) and short beam shear tests. The interfacial shear strength determined by short beam tests shows significant improvement when the glass fiber is appropriately functionalized. The DMA experiments also demonstrate that there is a significant increase in the storage modulus of the silane-treated composites compared to the composites with the unmodified glass fiber, indicating better interfacial stress transfer between the fiber reinforcement and the biorenewable polymer matrix in the composite with the silane-treated fiber. Dog-bone samples cut from the two types of composites were tested on a universal testing machine and the tensile strength and modulus are compared with theoretical models. Scanning electron microscopy of the fracture surface of the composites after tensile testing reveals improved adhesion between the glass fiber and the bio-based matrix for composite with the silane-treated fabric.
Stability of Elastic Composite Materials Having a Negative-stiffness Phase

Dennis Kochmann
University of Wisconsin - Madison
Department of Engineering Physics, 1500 Engineering Drive, Madison, 53706, US
Phone: 608-770-8108, Email: kochmann@wisc.edu

D. M. Kochmann
University of Wisconsin, Madison, WI

Abstract:

The rigorous classical bounds of elastic composite materials theory provide limits on the achievable composite stiffnesses in terms of the properties and arrangements of the composite’s constituents. These bounds result from the assumption, presumably made for stability reasons, that each constituent material must have positive-definite elastic moduli. If this assumption is relaxed, recently published elasticity analyses and experimental findings show that these bounds can be greatly exceeded, resulting in advanced materials of enormous engineering potential. The key question is whether a composite material having a non-positive-definite constituent can be stable overall in the practically useful situation of applied traction boundary conditions.

We determine the necessary conditions of stability for the elastic moduli of the fundamental elastic composite consisting of a circular cylinder of a non-positive-definite material firmly bonded to a concentric coating of a different, positive-definite material. This is accomplished via two different approaches: (i) an energy criterion, which permits a purely closed-form analytical treatment for thin coatings; and (ii) a full dynamic stability analysis, which permits treatment of the entire range of coating thicknesses. We determine quantitatively the full permissible range of inclusion and coating moduli, as a function of coating thickness, for which the overall composite is stable under dead traction boundary conditions. We confirm that both approaches yield identical results for thin coatings.

Among our results, we show that in the case of very thick coatings (corresponding to the dilute case of a matrix-inclusion composite), even an inclusion with merely strongly elliptic moduli can be stabilized by a positive-definite matrix satisfying weak requirements, for which we present analytical expressions. Overall, we show that surprisingly weak restrictions on the moduli and thickness of the positive-definite coating are sufficient to stabilize a non-positive-definite inclusion, even one whose moduli are merely strongly elliptic. These results legitimize expanding the search for novel materials with extreme properties to those incorporating a non-positive-definite constituent, and they provide quantitative restrictions on the constituent materials’ moduli and volume fractions, for the geometry examined here, that ensure overall stability of such composite materials.
Crushing Behavior of Composite Hexagonal Ring System

Elsadig Mahdi
Qatar University
College of Engineering, Qatar University, Doha, 2713, QA
Phone: 9746056768, Email: elsadigms@qu.edu.qa

A. M. S. Hamouda
Qatar University, Doha, Doha

Abstract:

An extensive experimental investigation of quasi-static lateral crushing of composite hexagonal ring system between platens has been carried out. Woven roving glass/epoxy hexagonal ring system with different angles and arrangement were employed. The rings angles are varying between 45 and 70 degrees. Typical histories of their crushing mechanism are presented. Behaviour of ring as regards the initial crushing load, post crushing load, energy absorbed and mode of crushing have been presented and discussed. Results showed that the crush failure loads and energy absorption capability are greatly affected by the hexagonal ring geometry, arrangement and loading conditions. As the ring angle increases the energy absorption capacity increases.
Thermal Efficiency Study of Heat Shield Materials in Automotive Applications

Venugopal Vengala  
Cummins Inc.  
2482 Thornybrook Dr., Columbus, 47203, US  
Phone: 8124478751, Email: venugopal.vengala@cummins.com

Abstract:

The demand for high performance heat shields is increasing in the automotive industry to meet the challenge of protecting heat sensitive engine components from the heat given off by the engine exhaust system. The introduction of new technology to improve engine performance and to meet stringent emission requirements made the heat shields to be the basic component of the engines to manage the higher temperatures of the exhaust system. High combustion temperatures to reduce emissions, tight packaging of exhaust side engine components, and switching engine components material from metal to plastic to lower the cost have driven the need for the heat shields. The primary function of the heat shields is to protect the components like rubber gaskets, plastic parts, wiring harness, electronic modules, and sensors from the excessive temperatures of exhaust manifolds, turbochargers, aftertreatment components and other components. The heat shield material selection is driven by temperature ratings of the engine, distance of the heat sensitive component from heat source and its temperature capability and most important is the space available to install the heat shield. In addition, meeting the resonant frequency requirements is key criteria. An experimental investigation was carried out to study the heat shielding capability of aluminum, steel and composite materials to provide a high performance heat shield for Cummins industrial engines. The goal of the study was to design a cost effective and light weight heat shield to protect valve cover gasket from the high temperatures of turbine housing within the space and mounting constraints. The temperature limit on the valve cover gasket material was 350 F max continuous and the maximum turbine housing skin temperatures were above 1000 F. The turbocharger arrangement on the hot side of the engine puts it within 34 mm of the valve cover gasket. The temperature data collected on the engine with no heat shield confirmed the requirement of a heat shield between turbine housing and valve cover gasket. The tapped holes available on cylinder head and rocker housing of the engine were used to mount the heat shield which placed it at a distance of ~ 18 mm from the turbine housing. The temperature data was collected on the prototype parts: aluminum 3 mm thick, steel 3 mm thick and composite material ~1 mm thick. The composite material comprises of three metal layers, corrosion resistant aluminized steel layers on the opposite sides of an aluminum layer. The experimental thermal data was collected on the engine running at abusive test conditions having high turbine inlet temperatures. The data predicted better thermal performance of composite material over other materials. Additive thermal resistance of three metal layers with the thermal insulation by the entrapped air between layers attribute to the better shielding performance of composite material. The factors like manufacturing cost, resonant frequency limits and bolted joint requirements were compared between the designs in the determination of final material.
Degradation Kinetics of Aerospace Wire Insulation Material

Peter Hondred
Iowa State University, Department of Materials Science and Engineering, 2220 Hoover Hall, Ames, IA
Phone: 515-564-9651, Email: phondred@iastate.edu

Sungho Yoon
Kumoh National Institute of Technology, Gumi, Gyeongbuk

Nicola Bowler
Iowa State University, Ames, IA

Michael R. Kessler
Iowa State University, Ames, IA

Abstract:
The past conventional wisdom that aerospace wire insulation failures such as cracks, fraying, and degradation are atypical and harmless has proven to be a costly liability exhibited in the tragic accidents of Swissair 111 (Nova Scotia, 1998) and TWA 800 (Long Island, NY 1996). These accidents have been attributed to damaged wiring insulation caused by degradation, cracking, and fraying; a problem for many miles of wire buried deep within their structures. As the aerospace industry matures, hundreds of failures are being discovered in typical aircrafts. Consequently, it is imperative to understand the cause of the failures. However, despite the importance of understanding the mechanisms and kinetics of wire degradation under various thermal, environmental, and mechanical loadings, no systematic studies has been reported on the thermal degradation kinetics of typical wire insulation materials.

This work investigates the thermal degradation kinetics of three commonly used wire insulation materials, poly(ethylene-alt-tetrafluoroethylene) (ETFE), poly(tetrafluoroethylene) (PTFE), and poly[(5,7-dihydro-1,3,5,7-tetraoxobenzo[1,2-c:4,5-c']dipyrrrole-2,6(1H,3H)-diyl]-1,4-phenyleneoxy-1,4-phenylene] (Kapton) through the use of thermogravimetric analysis (TG). Isoconversional kinetic models yield activation energy as a function of degradation, provide the number of steps, and elucidate the type of mechanism in the formulation of mathematical kinetic models of these insulation materials. This work uses model free kinetics (Friedman Analysis) to gain insight into the type of reactions and to develop multistep reactions models for each material. The resulting models provide excellent agreement with the experimental data, and can be used to gain insight and predictions for wire insulation degradation in aging aircraft for improved safety and risk assessment. The paper also investigates the derivative thermograms (DTG) to find the minimum number of reaction steps involved. Addition insight from Friedman Analysis compares the slopes of the isoconversional mass loss trend lines to the slopes of each peak at the beginning of the reaction step to determine whether the reaction is considered ‘accelerated’ (if the reaction step slope is steeper than the isoconversional trend line) by an autocatalytic mechanism or ‘retarded’ (if the isoconversional trend line is steeper than the reaction step slope).

During the onset of degradation, catastrophic failure due to subsequent short-circuiting of electrical wiring insulation may result. Therefore, it is our goal to correlate the degradation mechanism and model predictions to dielectric breakdown. As the insulation’s dielectric properties dwindle, the material becomes increasingly susceptible to these electrical failures.
Stability of Homogeneous and Periodic Media Under Coupled Electromechanical Boundary Conditions

Stephan Rudykh
Ben-Gurion University, P.O.B. 653, Department of Mechanical Engineering, Beer Sheva, 84105, IL
Phone: 97286477046, Email: rudykh@bgu.ac.il

Gal deBotton
Ben Gurion University, Beer Sheva, Israel

Kaushik Bhattacharya
California Institute of Technology, Pasadena, CA

Abstract:
Electroactive polymers (EAP) are soft dielectrics that change their shape and size in response to electric excitation. Various applications of EAP actuators have been considered in recent years [1, 2]. In this study, the behavior of homogeneous and periodic composite EAPs under coupled electromechanical boundary conditions in finite deformations is investigated with emphasis on the important aspect of instabilities phenomena.

First, we examine pure mechanical instabilities that may develop in fiber composites and detect the associated critical stretch ratios. In particular, we focus on macroscopic instabilities that are associated with long waves and considered as loss of ellipticity of the homogenized governing equations. Analytical estimations of the onset of ellipticity loss are given by making use of a new effective energy-density function for Gent fiber composites [3]. This model enables to capture the well-known "lock-up" effect of polymer molecular extensibility limit. The analytical estimations are compared with both 2D and 3D finite element simulations. For the 2D case the representative unit cell is a laminated structure. In the spatial case, we examine the responses of composites with periodic hexagonal unit cell [3]. It is demonstrated that the analytical estimations for the onset of failure are in fine agreement with the corresponding numerical results.

In the coupled electromechanical problems, instabilities may arise from geometry of a particular application, from material properties, or from a composite microstructure. These instabilities may be utilized as triggers for shifting actuators from one configuration to another. In other words, a relatively small value of electric excitation may lead to a significant actuation. Theoretical and numerical examples are considered.

References:
Multiscale Modeling of Micro/nano Structural Thin Films

ORGANIZERS:

George Voyiadjis, Louisiana State University
Co-optimization for Film on Substrate: Materials, Structure and Processes

Abraham Tesfamicael  
Huazhong University of Science and Technology (HUST)  
State Key Laboratory of Digital Manufacturing Equipment and Technology, Wuhan, 430074, CN  
Phone: 00862759835236,   Email: akabrish@gmail.com

YongAn Huang  
Huazhong University of Science and Technology, Wuhan, China

ZhouPing Yin  
Huazhong University of Science and Technology, Wuhan, China

YouLun Xiong  
Huazhong University of Science and Technology, Wuhan, China

Abstract:

This paper will discuss on the co-optimization for thin films bonded on substrate with particular reference to the evolution of interfacial stresses (peeling stress) during both thermal and mechanical cycling in roll-to-roll manufacturing. Following the earlier work by Y.A.Huang et al., we will model the system and develop co-optimization to improve its reliability by minimizing stress.

Thin film devices such as thin film transistor, exhibit relatively poor reliability, due to the existence of an inevitable residual stress along the interface generated during fabrication and service process. These stresses need to be minimized to reduce the damage in the thin film device and enhance its reliability. Interface is a key factor in controlling the reliability of thin films. It is particularly important in components within metallic films on elastomeric substrates where changes in composition and structure during processing and service can lead to interfacial failure. This paper will identify the condition for selecting favorable design parameters to enhance the reliability of thin film on substrate structures. Among these, the reliability is highly affected by the materials, structure and process. To this end, an optimization process will be implemented to adjust the three variables so that a reliable system might be designed and meet the demands of different applications. Mechanics modeling theory will be introduced to predict the interfacial stresses with respect to the selected design variables. The design may include evaluating the strain as a function of temperature and tension stress. Then the interfacial stress will be given in analytical expression related with temperature, thickness of substrate and film, tension stress of web, and the material of substrate. All these variables can be optimized to get a reliable device. In the end, FEM simulation will be adopted to show the validity of the optimization. With these information in hand, a preliminary optimal design for a better performance and reliable device may be achieved and serves as a prelude for further optimization design of flexible electronics.

Reference
Classical Molecular Dynamics Method Based Mechanics of Nanometer to Micrometer Sized Polycrystalline Silicon

Vikas Tomar
Purdue University-West Lafayette
3205 ARMS, 701 W Stadium Avenue, West Lafayette, 47907, US
Phone: 3172943251, Email: tomar@purdue.edu

Abstract:
Atomistic simulations of polycrystalline silicon (polysilicon) with grain sizes ranging from 3.4 nm to 135 nm are performed using a classical molecular dynamics method in an equivalent crystal lattice framework. The samples sizes range from 10 nm to 500 nm. The equivalent crystal lattice framework uses a new class of inter-atomic potentials by forming a series of equivalent crystal lattices that are larger-scale replicas of the original crystal lattice and have the same static and dynamic properties as approximated by the interatomic potential for the original crystal lattice. The use of equivalent crystal lattices increases the accessible length scale of MD simulations by up to 200 times and the accessible time scale by up to 500 times for analyzing molecular mechanics of bulk and thin film polycrystalline Si. One can perform microsecond and micrometer scale simulations at realistic experimental strain rates in the new framework. However, initial analyses focus on understanding the effects on Young’s moduli and fracture stress values caused by grain size and specimen size variation under two different strain rates: 0.01%/timestep and 0.001%/timestep. For the grain sizes analyzed neither Young’s modulus nor fracture stress values are affected appreciably by grain size variation in the case of the bulk nanocrystalline silicon. However, both Young’s modulus and fracture stress values are strong functions of grain size for polycrystalline Si thin films. Analyses show the mechanism of fracture changes from amorphization of grain interiors to brittle grain separation with changes in the grain sizes for bulk polycrystalline Si. Introduction of surfaces to simulated thin film fracture leads to the change in mechanism of deformation from being brittle to ductile at the same length scale. The simulation results are shown to agree completely with quantitative experimental findings.
Quantitative Nondestructive Evaluation for Adhesive Strength at an Interface of a Thin Film System with Opto-Acoustic Techniques

Bernhard R. Tittmann
The Pennsylvania State University
212 Earth-Engineering Sciences, Dept. of Engineering Science & Mechanics, University Park, 16802, US
Phone: 814-865-7827, Email: brt4@psu.edu

C. Miyasaka
The Pennsylvania State University, University Park, PA

I. Park
Seol National University of Technology, Seoul, Korea

Abstract:

A mechanical scanning acoustic reflection microscope (hereinafter called simply ‘SAM’) operating with a tone-burst wave having a center frequency ranging from 400MHz to 2GHz is a useful tool for nondestructively visualizing a defect (e.g., delamination, inclusion, micro-crack and the like) located at an interface between an opaque nano/micro scaled thin film and an isotropic/anisotropic substrate. The interior image obtained by the SAM clarifies a cause of a deterioration of adhesive strength at an interface of a thin film system. Further, a technique with the SAM for analyzing a velocity of a surface acoustic wave (hereinafter called simply ‘SAW’) obtained by monitoring a change of a transducer output (i.e., V(z) curve analysis) may quantitatively discriminate adhesive strength of the interface. This technique can be applied to evaluate a thin film system having no defect but having poor adhesion. However, the technique is limited for application to a small point region or a short line on the system. Therefore, for implementing the SAM technique in practice it is necessary to obtain the SAW velocities at as many different locations as possible for the same specimen to statistically reduce decision errors. Moreover, the SAM technique requires strict monitoring conditions (i.e., control of the center frequency of the transducer output, of the temperature of a coupling medium, and of the step size of a movement of an acoustic lens along Z-axis) to reduce the measurement error. Therefore, the evaluation procedure may be complicated, time consuming, and tedious. An opto-accoustical technique measuring a minute change of a displacement on a relatively large area of a thin film system may cover the above mentioned disadvantages of the SAM when the technique is included into the SAM. This article presents a basic principle and preliminary data obtained by a hybrid method for nondestructively evaluating adhesive strength at an interface of a thin film system. In the new technique the film is attached to a glass slide so as to allow laser based optics to impinge on the adhesive layer. The laser based method allows measurement of delaminations via optical path changes. The paper presents data obtained with both the SAM and the laser based optical techniques and compares the results for weak and strongly adhering thin films.
Molecular Dynamics Simulation of Conformational Transition and Associated Frictional Performance of Self-Assembled Monolayers

Xiao Ma
Iowa State University
0085 Black Engineering Building, Dept. of Mechanical Engineering, Iowa State Univ., Ames, 50010, US
Phone: 515-294-8020, Email: xma@iastate.edu

Pranav Shrotriya
Iowa State Univ., Ames, IA

Abstract:

Recently Self-Assembled Monolayers (SAMs) of organic molecules such as Poly Ethylene Glycol (PEG) terminated alkanethiols have attracted considerable attention due to their unique and flexible structure upon which conformational transition can be generated under external electrical field. By application of Molecular Dynamics (MD) simulation, the structural conformational transition of PEG terminated SAMs and corresponding frictional performance transition because of the polarity alteration of external electrical field were investigated and reported in this research. Harmonic/Class2 potentials with consideration of gold-thiol interaction as a Morse potential were applied in the model to simulate the atomic and molecular interaction during the conformational transition. Initialization and thermalization were performed at first to generate the initial movement freedom and achieve the required temperature and system stability, then electrical fields of different polarities were exerted to the SAMs respectively to induce the conformational transition. In the end, a repulsive indenter was applied to the system to generate frictional force. Simulation results indicate that significant conformational transition of close packed PEG terminated SAMs was formed due to the force couple of electrical fields with different polarities. Under positive electrical fields, the PEG groups were compressed and twisted into the helical form which is known as the $\psi$Gauche$_1^\pm$ conformation. While under negative electrical fields, the PEG groups were stretched into the straight form which is known as the $\psi$All-trans conformation. Such conformational transition can be profoundly related to the frictional performance transformation of PEG terminated SAMs. Interaction of SAMs with the repulsive indenter upon penetration and sliding shows that under positive electrical field, $\psi$Gauche$_1^\pm$ conformation caused the stiffness declination of the molecular chain, thus led to a comparatively lower frictional coefficient level. While under negative electrical field, $\psi$All-trans$_1^\pm$ conformation increased the stiffness of the molecular chain, and generated a higher frictional coefficient level. During the simulation of interaction of SAMs with indenter, two kinds of frictional phase were observed. Under shallow indentation and sliding, a lower level of frictional coefficient was obtained and the whole configuration of the molecular chains was not influenced by the indenter. While under deep indentation and sliding, the higher loads caused a higher level of frictional coefficient and the backbone chains can be dragged along with the indenter away from their original locations. The Molecular Dynamics simulation in this research provides meaningful insights and application potential upon the structural characteristics and frictional performance of the PEG terminated SAMs.
A Multiscale Model of Rate Dependence of Nanocrystalline Thin Films

Fernando Stump
University of Illinois at Urbana-Champaign
407 W. White St., Apt 14., Champaign, 61820, US
Phone: 1 (217) 778-8291, Email: fstump2@illinois.edu

Nikhil Karanjgaokar
University of Illinois at Urbana Champaign, Urbana, IL

Philippe H. Geubelle
University of Illinois at Urbana Champaign, Urbana, IL

Ioannis Chasiotis
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

Experimental observations have shown that nano-crystalline materials can exhibit strong rate dependency [1]. This phenomenon can be attributed to the fact the as the grain size decreases the ratio between grain boundary area and grain volume increases, and so the deformation mechanisms mediated by the grain boundary start to play a more important role. Simultaneously, the small free path between two grain boundaries constraints the dislocation movement, thereby decreasing the ductility of the material. The rate dependence can thus be explained by the competition between the two deformation mechanisms, the grain boundary diffusion and dislocation movement inside the grains.

Motivated by this observation, a multiscale finite element formulation has been developed to simulate thin film tensile and creep experiments. In a two-dimensional (plane stress) framework, a Voronoi tessellation is used to create a multi-grain representative volume element (RVE). The RVE is discretized in volumetric elements inside the grains and interfacial elements along the grain boundaries. The inter-granular processes are modeled by cohesive (interfacial) elements that account for diffusion-mediated sliding between grains. The intra-granular behavior is captured by a rate-dependent single-crystal plasticity model that represents the evolution of the various slips systems present in each grain. The key parameters entering the description of the grain interior and grain boundary models are calibrated through comparison with high strain rate tensile tests and creep experiments, respectively. The prediction of the viscoplastic response of gold thin films is validated against tensile test measurements obtained over seven decades of strain rate. The relative contribution of the two microstructural damage mechanisms is analyzed.

References:
Instabilities in Solids

ORGANIZERS:

Oscar Lopez, State University of New York, Stony Brook

Wei Hong, Iowa State University

Toshio Nakamura, State University of New York, Stony Brook
Localization Analysis of Porous Metals via Homogenization Models Incorporating Microstructure Evolution

Pedro Ponte Castaneda
University of Pennsylvania
220 S. 33rd. St., Towne Building, Room 235, Philadelphia, 19104-6315, US
Phone: 215-898-5046, Email: ponte@seas.upenn.edu

Kostas Danas
Ecole Polytechnique, Paris, France

Abstract:

In this presentation, we will make use of a recently developed homogenization model for elasto-plastic porous metals with evolving microstructure to investigate the possible development of localization instabilities as a function of the applied loading conditions and the elastic and plastic properties of the material. We find that the overall strain at localization depends strongly on the Lode parameter (i.e., the third invariant of the stress tensor), as well as on the stress triaxiality (i.e., the ratio of the hydrostatic and deviatoric stresses). In particular, the model predicts the collapse of voids at low stress triaxialities in such a way that the initially spherical pores tend to become oblate cracks or thin needles depending on the value of the Lode parameter. This void collapse mechanism leads to the formation of shear or dilation localization bands depending on the value of the Lode parameter. On the other hand, at large stress triaxialities the main mechanism of failure is the increase of porosity, which leads to the overall softening of the porous material. Our calculations show that these two different mechanisms of localization --- void collapse and porosity growth --- dominate the behavior of the porous solid at different levels of stress triaxialities, whereas the transition from the first localization mechanism to the second one is rather abrupt leading to sharp corners on the localization strain locus map in agreement with experimental results of Bao and Wierzbicki (2004). The predictions of this model will also be compared with the Gurson and other models recently developed models. In the context of these comparisons, it should be emphasized that unlike other models, the new micro-mechanically based model is fully predictive and need not be "calibrated" to experimental or numerical results for specific loading conditions (which may, or may not be appropriate for different loading conditions).
Inelastic Bending and Collapse of Tubes with Lüders Bands

Julian Hallai
University of Texas at Austin
210 East 24th Street, ASE/EM, C0600, Austin, 78712, US
Phone: 5125714167, Email: jfh@mail.utexas.edu

Stelios Kyriakides
University of Texas at Austin, Austin, TX

Abstract:

Hot finished carbon steel exhibits Lüders bands at the onset of yielding that is associated with inhomogeneous plastic deformation of about 1-4%. We investigate the influence of Lüders banding on the inelastic response and stability of tubes under pure bending. Tubes of diameter-to-thickness ratios (D/t) in the range of 33 to 14 and Lüders strains of 1.8% to 3.3% have been tested to collapse under rotation controlled pure bending. Collapse, was found to be governed by the tube D/t and by the extent of the Lüders strain in the material.

For lower D/t tubes and materials with shorter Lüders strain two curvature regimes were found to coexist, one that corresponds to the strain at the onset of yielding and the second to the strain at the end of Lüders stress plateau [1]. As the end rotation is increased the higher curvature zone(s) gradually spread while the moment remains essentially unchanged. When the whole tube has been deformed to the higher curvature the moment starts to increase while the deformation is uniform. The tube eventually fails at a higher curvature by localized diffuse ovalization without any apparent effect from the initial Lüders bands-induced inhomogeneous deformation.

For tubes with higher D/ts and/or longer Lüders strain the localization in curvature starts to develop and simultaneously a moment plateau is again traced. When the high curvature zone reaches a critical length the tube collapses catastrophically by developing a sharp inward local kink. This collapse is caused by an interaction of the higher curvature with naturally occurring wrinkles. A significant section of the test specimen is left in the low curvature regime.

This class of problems is analyzed using 3D finite elements while the material is modeled as an elastic-plastic solid with an ‘up-down-up’ response over the extent of the Lüders strain, followed by hardening. Mesh sensitivity and regularization by including rate dependence have been examined. It will be demonstrated that the solution procedure followed can simulate the experimentally obtained response as well as the onset of collapse with accuracy provided the unstable part of the material response is suitably calibrated. The presentation will include results from a study of the effect of the major parameters of the problem on the calculated response, e.g., D/t, Lüders strain, the strength of the material instability, initial geometric imperfections, etc.

Reference
Negative Stiffness and Negative Poisson's Ratio in Barium Titanate Ceramic

Liang Dong
Materials Science Program, University of Wisconsin-Madison
#212 Engineering Research Building, 1500 Engineering Dr., University of Wisconsin-Madison, Madison, 53706, US
Phone: 6083467275, Email: dong4@wisc.edu

Donald S. Stone
Materials Science Program, University of Wisconsin Madison, Madison, WI

Roderic S. Lakes
Engineering Physics, University of Wisconsin Madison, Madison, WI

Abstract:
Composite theory concludes that composite properties, such as stiffness, damping, and thermal expansion, cannot surpass either of the constituents. Such a conclusion is derived under the assumption that both matrix and inclusion possess positive stiffness. However, bounds can be exceeded provided the inclusion has negative stiffness. Negative stiffness is presented as the occurrence of a reaction force in the same direction as imposed deformation. Recent study on particulate BaTiO3-Sn composite revealed an extreme composite stiffness (greater than that of diamond) at temperatures where negative stiffness of the ceramic inclusion is constrained by the surrounding matrix. BaTiO3 has three structural phase transformations at specific temperatures: cubic-to-tetragonal (130°C, Curie point); tetragonal-to-orthorhombic (0°C); orthorhombic-to-rhomohedral (-80°C). Landau theory of ferroelastic phase transformation anticipates a negative stiffness in the vicinity of the Curie point. However, negative stiffness cannot be directly observed in a material without mechanical constraint, but only a softening even to zero is allowed.

Viscoelastic properties (damping and stiffness) of pure barium titanate ceramic (without mechanical constraint) have been studied (from 20°C to 150°C): significant softening in bulk stiffness by a factor of five and negative Poisson’s ratio (-0.25) have been observed in the vicinity of the Curie point. The effect is much more pronounced under electrical short circuited condition, low excitation strain and low excitation frequency. In addition, anelastic anomaly (undulation in damping and stiffness, softening in bulk stiffness and negative Poisson’s ratio) was observed in the tetragonal BaTiO3 after enough aging was performed below the Curie point; such anomaly disappeared after enough aging was performed above the Curie point. Relaxation model cannot account for this phenomenon as the anomaly does not shift in temperature with frequency. An oxygen vacancy mechanism has been proposed: stored elastic energy is introduced between defect dipole polarization and spontaneous polarization, gives rise to reversed curvature for the free energy curve at small strain levels in localized regions. The anomaly is the representation of constrained localized negative stiffness regions inside the ceramic.

The negative stiffness and negative Poisson’s ratio may also be possessed by other types of ferroelastic materials. The negative properties of ferroelastic materials will serve real purposes in the future.
Crater Function Analysis of the Ion Impact Angle Dependence of Surface Morphology Transitions

Md Hossain
University of Illinois at Urbana-Champaign
1206 W Green St, MC 244, Urbana, 61820, US
Phone: 2173778474, Email: hossain2@illinois.edu

Kallol Das
University of Illinois at Urbana Champaign, Urbana, IL

Jonathan B Freund
University of Illinois at Urbana Champaign, Urbana, IL

Harley T Johnson
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

The rearrangement of atoms during ion bombardment of solid surfaces is known to lead to the formation of regular nanometer-scale surface patterns. The nature of these patterns depends on a combination of ion energy, the types of target material and ion, and the angle of incidence. Dots or ripples oriented parallel or perpendicular to the ion direction have been observed, but the mechanisms of their formation is not well understood. By statistically averaging thousands of molecular dynamics simulations of ion impacts, we determine the average net change in surface shape due to individual ion impacts. We call this average change the "crater function" for a particular set of impact conditions. Such craters are calculated for Xe-ion bombardment of amorphous Si and Ge at 2keV for different ion incident angles ranging from 0°; to 70°; . These crater functions are then included in a continuum model for studying the evolution of the surface. We find that changes in the geometrical moments of the crater-functions correspond with the transitions between different surface morphologies computed using the continuum model. With a simple analysis of crater shapes a moments-based hypothesis is developed for explaining the morphological transitions. In particular it is found that when second-order moments about the projected ion beam direction are smaller than those about the transverse direction correspond to the formation of ripples parallel to the beam direction. This is confirmed for both the craters calculated via MD and for analytical functions constructed as crater models. The results are compiled in a phase diagram that shows the transition boundaries between different classes of surface morphologies as a function of the different crater moments.
Failure Surfaces for Fiber-Reinforced Elastomers Under General 3D Loading Conditions

Oscar Lopez-Pamies
State University of New York, Stony Brook
139 Light Engineering, Stony Brook, 11794-2300, US
Phone: 6316328249, Email: oscar.lopez-pamies@sunysb.edu

Abstract:

In this work, we carry out a thorough investigation of local instabilities, including matrix cavitation, fiber debonding, and fiber failure and global instabilities, defined as the loss of strict rank-one convexity of the effective properties, in fiber-reinforced elastomers subjected to finite deformations. Specifically, we consider isotropic hyperelastic solids reinforced with a random and transversely isotropic distribution of anisotropic hyperelastic fibers. The results are computed by means of an innovative iterated homogenization method, which incorporates direct microstructural information up to the two-point correlation functions and requires the solution to a Hamilton-Jacobi equation with the fiber concentration and the macroscopic deformation gradient playing the role of “time” and “spatial” variables, respectively. It is found that the manner in which the material fails depends greatly on the evolution of the underlying microstructure, which in turn depends directly on the type of applied loading conditions: i) for compressive modes of deformation, the material is found to become unstable via long-wavelength instabilities and fiber failure, ii) for tensile modes of deformation, the material undergoes cavitation and fiber debonding.
Failure and Fracture of Heterogeneous and Multilayer Materials

ORGANIZERS:

Pranav Shrotriya, Iowa State University
Ashraf Bastawros, Iowa State University
Nonlocal Boundary Layer Method for Overcoming Boundary Condition Ambiguity in Nonlocal and Statistical Models of Quasibrittle Structures

Christian Hoover
Northwestern University, 2145 Sheridan Road, Technological Institute Suite A123, Evanston, 60208, US
Phone: 1-847-491-4025, Email: ChristianHoover2010@u.northwestern.edu

Jialiang Le
Northwestern University, Evanston, IL

Zdenek P. Bazant
Northwestern University, Evanston, IL

Abstract:
The nonlocal models used in computational analysis for regularization of the boundary value problems of softening damage are still hampered by unresolved issues in the treatment of boundary conditions. The existing models are non-physical and treat the protrusion of the domain of the nonlocal weighting function beyond the structure boundary differently. For example, the protruding part is deleted while the interior part is either rescaled, or enhanced by a Dirac delta peak at the structure boundary or at the centroid of the domain. The boundary conditions are also unclear for gradient models. Various models can yield very different results.

A more physical approach to the numerical treatment of the boundaries, inspired by the weakest-link statistical size effect on structural strength, is proposed. Its modeling requires the structure (of positive geometry) to be subdivided into elements roughly equal to the representative volume element (RVE) of material. The RVE is defined as the smallest material volume whose failure causes the entire structure to fail. In the proposed nonlocal boundary layer model (NBL), the structure is divided into two parts: an interior domain, and a boundary layer of a thickness equal to the RVE size, which approximately equals the fracture process zone width. In the boundary layer, the stress depends solely on the average strain over its thickness, which is approximately given by the continuum strain at the middle surface of the layer. In the interior domain, nonlocal averaging may be applied without modification because the nonlocal integral domain cannot protrude outside the structure boundary.

Since statistically the structure is equivalent to the weakest link model, its survival probability 1 - Pf is the joint probability of survival of all the RVEs. The subdivision into RVEs is generally non-unique and for irregular geometries, exactly equal RVE sizes are impossible. This gives inconsistent estimates of failure probability Pf. One way to overcome the problem is to calculate the nonlocal stress in the joint probability expression by averaging the strains over the zone of influence using a weighting function. Five different methods of boundary treatment were used for comparing the size effect on structure strength: 1) calculating Pf based on the weakest-link model, 2) redistributing the protruding volume by placing it into a Dirac delta function at either the structure boundary or 3) at the center nonlocal domain, 4) uniformly rescaling the weighting function, 5) and the present NBL method. The last three methods were also used in and integral type formulation of deterministic nonlocal softening damage. These models were compared by simulating the size effect on the modulus of rupture due to crack initiation, which is a problem experimentally studied by Rocco (1995), and the size effect in the notched specimens of Bazant and Pfeiffer (1987). The NBL model and the implicit gradient model of Peerlings et al. were also compared by simulating the size effect tests of Rocco (1995).
Micromechanical Simulations of the Dynamic Response of Polymer Bonded Explosives using a Cohesive Finite Element Method

Ananda Barua  
Georgia Institute of Technology  
801 Ferst Drive, Woodruff School of ME, MRDC, Atlanta, 30332, US  
Phone: 404-242-7187,   Email: abarua@gatech.edu

Min Zhou  
Georgia Institute of Technology, Atlanta, GA

Abstract:

A framework for quantifying the thermo-mechanical response of HMX/Esta ne, a Polymer Bonded Explosive (PBX), at the microstructural level is developed. The analysis concerns impact loading with strain rates on the order of 10e4 - 10e5 /s and uses a cohesive finite element method (CFEM). Issues studied include large deformation, thermo-mechanical coupling, failure in the forms of micro-cracks in both bulk constituents and along grain/matrix interfaces, and frictional heating. The Estane matrix is described by a fully coupled thermo-elasto-viscoelastic constitutive formulation, accounting for temperature dependence, strain rate sensitivity and strain hardening. The HMX crystals are assumed to be elastic under the conditions analyzed and are modeled using a finite deformation hyperelastic formulation. The CFEM framework allows the contributions of individual constituents, fracture and frictional contact along failed crack surfaces to heating to be analyzed and tracked. Thermal conduction across the cohesive surfaces is accounted for. Digitized micrographs of actual PBX materials as well as idealized microstructures having mono or bi-modal distribution of grain sizes are used in the analysis. The formation of local hot spots as potential ignition sites is primarily due to the viscoelastic dissipation in the matrix in early stages of deformation and frictional heating along crack surfaces in later stages of deformation. At temperatures below the glass transition temperature (Tg) of Estane, debonding along the interfaces and cracking in the bulk phases dominate. At temperatures above Tg, shear banding and grain-grain interactions are the primary modes of deformation. Imperfections such as voids and inclusions are invariably found in tomographic scans of PBX microstructures. A quantitative understanding of the effect of voids on both the overall mechanical strength and formation of stress concentration regions in the microstructure is explored by using a range of idealized samples containing a range of spherical voids. Finally, microstructure-response relations that can be used in the design of soft energetic composites are established.
An Exact Solution for History-Dependent Material and Delamination Behavior of Laminated Plates Subjected to Cylindrical Bending

Todd Williams
Los Alamos National Laboratory
Lost Alamos National Laboratory, Theoretical Division, T-3, MS B216, Los Alamos, 87545, US
Phone: 505 665 9190, Email: oakhill@lanl.gov

Abstract:

The exact solution for the history-dependent behavior of laminated plates subjected to cylindrical bending is presented. The solution represents the extension of Pagano’s solution to consider arbitrary types of constitutive behaviors for the individual lamina as well as arbitrary types of cohesive zones models for delamination behavior. Examples of the possible types of material behavior are plasticity, viscoelasticity, viscoplasticity, and damaging. Examples of possible CZMs that can be considered are linear, nonlinear hardening, as well as nonlinear with softening. The resulting solution is intended as a benchmark solution for considering the predictive capabilities of different plate theories. Initial results are presented for several types of history-dependent material behaviors. It is shown that the plate response in the presence of history-dependent behaviors can differ dramatically from the elastic response. These results have strong implications for what constitutes an appropriate plate theory for modeling such behaviors.
Modeling Dynamic Fracture and Damage in Unidirectional Fiber-reinforced Composites with Peridynamics

Wenke Hu
University of Nebraska Lincoln
Department of Engineering Mechanics, W317.4 Nebraska Hall, Lincoln, 68588, US
Phone: 4024707056, Email: wenke.hu@huskers.unl.edu

Florin Bobaru
University of Nebraska Lincoln, Lincoln, NE

YounDoh Ha
University of Nebraska Lincoln, Lincoln, NE

Abstract:

Traditional methods may not be suitable for modeling fracture and damage because of the displacement discontinuities, over which partial derivatives fail to exist. Thus, additional techniques and criteria need to be used to deal with this problem. The Peridynamic theory, which is a non-local extension of the classical continuum theory which uses integration of forces per unit volume instead of the divergence of stresses in the equations of motion, has been developed in order to treat damage and fracture in a direct and unified way. The Peridynamic formulation has been successfully used for modeling dynamic fracture and crack branching in homogeneous isotropic materials. In the present study, a peridynamic formulation for unidirectional (UD) fiber-reinforced composites is proposed based on homogenization and mapping between the peridynamic bond micro-scale and the macro-scale elastic parameters of the composite lamina. The model is used to analyze the dynamic fracture of UD fiber-reinforced composites. We perform a detailed analysis of convergence for UD fiber reinforced lamina. We also show simulations of crack growth in a UD composite lamina and laminates under dynamic loading condition. The complex modes of dynamic fracture in these laminates are captured by the peridynamic model without the need for extra criteria of failure. The results show that peridynamics is a promising tool for modeling dynamic fracture and damage in fiber-reinforce composites.
Development of an Internal State Variable Theory of Inelasticity by Repeated Imposition of Equilibrium at Each Length Scale

Douglas Bammann
Mississippi State University
217 Carpenter Hall, Mississippi State, 39760, US
Phone: 9256984792, Email: bammann@me.msstate.edu

Abstract:
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. Increasing degrees of freedom and defects at smaller scales are included by repeated application of this structure, including the essential balance laws ensuring equilibrium of conjugate thermodynamic forces at each length scale.

Examples are given for the construction of such theories ranging from the simplest model incorporating a scalar measure of statistically stored dislocations and mobile dislocations (both elastic and plastic parts), coupled transport theories for hydrogen and a multi-phase model for steels in which a repeated application of the balance laws is necessary to bridge the various length scales.
Effect of Curvature Dependent Surface Energy upon Fracture along a Bi-Material Interface

Jay Walton
Texas A&M University
Department of Mathematics, College Station, 77843-3368, US
Phone: (979)845-7242, Email: jwalton@math.tamu.edu

Tsvetanka Sendova
IMA, University of Minnesota, Minneapolis, MN

Abstract:

We discuss mixed mode de-bonding of a material interface within the context of a new theory of fracture incorporating curvature dependent crack surface energy and interfacial boundary conditions coming from the jump momentum balance (a generalization of the classical Gibbs/Thompson relation). It is shown that if the curvature dependence of surface energy is sufficiently strong relative to the surface energy of a flat bi-material interface, then the model predicts bounded crack-tip stress and strain in stark contrast to the oscillatory, singular crack-tip stress and strain predicted by classical fracture models.
A Study of Highly Crosslinked Epoxy Molding Compound and its Interface with Copper Substrate by Molecular Dynamic Simulations

Shaorui Yang
Northwestern University
2145 sheridan rd, evanston, 60201, US
Phone: 847-491-5164, Email: shaoruiyang2009@u.northwestern.edu

Jianmin Qu
northwestern university, Evanston, IL

Abstract:

Epoxy resin is widely used in microelectronic packaging, either in the bulk form such as encapsulants and carriers, or as adhesives, for example die-attach and underfill. The performance of the material itself and its interface with other components, such as metals and metal-oxides, is critical to the reliability of electronic packages. To prevent extensive trial-and-error testing efforts, quantitative simulation techniques need to be developed to predict material properties of epoxy resins and their adhesions to metal/metal oxide substrates. Molecular dynamics (MD) simulation studies material behaviors at an atomistic level thus could be promising in establishing a structure-property correlation of the bulk epoxy resin and constitutive law of the interface. This paper is devoted to utilize MD simulation to determine the material properties of a novel epoxy resin and their dependence on atomistic structure. The traction-separation law of epoxy/copper interface is also extracted based on MD simulation, which can be incorporated into a cohesive zone finite element method to simulate the interface delamination.

A novel Epoxy Molding Compound (EMC) with a crosslinked network structure was formed by curing tri-/tetra-functionalized EPN1180 with Bisphenol-A. A fully atomistic model reflecting the network nature of the material was constructed by applying a cyclic crosslinking algorithm to a 3D periodic amorphous cell containing the stoichiometric mixture of constitutive monomers. The geometry of the model was then optimized using COMPASS force-field in Materials Studio software. The variation of system density and volume against the temperature was simulated using a specific cooling down profile, which was employed to derive the glass transition temperature and coefficient of thermal expansion of the system. Furthermore, the Young’s modulus and Poisson’s ratio as a function of temperatures were calculated by the uni-axial tensile MD simulation. The material properties computed by MD simulation were in good agreement with experiment measurements. In the meantime, a series of models with different crosslinking conversion ratios were constructed to investigate the property dependence on the structure. An epoxy resin/copper interface model was constructed and the geometry optimization was also performed for the subsequent MD simulation. The traction-displacement relation of the interface was derived when the system was subjected molecular statics simulation of uni-axial tensile test. The peak traction and separation work were extracted from the traction-displacement law. These two parameters can be incorporated into cohesive zone finite element method to facilitate multi-scale simulations of interfacial delamination.
Evolution of Void Size Distribution in Initially Porous Materials

Ali Ghahremaninezhad
Center for Mechanics of Solids, Structures and Materials, The University of Texas at Austin
210 East 24th Street, W. R. Woolrich Laboratories, Austin, 78712, US
Phone: (512) 363-8754, Email: a_ghahremani@mail.utexas.edu

K. Ravi Chandar
Center for Mechanics of Solids, Structures and Materials, The University of Texas at Austin, Austin, Texas

Abstract:

Damage models based on void nucleation, growth, and coalescence, such as the modified Gurson-Tvergaard-Needleman (GTN) model, have been developed over the past four decades with the goal of capturing material response all the way to final failure. Many analytical and numerical studies related to statistical homogenization have also been reported. However, the few experimental studies of damage have primarily restricted attention to qualitative identification of damage mechanisms and hence there are very few quantitative studies characterizing the quantitative evolution of microstructural features and voids during plastic deformation. In this presentation, we report on a detailed examination of the response of an initially porous material. The void size distribution and its evolution are examined through direct measurements in a tensile test. These measurements are then used to propose a modification of the GTN model. The comparisons between experimental results from tensile test and flat-notched specimens made of sintered iron and results from numerical simulations will be reported.
Convergence and Scaling in Peridynamics for Modeling of Fiber-Reinforced Composites

Wenke Hu
University of Nebraska Lincoln
Department of Engineering Mechanics, W317.4 Nebraska Hall, Lincoln, 68588, US
Phone: 4024707056, Email: wenke.hu@huskers.unl.edu

Florin Bobaru
University of Nebraska Lincoln, Lincoln, NE

YounDoh Ha
University of Nebraska Lincoln, Lincoln, NE

Abstract:

The Peridynamics theory is a new non-local method which does not involve spatial partial derivatives, and is capable of correctly modeling fracture initiation, unguided propagation and coalescence of cracks. Recently, the peridynamic formulation has been used for modeling of damage in composites. Simulations of damage in composites performed with the peridynamic model compare well with experiments. However, the model for composite laminates is not given in detail and no study of convergence is performed. In the present study, a peridynamic formulation for unidirectional (UD) fiber-reinforced composites is used to analyze the dynamic fracture. A scaling procedure is developed in order to have the elastic strain energy, for a fixed horizon, converges to the classical one under grid refinement. Convergence studies under uniform grid refinement for a fixed horizon size (m-convergence) and under decreasing the peridynamic horizon (h-convergence) are performed. We also show simulations of crack growth in UD composite lamina panels with 0, 45, and 90 degree under dynamic loading condition. The crack pattern in these panels under dynamic loading is different from quasi-static loading. We notice that because of the dynamic loading, the crack growth and propagation speed is strongly affected by the stress waves in the body. The results show that peridynamics is a useful tool for modeling crack propagation in fiber-reinforce composites.
Mechanics of Materials and Structures in Emerging Technologies

ORGANIZERS:

Pradeep Guduru, Brown University

Baskar Ganapathysubramanian, Iowa State University

Wei Hong, Iowa State University
Graphene Fracture

Kyug-Suk Kim
Brown University
Box D Engineering, Brown University, 182 Hope Street, Providence, 02912, US
Phone: 401-863-1456, Email: Kyung-Suk_Kim@brown.edu

Invited Presentation

Abstract:

The dynamic fracture of homogeneous materials is historically known to be caused by crack-opening tension near the crack-tip, even when the apparent far-field loading is compressive. While the dynamic crack growth under crack-closing compression is theoretically admissible in fracture mechanics, the phenomenon has never been observed in any material systems so far. Here, we report that a graphene sheet can be cut by in-plane compression which is able to eject a row of atoms out-of-plane, thereby dynamically growing the crack under crack-closing compression. This unusual mode of atomic-scale fracture is due to the structural peculiarity of the graphene sheet, i.e. single sheet of atoms. We show that the compressive atomic-sheet fracture is the critical precursor mechanism of cutting single-walled carbon nanotubes by sonication.

Fracture mechanics stipulates that the available energy per advancement of the crack, i.e. the energy release rate, must be sufficient to create the fracture surfaces. This energy release rate is proportional to the square of the stress intensity around the crack-tip, and thus is indifferent to the sign of the stress intensity. Therefore, both crack growth by crack opening tension and crack-closing compression, which create positive and negative stress intensities respectively, are theoretically possible provided the mechanisms for crack growth are available. However, crack growth under crack-closing compression has never been observed so far. Unlike conventional bond-breaking fracture under crack-opening tension, a mechanism is required to continuously remove atoms to prevent overlapping of the crack-faces under crack closing compression. For the first time, we have observed that such mechanism ‘atom shooting fracture’ is possible in a sheet of atoms, and is operative in the cutting of single-walled carbon nanotubes (SWCNTs) under sonication. Knowing the fundamental cutting mechanism provides insights to develop new manufacturing and sorting processes of SWCNTs with different diameters, lengths and chiralities. More importantly, we have discovered for the first time that cracks can dynamically grow under crack-closing compression in graphene-like nanostructures. This unique atomic-sheet fracture mechanism is expected to play an important role in furthering our understanding of other compressive atomic scale events such as ion beam bombardment, laser ablation, shock wave loading, and focused ion beam milling of graphene-like structures.
Multiscale Modeling of Fabrication Process for Organic Photovoltaics

Olga Wodo
Iowa State University,
Department of Mechanical Engineering, Black Engineering, Ames, 50011-2161, US
Phone: 515 441 2602, Email: owodo@iastate.edu

Abstract:

Organic solar cells have become a new hope as an inexpensive and disposable source of energy. Significant advances in this area have led to 7.9% power conversion efficiency and have revealed that the active layer morphology is a key element in achieving high efficiency. Current approaches to understanding and designing high efficiency organic solar cells involve mainly combinatorial, trial and error based experimental investigations, which are expensive and time consuming. Moreover, experimental techniques has limited capabilities to trace intermediate stages of the process. Thus, analysis is usually restricted to investigation of final morphology only. A computational framework to simulate morphological evolution during fabrication process would provide unique means to trace intermediate stages of the process and the final morphology. Moreover, such framework could be used to perform high throughput analysis of system variables phase space to determine which variables has minor and major effect on the final morphology and in this way enable tailoring of the final morphology of the active layer.

The photoactive layer for organic solar cells is fabricated mainly by deposition from solutions via spin-coating. In this process the volatile solvent evaporates and this induces a phase separation between polymer and fullerene. One of the challenges in the simulation of the spin-coating process is the ability to encompass phenomena on different length scales. During spin-coating the volume of the solution undergoes a rapid change due to evaporation and may decrease even by two orders of magnitude. Finally, the parameters that govern the phase separation cannot be described without understanding pair-wise interactions between components at the molecular level.

We construct a computational framework that simulates morphology evolution during the fabrication process. The computational frame is multiscale in nature in the sense that it resolves nanometer scale features while still having possibility to mode device scale phenomena. The framework is based on the phase field approach, which is used to trace the phase separation into polymer-rich and fullerene-rich regions. The phase field solver involves the efficient, parallel, solution to the Cahn-Hilliard equations using a finite element method with an adaptive time stepping.

Our framework can be used to determine the distribution of the polymer and fullerene sub-regions during consecutive stages of fabrication process. We showcase the framework by analyzing the morphological evolution of polymer:fullerene organic solar device using various statistical descriptors. The flexibility of the computational framework provides an enhanced understanding into how kinetic and thermodynamic parameters affect morphology evolution. This is especially important taking into account limited applicability of purely experimental methods.

Hari Krishna Kodali
Iowa State University, 2025 Black Engineering Building, Ames, 50011, US
Phone: 5154502891, Email: hari@iastate.edu

Baskar Ganapathysubramanian
Iowa State University, Ames, Iowa

Abstract:

Introduction: Organic solar cells (OSC) offer a promising low-cost strategy for harnessing solar energy. Efficiencies of ~ 7.8% have been achieved recently in conjugated polymer based organic solar cells. These devices were fabricated by spin coating an active layer from a blend of p-type photoactive polymer and n-type derivatives of fullerenes into the so called ‘blend-heterojunction’ architecture. Experimental evidence suggests that a key property determining the solar efficiency of such devices is the final morphological distribution of the organic phases. Furthermore, there is a complex relationship between device topology (device scale), morphological distribution of the polymers (nano-scale) and the device efficiency. Computational techniques can help unravel these relationships to accelerate the fabrication of high efficiency OSC. We showcase a computational engine that efficiently interrogates virtual organic solar cell devices to investigate relationships between the morphology at the nano-scale and topology at the device scale with the electrical and optical characteristics.

Methods: Simulation of OSCs requires determination of electrostatic potential and electron/hole densities, which is described by Boltzmann Transport Equation (BTE). As the direct solution of BTE is computationally challenging, the drift-diffusion model is used for modeling these devices. We utilize the Finite element method to model the topological and morphological details. A ‘Streamline Upwind Petrov Galerkin’ (SUPG) based stabilization method is used to minimize numerical instabilities. The absorptivity is calculated by solving Maxwell's equations. A method of continuation is used to aid convergence of the strongly coupled nonlinear equations. In this method, initially spatially averaged material properties are used for calculating the variables. The morphological variations are introduced gradually, one property at a time. Domain Decomposition is utilized to solve the large computational problem arising (out of the necessity to resolve the microstructure details).

Results: The effect of microstructure on the distribution of electrons, holes and electrostatic potential is investigated. The electron density was observed to be diminished in the polymer rich regions (PRR) and enhanced in fullerene rich regions (FRR). This results in uneven current density in FRR and PRR at electrodes. The accumulation of electric field at corners due to undulations in the topology of the polymer-fullerene film has been captured.

Conclusions: The scalability studies show the effectiveness of the domain decomposition strategy. A method of continuation is proposed to solve the stiff drift-diffusion problem with morphological property variation. Trends between the metrics associated with morphology and overall current generated reveals the property-performance relationships for OSC.
Focused Electric Field Induced Ion Transport (FEFIIT): Experiments and Modeling

Andrey Semichaevsky
UIUC, 1206 W. Green St., 362D, MechSE department, Urbana, 61801, US
Phone: 217-244-4488, Email: avsemych@uiuc.edu

Harley T. Johnson
UIUC, Mechanical Science and Engineering Department, Urbana, IL

Ashraf Bastawros
Iowa State University, Mechanical and Aerospace Engineering Departments, Ames, IA

Abhijit Chandra
Iowa State University, Mechanical and Aerospace Engineering Departments, Ames, IA

Abstract:
A novel approach to the microscale patterning of metal surfaces called ‘Focused Electric Field-Induced Ion Transport’ (FEFIIT) is introduced. This process is a modification of the non-contact through-mask electrochemical etching method, in which an ion-selective membrane separates the anodic and cathodic electrolyte volumes. The ion-selective Nafion membrane allows for a low initial metal ion concentration near the anode. The electric field near the workpiece can be modified by means of a perforated insulated mask parallel to the membrane surface.

In this presentation, we study the performance of the FEFIIT process both experimentally and computationally. The time-dependent governing Poisson-Nernst-Planck equations [1] with appropriate boundary conditions are solved for the three ionic species present in the system: copper, sulfate, and hydrogen. Based on these solutions we find spatial distribution of the material removal rate due to copper oxidation at the anode and predict the evolution of the anode profile during the etching.

Predicted anode profiles are compared to the results of profilometric characterization of the actual etched surfaces. A good qualitative agreement is observed between our simulations and experiments. From our model we also find that during the DC etching, the wall angle of the etched features is low, which is also consistent with experimental observations. This limitation, inherent to all through-mask electrochemical etching methods, is attributed to the diffusive transport of the copper ions transversely to the electric field streamlines and to the spatially-varying negative feedback on the anodic current because of the current-density-dependent surface overpotentials.

One of the solutions shown by our model to improve the spatial resolution of FEFIIT is the use of bipolar pulsed etching instead of DC etching. Under this approach, the electrochemical cell is repeatedly returned to the low copper concentration near the anode by reverse-polarity pulses, while the direct-polarity pulses are used for the focused material removal. Our model predicts a substantial increase in the wall angles in the case of bipolar pulsed etching.

Reference
Measurement of Mechanical Properties and Stress-Potential Coupling in Lithiated Silicon for Energy Storage Applications

Pradeep Guduru
Brown University
182 Hope St, Providence, 02912, US
Phone: 401 863 3362, Email: Pradeep_Guduru@Brown.edu

V. Sethuraman
Brown University, Providence, RI

A.F. Bower
Brown University, Providence, RI

V. Srinivasan
Lawrence Berkeley National Laboratory, Berkeley, CA

Abstract:

Silicon is considered to be a promising anode material to increase the specific energy of lithium-ion batteries by as much as 50% - 100%. For accurate modeling of battery performance, cycle life and reliability, there is a need to characterize the mechanical properties of lithiated silicon (an amorphous alloy of silicon and lithium). This work presents experimental determination of biaxial modulus and strain rate effects of lithiated silicon as a function of lithium concentration. Further, an analysis of the dependence of electric potential on the state of stress of a lithiated-silicon electrode is presented. Based on Larche and Cahn chemical potential for a solid solution, a thermodynamic argument is made for the existence of the stress-potential coupling in lithiated-silicon and, based on the known properties of the material, the magnitude of the coupling is estimated to be around 60 mV/GPa in thin film electrode geometry. An experimental investigation has been carried out in which the stress was varied incrementally while measuring the electrode potential simultaneously; the relation between stress change and electric potential change is measured to be 60 - 80 mV/GPa, which agrees very well with the prediction. The importance of this coupling is discussed in the context of interpreting the hysteresis loops observed in potential vs. state of charge plots.
A Continuum Model of Coupled Deformation, Stress, Diffusion, and Electrochemical Reactions in an Electrochemical Half-cell

Allan Bower  
School of Engineering, Brown University, Providence, 02912, US  
Phone: 4018631493,   Email: Allan_Bower@brown.edu

Pradeep Guduru  
School of Engineering, Brown University, Providence, RI

Abstract:

We formulate the continuum field equations and constitutive equations that govern deformation, stress, and electric current flow in a Li ion half-cell, which consists of a solid cathode, a solid intercalation anode, separated by a fluid electrolyte. The model accounts for mass transport through the system, deformation and stress in the anode and cathode (accounting rigorously for finite geometry changes), electrostatic fields, as well as the electrochemical reactions at the electrode/electrolyte interfaces. In particular, expressions are derived for the effects of stress on the electrochemical potential differences driving reactions at the anode and cathode. Representative boundary value problems are solved to illustrate features of the model. Predictions of the model are shown to be in good agreement with experimental measurements.
The Role of Electrons in Nanostructured Si1-xGex/Si for Energy Conversion

Md Hossain
University of Illinois at Urbana-Champaign
1206 W Green St, MC 244, Mechanical Engineering Bldg, Urbana, 61801, US
Phone: 12173778474, Email: hossain2@illinois.edu

Harley T Johnson
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:
Nanostructured materials such as Si1-xGex/Si have attracted significant attention in the recent literature because of their potential for on-chip heat management or energy conversion utilizing waste heat. Maximizing the efficiency of energy conversion involves optimizing several interdependent transport properties of electrons as well as phonons. Nonetheless, because of the limitations in experimental measurements of conductivities on the nanoscale, especially for lengths on the order of a few Angstroms, ascertaining the influence of physical dimension on energy conversion is a challenging task. Consequently, efforts on improving ZT have mainly been focused on phonons, disregarding the prospects of enhancing thermopower that originate solely from electrons.

In this work, using a combination of first-principles calculations and a semi-classical Boltzmann transport formalism, the role of electrons on energy conversion is studied for Si1-xGex/Si heterostructures. In addition to providing quantitative measures for the role of electrons on nanoscale energy conversion in Si1-xGex/Si, a rigorous computational framework is developed for computing electronic contributions to thermopower and electron thermal conductivity, taking into account the influences of various relaxation time functions or scattering events, temperature, doping, and layer thickness ratio. It is found that alloying can substantially improve thermopower while nanoscale lengths can lead to degradation and adversely affect ZT values. At room temperature, the maximum thermopower for a 3.3 nm Si0.5Ge0.5/Si heterostructure with layer thickness ratio of 1:1 is obtained as 336 V/K, while for a similar size Si0.0Ge1.0/Si heterostructure with the same layer thickness ratio the maximum thermopower is only 129 V/K. Furthermore, the maximum values occur at different chemical potentials or carrier densities: 0.0025 Ry (6x1018 cm-3) for Si0.5Ge0.5:Si = 1:1 and 0.0058 Ry (3x1019 cm-3) for Ge:Si = 1:1. Thus, the results indicate that nano-structuring alone does not offer beneficial effects for maximizing the efficiency of energy conversion in nanostructured thermoelectrics. Rather, alloying and a proper choice of carrier density and type of carriers - which can create a sharp increase in the density of states around the Fermi energy of the system - are also essential for enhancing thermoelectric efficiency. Moreover, because of a difference in mean free path for electrons and phonons, it is important to identify length scales that can amplify the combined effects of phonons and electrons on ZT. It has already been reported in the literature that a reduction in phonon thermal conductivity results in improved energy conversion in nanoscale materials; nonetheless, the limiting values of lengths at which the thermal conductivity can be a minimum and transport becomes ballistic are still under investigation. Our study on the role of electrons on thermopower and electron thermal conductivity at different lengths can help identify the length scales that play the biggest role in achieving optimum ZT values in nanoscale materials.
Transport of Hydrogen in Materials Undergoing Finite Straining

Mohsen Dadfarnia  
University of Illinois at Urbana-Champaign  
158 Mechanical Engineering Building, 1206 West Green Street, Urbana, 61801, US  
Phone: 2174196028, Email: dadfarni@illinois.edu

Petros Sofronis  
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

A key element for the realization of the hydrogen economy is the large scale gaseous hydrogen transport and storage from production facilities to local distribution sites. Among the technical barriers to the implementation of hydrogen transport and storage technologies is hydrogen embrittlement, a severe degradation of the mechanical properties of materials in the presence of hydrogen. In an effort to understand the mechanics of hydrogen embrittlement in structural materials, we study the hydrogen/microstructure interaction in a material undergoing elastoplastic straining. With the use of a hydrogen diffusion formulation which accounts for large geometry changes, we present numerical simulation results for hydrogen accumulation profiles ahead of a blunting crack tip. For ferritic steels, we find that using an updated Lagrangian formulation for the material deformation and ignoring the geometry changes for the diffusion process, we can predict the hydrogen distribution ahead of the crack very reliably. For austenitic steels with much smaller hydrogen diffusivity than the ferritic systems, we observe small deviations when we neglect the effect of large geometry changes under slow loading rates. We resolve the issue over a range of applied strain rates through a Streamline Upwind Petrov-Galerkin formulation.
Thermoresponsive Microcapsules for Autonomic Lithium-Ion Battery Shutdown

Marta Baginska
University of Illinois Urbana-Champaign
104 S. Wright Street, Room 306, Urbana, 61801, US
Phone: 217-265-6261, Email: mbagin2@gmail.com

Benjamin J. Blaiszik
University of Illinois Urbana Champaign, Urbana, IL

Susan A. Odom
Illinois Urbana Champaign, Urbana, IL

Jeffrey S. Moore
Illinois Urbana Champaign, Urbana, IL

Nancy R. Sottos
University of Illinois Urbana-Champaign; Urbana, IL

Scott R. White
University of Illinois Urbana-Champaign; Urbana, IL

Abstract:

Lithium-ion batteries are used in a variety of applications ranging from consumer electronics such as cellular phones and computers to hybrid vehicles, but safety remains an important issue when lithium ion batteries undergo external heating, over-charging, high current charging, or physical damage. Lithium-ion batteries must be safe and damage tolerant for full market penetration.

Functionalization of battery electrodes with thermoresponsive microcapsules is proposed as a fail-safe mechanism for autonomic shutdown of unsafely operating lithium ion batteries. Battery electrodes are functionalized with monomer-filled microcapsules that can be triggered to rupture within a desired temperature range and deliver a thermally polymerizable core to the electrode surface. This release and thermal polymerization may prevent ionic conductivity by forming an insulating film, thus, shutting down the battery cell.

Capsules containing thermally polymerizable monomers must satisfy a rigorous set of requirements for autonomic shutdown including: (1) long term stability in the electrochemical environments typical for lithium-ion batteries, (2) survival of battery processing conditions, and (3) thermal triggering of capsules in the target temperature range. Initial work on the selection and microencapsulation of thermally polymerizable monomers and design of thermally triggered microcapsules is described.
Continuum and Atomistic Models of Strongly-coupled Diffusion, Stress, and Solute Concentration: Applications to Battery Electrodes

Huajian Gao
Brown University
Division of Engineering, Providence, 02912, US
Phone: 4018632626, Email: Huajian_Gao@Brown.edu

Jun Song
Brown University, Providence, RI

William Curtin
Brown University, Providence, RI

Invited Presentation

Abstract:

Poor cyclic performance of electrodes in lithium-ion rechargeable cell batteries has seriously restricted their application. Recent experiments suggest that substantially improved performance is attainable using nano-sized electrodes. A lack of a clear continuum modeling framework is currently impeding efforts to optimize design of electrodes. The present work provides an underlying comprehensive understanding for continuum modeling of diffusion at high solute concentrations. Compared to the existing models in the literature which are only applicable for dilute solutions, we present a continuum model which accommodates four fundamental features of highly nonlinear behavior associated with diffusion at high solute concentrations. First, the effect of very large solute-induced stresses on the activation energy of solute diffusion is considered. Second, the stoichiometric maximum concentration is explicitly recognized as a saturation limit for solute. Third, the strong influence of the change in local chemical environment on the interaction energy between solute and host atoms is accommodated. Fourth, the effect of the solute concentration on the Young’s modulus of the host material is considered. The continuum model is validated using hydrogen diffusion in nickel as a test system, and the influences of each feature above are clearly demonstrated through parametric studies. We then discuss the applicability of the model to the case of lithium diffusion in silicon.

As an example of new phenomena associated with the model, we show that, with the introduction of a coupling between internal stresses and activation energy for diffusion in the classical theory of diffusion induced stresses, there exists a class of nonconventional solutions for atomic intercalation into a solid electrode, indicative of a surface locking instability once the product between electrode dimension and charging rate exceeds a critical value.
Elastic Softening of Amorphous and Crystalline Li-Si Phases with Increasing Li Concentration: A First-Principles Study

Vivek Shenoy
Brown University
Brown University, Division of Engineering, Providence, 02912, US
Phone: 401-863-1465, Email: Vivek_Shenoy@brown.edu

Abstract:

Knowledge of the elastic properties of Li-Si alloys as a function of Li concentration is crucial in the development of reliable deformation and fracture mechanics models for Si anodes in Li-ion batteries. Here [1], we have studied these properties using first principles calculations for both amorphous and crystalline phases observed during lithiation of Si anodes. In the case of crystalline alloys, we present the anisotropic elastic tensors as well as the homogenized Young’s, shear, and bulk moduli and the Poisson’s ratios. We find that while these moduli decrease in an approximately linear manner with increasing Li concentration leading to significant elastic softening (by about one order of magnitude) in both crystalline and amorphous systems, the Poisson’s ratios remain in the range of 0.05-0.20 and 0.20-0.30 in the case of crystalline and amorphous systems, respectively. Further, for a given Li concentration, we find that the amorphous structures are elastically somewhat softer than their crystalline counterparts, the difference being more significant (about 30-40 %) in Li-poor phases. Our results underscore the importance of including the concentration dependence of elastic constants in the analysis of stress and deformation fields during lithiation and de-lithiation of Si anodes.

First-principles Calculation of Elastic Properties of Ni-Cu-Sn Crystal Structures

Feng Gao
Northwestern University
A156, 2145 Sheridan Road, Evanston, 60208, US
Phone: 847-491-5164, Email: feng-gao@northwestern.edu

Jianmin Qu
Northwestern University, Evanston, IL

Abstract:

The properties of intermetallic compound (IMC) are crucial to the solder joint reliability. This issue tends to be more pronounced following with the solder joint size scaling down to micros level. However, the IMCs distributed at the solder/substrate interface or within the solder matrix often exhibits complex crystal structures due to the doping element participation. It is still challenging to evaluate the change of the IMC crystal structure property precisely. Ni-based finishes, e.g., electroless nickel immersion gold (ENIG) are widely utilized in electronic packaging. The Ni3Sn4 intermetallic compound (IMC) is often found at the interface between Sn-based lead-free solders and ENIG. It has been found that a trace amount of Cu can substitute for Ni atoms in Ni3Sn4 to form (Ni, Cu)3Sn4. In this talk, by using first-principles approach within density functional theory (DFT), we studied the (Ni,Cu)3Sn4 properties due to the Ni occupancy in the crystal structure. In order to study the thermodynamic stability, the total energy of (Ni,Cu)3Sn4 crystal was first computed. Then the total energy was used to calculate the heat of formation to determine the thermodynamic stability. The heat of formation is related to the composition-average energies of the pure component elements in their equilibrium crystal structure. In terms of heat of formation, the thermodynamic stability of (Ni,Cu)3Sn4 is found to be reduced when the Cu concentration is greater than 14.3 at.%. The Ni3Sn4 crystal structure exhibit anisotropic elastic properties. This is because the changes of the electronic states are different against different applied strains. It is demonstrated that the changes of both Ni-d and Sn-p states in Ni3Sn4 are more significant against the strain along the larger stiffness directions. Furthermore, the elastic properties of (Ni,Cu)3Sn4 polycrystalline are extracted by using the elastic constants of single crystal. It is shown that the presence of Cu in the crystal structure reduces the moduli of (Ni,Cu)3Sn4 due to the deterioration of Ni and Sn states hybridization.
Autonomic Restoration of Conductivity for Li-ion Battery and Microelectronic Applications

Benjamin Blaiszik
University of Illinois at Urbana-Champaign
405 N. Mathews Ave., Urbana, 61801, US
Phone: 6306391957, Email: blaiszik@illinois.edu

Sharlotte L.B. Kramer
University of Illinois at Urbana Champaign, Urbana, IL

David A. McIlroy
University of Illinois at Urbana Champaign, Urbana, IL

Marta Baginska
University of Illinois at Urbana Champaign, Urbana, IL

Abstract:

A variety of complex damage mechanisms in Li-ion batteries and microelectronics can lead to a significant loss of conductivity, and eventual system failure. For Li-ion batteries, cracking, deterioration, and electrochemical pulverization occur during the massive volume changes associated with the intercalation/deintercalation of Li+ ions during charge and discharge. As this damage accumulates, there is a significant degradation of the efficiency, and eventually failure of the battery. In microelectronics, mechanical or thermal damage can lead to a loss of conductivity across a damaged pathway and performance degradation of the overall circuit. Deriving from bioinspired concepts, we propose to use damage in the material as a trigger to autonomically initiate a self-healing response for restoration of conductivity in both Li-ion battery electrode and microelectronic applications. Through restoration of conductivity in these damaged materials, battery and microelectronic device lifetime and reliability may be increased.

In this presentation, we describe the development of a self-healing system for restoration of conductivity and preliminary test results. The testing apparatus includes a custom-built four-point bend fixture with simultaneous load-displacement and Wheatstone bridge resistance measurement. This testing apparatus is used to initiate damage and also to monitor the conductivity in undamaged, damaged, and the healed samples. The autonomic system development includes the investigation, screening, and characterization of several potential mechanisms for conductivity restoration. We describe in detail a novel urea-formaldehyde (UF) encapsulation technique for sequestration and delivery of a conductive liquid metal, such as elemental gallium (Ga) or common Ga eutectic alloys (Ga-In, Ga-In-Sn), to the site of mechanical damage in a conductive material. Further, we describe alternative methods to achieve conductivity restoration such as solvent-aided delivery of highly conductive silver particles, and the in situ formation of conductive polymers.
Full-field Imaging Methods for Validation of a Multiscale Model for Polycrystalline Plasticity

Laurence Bodelot
California Institute Of Technology
1200 E. California Boulevard, MC 105-50, Pasadena, 91125, US
Phone: 617 899 9395, Email: lbodelot@caltech.edu

G. Ravichandran
California Institute Of Technology, Pasadena, CA

Abstract:
The assumption of homogeneity in deformation for metallic materials only holds at a macroscopic scale. Most metals actually have a polycrystalline structure made of grains of different orientations. As a consequence, even under uniform loading, the mechanical behavior of a polycrystal is highly heterogeneous at the grain scale, featuring the appearance of early and localized plasticity. Such heterogeneities in static and kinematic quantities at a local scale contribute to the macroscopic behavior of the material and need to be better understood and accounted for in constitutive laws and in numerical modeling in order to lead to accurate predictions of the macroscopic behavior.

The objective of this work is to use advanced full-field measurements methods so as to have an insight on localization phenomena and their relationship to the microstructure. Furthermore, accessing polycrystalline structure characteristics as well as mechanical data at the grain scale will give information of interest in the validation of numerical models aiming at taking into account multiscale plasticity.

Quasi-static experiments are thus designed to validate a fast multiscale model for polycrystalline plasticity developed in Caltech by first providing the microstructure and orientation data of a sample before and after loading, in addition to the strain fields at the grain level during loading.

Accessing microstructural information requires high-resolution and full-field advanced imaging methods. A module Electron Backscatter Diffraction (EBSD) is used inside a Scanning Electron Microscope to establish the orientation of the grains of polycrystalline metallic samples which have been polished as perfect mirrors beforehand. This technique, performed on the sample prior to and after loading, thus enable to monitor any texture evolution of the microstructure induced by the mechanical deformation.

Mechanical data, and in particular strain fields, are obtained through a Digital Image Correlation technique. This method involves taking images of the sample during loading. For this purpose, a high resolution camera is used in-situ during quasi-static loading of a dog-bone shaped sample on an Instron tensile machine in order to obtain strain fields evolutions at the grain level in zone of interest previously analyzed by EBSD.

The material used in this study is a face centered cubic structured austenitic stainless steel. Orientation data and strain fields at the microstructure scale obtained during the loading of this material are analyzed in order to enlighten the relevant relationship existing between them. They are further used to validate predictions of the aforementioned fast multiscale model developed for polycrystalline plasticity.
Response of Composite Structures to Underwater Shock Loading

Siddharth Avachat  
Georgia Institute of Technology  
Woodruff School of Mechanical Engineering, 801 Ferst Drive, MRDC 4113, Atlanta, 30332-0405, US  
Phone: 4048943647, Email: sidavachat@gatech.edu

Min Zhou  
Georgia Institute of Technology, Atlanta, GA

Abstract:

The objective of this combined numerical and experimental study is to analyze the dynamic response of sandwich structures which play an important role in applications requiring shock resistance, high capacity for energy-absorption and out-of-plane shear strength. This investigation focuses on the overall structural response, deformation, damage, and energy-absorption through delamination and core crushing. Air-backed and water-backed/submerged composite structures are subject to a range of blast loading. The damage and failure characteristics of individual components of the sandwich structures are studied using laser-based in-situ diagnostics and postmortem analysis. In the 3-D finite-element simulations, the underwater blast loading intensity is considered using the Mie-Gruneisen equation-of-state of a linear Hugoniot form. Configurations analyzed include metallic honeycomb core structures with planar and cylindrical geometries. Core crushing is accounted for through the Johnson-Cook ductile damage model. Calculations reveal a significant difference between the response of air-backed and water-backed/submerged structures in terms of deflection, core crushing and energy-absorption. The experiments and computations offer approaches for improving the blast mitigation capabilities of submerged composite sandwich structures in the critical parts of a ship structure like keel, turbine-blades and rudders.
Anomalous Loss of Toughness with Physical Aging of Work Toughened Polycarbonate

Shawn Meagher
University of Nebraska-Lincoln
2501 S 79 ST, Lincoln, 68506, US
Phone: 402-304-2562, Email: shawn.meagher@gmail.com

Kyle Strabala
University of Nebraska Lincoln, Lincoln, NE

Charles Landais
University of Rouen, Rouen, France

Mehrdad Negahban
University of Nebraska Lincoln, Lincoln, NE

Abstract:

We have studied the response of mechanically toughened and physically aged polycarbonate using Charpy impact and ultrasonic wave speed measurements. The toughening was conducted through plastic compression. As expected, the toughened material showed anisotropic elastic response. The Charpy impact tests also showed anisotropic toughening both in the absorbed energy and in the mode of fracture. There was an anomalous drop in the toughness of the sample with aging, which was anisotropic and uncorrelated in the different directions, and which disappeared for the highly toughened samples. The transition was bimodal and statistically distributed between either ductile or brittle transitions. The transition time indicated a temperature dependence that was logarithmic.
Lateral Vibration of a Travelling Tensioned Euler-Bernoulli Beam with
Stick-Slip End Condition

Sameer Jape
Iowa State University
102, Nuclear Engineering Laboratory, Iowa State University, Ames, 50011, US
Phone: 5152031890, Email: ssjape@iastate.edu

Jonathan A. Wickert
Iowa State University, Ames, IA

Baskar Ganapathysubramanian
Iowa State University, Ames, IA

Abstract:
Magnetic tape libraries which are used for long-term archival and backup of the digital data, face the need to offer the least expensive storage for huge quantities of data. Lateral in-plane vibration of the tape can cause misalignment (and data loss) between the data tracks and the position of the read/write head, and hence need to be investigated, understood and minimized. Lateral vibration can be caused by excitation sources viz. pack runout, flange impacts, pack tilts and tape edge weave. To attenuate this vibration, surface guides, which include grooved rollers, porous rollers, or roughened rollers, are used. A good understanding of the physical phenomena involved will allow the appropriate and optimal choice of roller characteristics.

We develop a mathematical model to study the frictional interaction between the roller surface and the tape that travels over it. The tape is modeled as an axially moving, tensioned, viscoelastic Euler-Bernoulli beam subjected to boundary disturbances arising from supply and take-up pack runout along with Coulomb friction between the tape and the roller surface. Because of the friction constraints between the roller surface and the Euler-Bernoulli beam, the beam will have two states in axial motion: if the axial force is smaller than the frictional force, stick occurs; if the axial force increases to the frictional force, the beam starts slipping. The governing equations of lateral vibration of the beam are discretized through the finite element method by using the Galerkin approximation and hermite polynomials of order three for the element basis functions. Considering a periodic stick-slip motion, the axial force is represented by a saw-tooth waveform.

The model is used to quantify the possibility of sticking or slipping between the surfaces in contact, as a function of the tape parameters -- speed, tension and span length. An experimental setup is used to control these beam parameters and obtain lateral vibration measurements for validation of the model. This experimentally driven analysis framework is used to construct and understand the dynamic phase diagram, i.e. to determine the regions in the stiffness-velocity plane where steady stick-slip motion occurs and its effects on the lateral vibration in the magnetic tape. This phase diagram can subsequently be used as a look-up table to choose roller characteristics.
Atomistic Simulations of the Interfacial Behavior of Carbon Nanotube Contacted with Si

Ajing Cao
Northwestern University
A156 Technological Institute, 2145 Sheridan Road, Evanston, 60208, US
Phone: 847-491-5164, Email: a-cao@northwestern.edu

Jianmin Qu
Northwestern University, Evanston, IL

Abstract:

With the promising applications of carbon nanotubes in future micro-electronic devices, it is desirable to know the mechanical stability of carbon nanotube attached to Si substrates. In this paper, the results of mechanical response of a single-walled carbon nanotube contacted with a Si substrate when subject to both tensile and shear loading are presented using molecular dynamics simulations with the Brenner potential. Interesting, our results show that atomic chain formed with large elongation after the yield (peak) stress. The jerky stress-strain curve corresponds to each bond breaking event, followed by consecutive elastic loading of each chain, rendering the novel plastic deformation behavior. The bond strength of C-Si and Si-Si are compared to determine the interfacial strength. The temperature effects on yield strength are also discussed. The simulation work is expected to gain some understandings on the mechanical behavior of perfect interfaces and offers new means for their realistic applications.
Abstract:

A new strategy is employed to impart productive mechanochemical response to an elastomeric polymer [1]. Force sensitive molecules, termed mechanophores, are successfully incorporated as cross-linkers into poly-(methyl methacrylate) (PMMA) through a free radical polymerization initiated with benzoyl peroxide [2]. Evidence of local chemical reaction is provided by a color and fluorescence generating spiropyran (SP) mechanophore that undergoes an electrocyclic ring opening reaction under mechanical deformation. This ring opening can be driven by mechanical force, certain wavelengths of light, and heat and is also reversible. Here, we investigate the role of shear loading on bulk polymer specimens and the mechanical force required to perform this ring opening process.

Cross-linked PMMA was synthesized with a total cross-link density of 1%. For all polymers, the spiropyran cross-linker content was held at 0.018 mol% with the remaining balance being made up of either ethylene glycol dimethacrylate (EGDMA) or polyethylene glycol (PEG-550). Polymerization was carried out in 1 mL syringes which had been compression molded into a tapered cylinder with a gauge length of 10 mm and a diameter of 2 mm.

Shear testing was performed on the mechanophore cross-linked PMMA. All specimen types were tested using a torsion test fixture and a TA Instruments AR-G2 rheometer. Shear rates were held constant at 0.1 sec-1, 0.01 sec-1, and 0.001 sec-1 to allow the sample to undergo larger strains in torsion and to produce color change and fluorescence in the active samples. The activation strain, activation stress and activation strain energy were higher at higher shear rates and were linearly related to shear rate. In an effort to lower the activation parameters, the major cross-linker (EGDMA) was replaced with PEG-550. We hypothesized that the longer length of the PEG chains compared to the spiropyran molecule would enhance load transfer to the spiropyran, thus leading to mechanical activation at a lower bulk shear stress and strain. The result of changing the major cross-linker from EGDMA to PEG was a lower activation shear strain, shear stress and strain energy for all shear rates.

Control tests were performed on PMMA with monofunctional spiropyran [2] and PMMA with no spiropyran. As expected, no color change resulted from the shear testing. Experiments are in progress.
to understand the role of cross-link length, cross-link density, and the incorporation of other mechanophores on the shear-induced chemical reactions.

Reference:
Cooling Effects on the Vibronic Bands of Photo-Stimulated Luminescence Spectroscopy for 3-D Stress Characterization

Hugo Pelaez
Purdue University
701 W Stadium, ARMS 1333, West Lafayette, 47906, US
Phone: (765) 496-7225, Email: hpelaez@purdue.edu

P.K. Imbrie
Purdue University, West Lafayette, IN

Hugo Pelaez
Purdue University, West Lafayette, IN

Abstract:

Photo stimulated luminescence spectroscopy (PSLS) has been extensively used in recent years in an attempt to characterize a 3-D stress state of thermally grown oxide layers (TGO) in thermal barrier coatings (TBC) used in jet engine turbine blades. Recent studies have shown a strong correlation of the vibronic band regions, along with their corresponding R-lines of the spectral readings to applied stresses in chromium-doped alumina (Al₂O₃ [Cr]³⁺). This research is aimed at establishing the relationship between the thermally-induced peak shifts of the vibronic bands and the R-lines. The spectral signal for the three principle crystallographic orientations of single crystal chromium-doped alumina was analyzed using the GA spectral analysis method for both room temperature and cold temperature experiments. R-line shifts with stress were verified by comparing them to other results obtained by previous research. The fitness function value for the R-lines increased from 0.99 to 0.999 when data was taken at -60°C compared to 23°C. R-line peak shifts differed among the three crystallographic orientations with applied stress. Both the R-line and vibronic band peak shifts have shown to differ by the three principle crystallographic orientations with applied stress. Linear relationships of several peakshifts of the vibronic bands have been quantified in the polycrystal specimen. An average shift of the vibronic band peaks were calculated as -.07cm⁻¹/°C with data taken between -50°C and -176°C, which is about half of that observed from the ruby polycrystal R-lines thermal shifts observed between 23 oC and -176oC. The data obtained in this study suggests that vibronic band thermally-induced peak shifts are linear, however these shifts with respect to each other differ in magnitude. Results of the correlation between the R-lines and vibronic bands thermally-induced peakshifts will be presented. Ultimately, the relationship between the room temperature and cold temperature data will be needed to accurately predict 3-D stress states within the TGOs of TBCs.
Modeling and Simulation of a Novel Dual-stack Piezoelectric Actuator

Xinong Zhang
Department of Engineering Mechanics /MOE Key Laboratory for Strength and Vibration
School of Aerospace Engineering, Jiaotong University, Xi’an, 710049, CN
Phone: +86-29-82668482, Email: xnzhang@mail.xjtu.edu.cn

Abstract:

Generally, piezoelectric stack actuators are mainly designed for the push-only actions because it can normally take remarkable compressive loads but cannot tolerate tension. For achieving bidirectional outputs, a common method is that a compressive preload mechanism is embedded into the actuator. However, it may reduce the holistic actuated capability. In this research, a new type dual-stack piezoelectric actuator is designed in order to obtain a smart structure with perfect bidirectional output (both push and pull). In this actuator, two matching piezoelectric stacks are utilized and alternatively extended and shortened by applying opposite driving voltages. That is, there is always a piezoelectric stack to take compressive loads in either push or pull directions. Further, the dynamic modeling is developed and the actuated performance is simulated. To analyze the performance of the new actuator, both linear model and hysteresis model are built based on the structural characteristics and operating principle. The ideal operation is that the two stacks generate an output with the same amplitude and opposite direction, and then the whole actuator is able to obtain maximum output capacity. However, because of the different output capacity in the positive and negative driving directions and the hysteretic attribute of piezoelectric stacks, the operation of two piezoelectric stacks is not coordinated and the contact-detachment motion phenomenon will appear in the actuator. In order to decrease the effect of the contact-detachment motion on the output of the actuator, the method of applying pre-pressure is adopted. Thereupon, the effect of the pre-pressure is also considered in the dynamic modeling. Moreover, the contact-detachment conditions are derived and the corresponding motion equations are obtained. Finally, some numeric simulation examples are completed to compare the two models and analyze nonlinear actuated behavior. These simulated results validate the dynamic model of the novel actuator and its actuated law, and point out the good application prospect in high performance intelligence structures.
Dynamoic Damage Tolerance of Aeronautical Sandwich Structures

Nathan Bailey
The University of Auckland
537 Ethel St NW, Atlanta, 30318, US
Phone: 404-316-6966, Email: nbai010@aucklanduni.ac.nz

Siddharth Avachat
The Georgia Institute of Technology, Atlanta, GA

Abstract:
Requirements for increased performance and efficiency and reduced emissions have necessitated the use of advanced composite materials in fixed wing aircraft and helicopters. While these materials have good fatigue performance, damage tolerance of the structures is a major concern. Design and certification requirements for interior aircraft structures are typically based on dynamic load cases with specified acceleration levels in defined directions to represent crash scenarios. There is limited knowledge available about the residual strength of damaged sandwich composite materials subjected to dynamic loads.

This study outlines the design, fabrication and verification of a new test method to characterize the damage tolerance of aeronautical sandwich composites materials under dynamic loads using a modified Split-Hopkinson bar experiment. In-situ diagnostics include laser vibrometers, high speed photography and embedded strain-gage based measurements. A computational framework is developed to account for core crushing, fiber and matrix damage and failure. The energy absorption characteristics of the individual components of the sandwich structure are evaluated using computational calculations. This combined experimental and computational approach will give insights into the dynamic response of composite sandwich structures subjected to impact loading and enable the design of newer and better aeronautical structures.
On the Loss of Ellipticity in Electroactive Polymer Composites

Stephan Rudykh
Ben-Gurion University
P.O.B. 653, Department of Mechanical Engineering, Beer Sheva, 84105, IL
Phone: 97286477046, Email: rudykh@bgu.ac.il

Gal deBotton
Ben Gurion University, Beer Sheva, Israel

Kaushik Bhattacharya
California Institute of Technology, Pasadena, CA

Abstract:

Electroactive polymers (EAP) are soft dielectrics that change their shape and size in response to electric excitation. Various applications of EAP actuators have been considered in recent years [1, 2]. In this study, the behavior of homogeneous and periodic composite EAPs under coupled electromechanical boundary conditions in finite deformations is investigated with emphasis on the important aspect of instabilities phenomena.

First, we examine pure mechanical instabilities that may develop in fiber composites and detect the associated critical stretch ratios. In particular, we focus on macroscopic instabilities that are associated with long waves and considered as loss of ellipticity of the homogenized governing equations. Analytical estimations of the onset of ellipticity loss are given by making use of a new effective energy-density function for Gent fiber composites [3]. This model enables to capture the well-known "lock-up" effect of polymer molecular extensibility limit. The analytical estimations are compared with both 2D and 3D finite element simulations. For the 2D case the representative unit cell is a laminated structure. In the spatial case, we examine the responses of composites with periodic hexagonal unit cell [3]. It is demonstrated that the analytical estimations for the onset of failure are in fine agreement with the corresponding numerical results.

In the coupled electromechanical problems, instabilities may arise from geometry of a particular application, from material properties, or from a composite microstructure. These instabilities may be utilized as triggers for shifting actuators from one configuration to another. In other words, a relatively small value of electric excitation may lead to a significant actuation. Theoretical and numerical examples are considered.

REFERENCES:
Laser and Multi-Energy Interactions with Materials

ORGANIZERS:

Judith Todd, Pennsylvaia State University

Yongfeng Lu, University of Nebraska - Lincoln

Xinwei Wang, Iowa State University
Near-field Heating of Nano-tips in Laser-assisted SPM
Surface Nanostructuring

Xiangwen Chen
Iowa State University
2025 Black Engineering Building, Dept. of Mechanical Engr., ISU, Ames, 50011, US
Phone: 515-294-2085, Email: xwchen@iastate.edu

Abstract:

In surface nanostructuring using laser-assisted scanning probe microscope (SPM), the focused sub-10 nm optical field could heat both the substrate and SPM simultaneously. In this work, we carry out systematic study of highly enhanced optical field between scanning probe tips and silicon substrate system under laser illumination. The effects on optical field distribution caused by curvature radii, aspect ratios of tips, and polarization directions of incident laser are studied. The heating effect inside tungsten SPM tips because of absorption of incident laser is also explored using the finite element method with the optical field provided by the optic simulation. The temperature distribution inside the SPM tips, temperature change verse time, and the effect of tip curvature radii and aspect ratios on temperature distribution inside the tips are investigated.
Abstract:

The objective of this study is to determine the required laser parameters for producing the desired free radicals and conditions that may facilitate the formation of diamond or diamond-like thin films. In order to efficiently produce the desired free radicals, one needs to either choose an appropriate laser frequency (one-laser-dissociation case) or include another laser to excite the molecule to a particular intermediate state (two-laser-dissociation case). In this work, we use an ab initio model for two-laser dissociation of CO\(_2\) molecules to investigate the influences of different combinations of laser parameters (laser intensity, laser pulse duration, and time delay between the two laser pulses) on the population of free radicals. In the simulation, laser is considered as a classical electromagnetic wave and molecule is modeled as a linear combination of wave functions of different molecular energy states. The time evolution of population of molecules at different energy states during the laser irradiation is studied by solving the time-dependent Schrödinger equation which includes a laser-molecule interaction term. It is found from the simulation that the photo-dissociation process is more controllable and efficient by using a combination of one infrared laser which excites the molecule to particular vibrational states and one UV laser which excites the molecule to continuum states, providing that the energy of both lasers can be resonantly absorbed by molecules. The maximum free radical population is obtained when two lasers are applied to the gas simultaneously. With the increase of pulse duration of the infrared laser, the population of free radicals becomes less sensitive to the time delay between the two laser pulses. But the maximum population of free radicals is almost not affected. The current model can be extended to the photo-dissociation of other molecules if the molecular properties like transition dipole moments and transition energies for the corresponding molecules are available from either ab initio calculations or experiments.
Fundamental Studies of the Role of UV Laser Defect Production on the Modification of Surfaces: Single Crystal ZnO and CaF$_2$

Tom Dickinson
Washington State University
Department of Physics, Pullman, 99164-2814, US
Phone: 509 335 4914, Email: jtd@wsu.edu

Abstract:

UV-Laser interactions with wide bandgap insulators and semiconductors has generated a number of examples of point defect production, surface and bulk modification, etching and re-deposition processes, as well as numerous PLD related applications involving the emitted particles. In metal containing compounds such as oxides and halides, aggregation of metals into nanoparticles has been observed. In this talk we examine the fundamental mechanisms required to explain the formation of such nanoparticles. We examine these modifications in oriented single crystals of semiconducting ZnO with a band-gap of ~3.4 eV We first discuss results on interactions of strongly absorbing 248 nm (5 eV), 193 nm (6.3 eV), and 157 nm (7.8 eV) excimer laser light with high purity ZnO surfaces in UHV. Using time resolved quadrupole mass spectroscopy, we show examine atomic and molecular emissions (Zn, O, and O$_2$) generated at fluences below plasma formation threshold. Although the atomic Zn emission is robust, more total oxygen is observed to leave the surface. One possible emission mechanism we are pursuing is the ejection of O by localized electron hole pair annihilation. Accompanying exposure of these single crystals to 193 nm light is coloration: i.e. gray to black spots (some preliminary evidence is showing detectable but less coloration at 248 nm); we show conclusively that this coloration is due to surface metallic zinc in the form of nanoparticles, typically 10-20 nm in diameter. We discuss formation mechanisms and the role of strong interactions of the laser with these nanoparticles. Finally, we show preliminary results on the production of defects in the VUV region of the spectrum induced by 157 nm light on single crystal CaF2 light that results in significant and novel first order interactions with the laser light itself. This may enter into the processes that lead to high density Ca metal nanoparticle generation inside the crystal by 157 nm exposure.
Laser Texturing of Polyimide for Altering the Contact Angle of Water

David Willis
Southern Methodist University
PO Box 750337, Dallas, 75275, US
Phone: 214-768-3125, Email: dwillis@lyle.smu.edu

David A. Willis
Southern Methodist University, Dallas, TX

Abstract:

Laser ablation of Kapton HN polyimide was performed at low fluences using a neodymium-doped yttrium lithium fluoride (Nd:YLF) laser operating at the third-harmonic wavelength (349 nm). Surface texture with cone-like and hemispherical bump-like shapes were formed, with the areal density and size of the textured features dependent upon the laser fluence and number of laser pulses. As the laser fluence and number of pulses increased, the size of cones and bumps increased. For a given fluence, the areal density of the bumps decreased with number of laser pulses, while the areal density of cones increased. The contact angle of de-ionized water on polyimide was measured before and after laser irradiation to quantify the effect of surface texture. The polyimide was converted from an initially hydrophilic state to a hydrophobic state for some samples, while for other samples the surfaces became more hydrophilic. The contact angle modification was a result of both changes in the surface roughness and the laser-induced alteration of the polyimide carbon composition. X-ray photoelectron spectroscopy (XPS) was performed on both textured and un-textured regions of samples. The results showed that the textured regions had a higher carbon content that the native polyimide, and that the carbon content was higher at the tips of the bumps and cones than at the bases of the structures. Thus the lower oxygen content on the textured features likely increased the native contact angle. The formation of surface structures will be explained in terms of existing models, including the radiation hardening model, impurity model, and debris model. The results will also show that the contact angle depends upon the ratio of the feature spacing to feature size. Small values of this ratio (closely packed features) resulted in an increased contact angle, while large ratios (widely spaced features) resulted in a decreased contact angle.
Generation of Crystal Defects and Microstructure in Laser Processing of Metals: Molecular Dynamics Study

Leonid Zhigilei  
University of Virginia  
395 McCormick Road, P.O. Box 400745, Charlottesville, 22904, US  
Phone: 434 243 3582,  Email: lz2n@virginia.edu

Chengping Wu  
University of Virginia, Charlottesville, Virginia

Eaman Abdul Karim  
University of Virginia, Charlottesville, Virginia

Zhibin Lin  
Colorado School of Mines, Golden, Colorado

Abstract:  
Atomic-level computer modeling has the ability to provide detailed information on the complex processes induced by short pulse laser irradiation of metal targets and can assist in the advancement of laser-driven applications. Recent results obtained in simulations of laser interactions with metal targets (Au, Ni, Cr, AuCu bilayer) [1-5] will be reviewed in the presentation, with a particular focus on the laser-induced generation of crystal defects and the role of the microstructure of the target on the material response to the fast laser energy deposition. In particular, the results of a detailed analysis of the mechanisms and driving forces responsible for the generation of point defects (vacancies and interstitials) and dislocations in femtosecond laser interactions with metals will be presented. The implications of the computational predictions for atomic mixing and damage accumulation in multi-pulse irradiation regime will be discussed. The processes responsible for the formation of a nanocrystalline structure in regions of the irradiated target experiencing ultrafast melting and resolidification under conditions of localized laser energy deposition will be analyzed based on the results of large-scale molecular dynamics simulations.

Surface Modification of Titanium Via Laser-Sustained Plasma

Ravindra Akarapu
The Pennsylvania State University - Department of Engineering Science & Mechanics
212 EES Building, University Park, 16802, US
Phone: 8605503096, Email: anb191@psu.edu

Ravindra Akarapu
Center for Multiscale Wave Material Interactions, Department of Engineering Science & Mechanics, Penn State University, University Park, PA

Judith Todd
Center for Multiscale Wave Material Interactions, Department of Engineering Science & Mechanics, Penn State University, University Park, PA

Stephen M. Copley
Applied Research Lab, Penn State University, University Park, PA

Abstract:

A laser-sustained plasma (LSP), which can be maintained indefinitely by a laser beam away from interacting surfaces, has been investigated as a means of surface modification. Previous research efforts have focused on the characteristics of the LSP and its use as a deposition process. The current research investigates the effect of the LSP coupling on commercially pure titanium substrates and its effectiveness as a surface modification technique. Variables explored include plasma composition, gas flow rate into the plasma, substrate translational speed, and process setup. The products of processing methods were subjected to a variety of material characterization techniques to discover the constitution, surface features, microstructures, and mechanical properties of LSP processed titanium. Comparisons are made between the results of comparable runs by the laser with and without the plasma and relationships between processing parameters and resulting surface properties are explored.
Femtosecond Laser Processing of Graphene Oxides for Fine Patterning of Novel Electronic Devices

Hong-Bo Sun
Jilin University
College of Electronic Science and Engineering, 2699 Qianjin Street, Changchun, 130012, CN
Phone: 86 431 85168281, Email: HBSUN@JLU.EDU.CN

Yong Lai Zhang
Jilin University, Changchun, Jilin

Li Guo
Jilin University, Changchun, Jilin

Qi Dai Chen
Jilin University, Changchun, Jilin

Abstract:

In recent years, interests in graphene-based materials are exploding due to their unique properties. Especially, for electronic applications, two-dimensional graphene sheets demonstrate great potential for future use in microdevices. Generally, graphene sheets synthesized through chemical-oxidative exfoliation of graphite were of benefit to solution-processing compatibility, which imparts tractable nature to graphene for further applications. However, the oxygen-containing graphene suffers from poor electric conductivities due to the presence of abundant defects, which significantly hinders its electrical applications, and therefore, post-reduction was essential. On the other hand, the use of graphene in electronic microdevices requires refined control of various complex patterns of integrated circuits. Novel transfer printing methods were developed for fabricating graphene patterns by employing elastomeric stamps. Shadow mask was used for patterning solution-processed graphene oxide (GO) films through etching or reducing the exposed part of the GO films. In addition, patterned graphene was also prepared by a successful epitaxial growth on a pre-patterned substrate. However, it is still difficult to fabricate complex patterns with higher resolution and smaller size on graphene films. The lack of micronanoprocessing technologies for fabricating graphene into complex patterns constitutes the main trammel of its applications in electronic microdevices. Therefore, it would be of interest to develop new method for patterning and reduction of solution-processed graphene oxides through a simple process. In this talk, a femtosecond laser direct writing (FsLDW) technology is proposed to reach the above end. FsLDW has been widely used for producing micrometer-sized feature and three-dimensional (3D) microdevices due to its advantages of nanometre spatial resolution and 3D prototyping capability. The extremely high transient power benefits the photo-reduction of graphene oxides (GO) to graphene, while the pinpoint irradiation was performed with a digital scanning means, as leads directly to fine patterns. Various complex patterns were successfully created through this simple nanowriting pathway. The patterned graphene was synchronously reduced and thus represent well conductivity for electrical applications.
Coating Deposition via Insertion of Metallic Rods into a Laser-Sustained Plasma

Abdalla Nassar
Penn State University
212 Earth Engineering Sciences Building, University Park, 16802, US
Phone: 8148671571, Email: arn5000@psu.edu

Ravindra Akarapu
Penn State University, University Park, PA

Stephen M. Copley
Penn State University, University Park, PA

Judith A. Todd
Penn State University, University Park, PA

Abstract:

A laser-sustained plasma (LSP), also known as a continuous optical discharge or a laser plasmatron, can be generated and sustained in a coaxial gas flow using a high-powered, continuous-wave carbon dioxide laser. Previous authors have shown that species can be introduced into a LSP, for coating deposition, via the gas phase. We propose a more general means to introduce species, for coating deposition, into a laser-sustained plasma-direct insertion of thin rods into the LSP. This method eliminates the need for toxic precursors, e.g. titanium tetrachloride (TiCl4) is often used as a precursor to deposit titanium nitride (TiN) films via chemical vapor deposition. Here, we present the findings of a set of experiments investigating the interaction of a LSP, sustained by a 5kW CO2 laser in a coaxial flow of nitrogen gas at atmospheric pressure, and a titanium rod. Parameters including the rod feed rate and substrate location are investigated.

Using a high-speed CCD camera, a maximum feed rate for stable plasma sustainment is identified. Above the threshold feed rate, the LSP is observed to fluctuate wildly and extinguish. The threshold feed rate is also heavily dependent on the composition of the rod. The LSP structure and threshold feed rate is found to depend on the locations of the feed and the substrate. The plasma composition before and during insertions of the titanium rod is studied via optical emission spectroscopy. The spectra of a nitrogen LSP in open atmosphere shows the presence of excited oxygen species. This suggests that oxygen is entrained into the LSP. We show that oxides of titanium can be readily deposited in open atmosphere without a chamber using a nitrogen LSP. However, deposition of nitrides and oxynitrides of titanium is not observed in open atmosphere due to oxygen entrainment. We show that oxygen entrainment can be reduced by performing deposition within an aluminum bell jar.

Xiangnan He
University of Nebraska, 209N WSEC, Lincoln, 68588-0511, US
Phone: 402-472-8323, Email: ylu2@unl.edu

Z. Q. Xie

T. Gebre

Y. F. Lu

Abstract:
Optical emission spectroscopy (OES) and spectroscopic temperature determination were carried out to study C2H4/C2H2/O2 flames used for diamond deposition with and without an excitation by a wavelength-tunable continuous-wave (CW) CO2 laser. This diamond deposition process is a multi-energy process with both flame and laser energy. In this study, strong emissions from C2 and CH radicals were observed in the visible range in all the acquired OES spectra. When the flames were irradiated using the CW CO2 laser at a wavelength of 10.591-μm, the emission intensities of OH, CH and C2 radicals in the flames increased owing to the laser excitation, resulting in higher radical intensities which are a key factor in diamond deposition process since they affect the deposition of diamond by affecting the concentrations of atomic H and OH radicals. High-resolution spectra of OH, CH, and C2 after CO2 laser excitations were also taken to compare with those without CO2 laser excitations. The CO2 laser was also tuned to a wavelength of 10.532-μm to precisely match the resonant frequency of the CH2-wagging vibrational mode of the C2H4 molecules. OES spectroscopy of the C2 and CH radicals were performed at different laser powers, and OES spectra taken were collected for comparison. Comparison shows that 10.532-μm CO2 laser excitations were much significant than 10.591μm CO2 laser excitations. The rotational temperatures of CH radicals in the flames were determined by analyzing the spectra of the R branch of the A2Δ→X2Π; (0, 0) electronic transition near 430 nm. The equation used for temperature calculation is \( \ln(I/\lambda^{4}/SJ) = -(1/Tr)(EJ/kB)+\ln C \), which is derived from \( I=CSJ \lambda^{4}\exp(-EJ/kBT) \), in which I is the relative emission intensity of a rotational line obtained from the experimental spectra, \( C \) is a proportionality constant which is the same for all rotational transitions within a band, \( SJ \) is the rotational intensity factor or Hönl-London factor, \( \lambda \) is the wavelength of the emitted spectral line, \( EJ \) is the rotational energy of the initial level, \( kB \) is the Boltzmann constant, and \( Tr \) is the rotational temperature. Afterward, Boltzmann plot, the negative and inverse of whose slope is rotational temperature, will be generated for temperature determination. Both intensity and temperature distributions were plotted along the flame axial direction from nozzle to substrate. When the laser wavelength was kept at 10.591 or 10.532 μm, curve plots were generated with laser power changed from 0 to 1000 W with an interval of 200 W. Besides, the deposited diamond thin-films were characterized by scanning electron microscopy, stylus profilometry, and Raman spectroscopy. All the characterization results were collected and compared to better explain this multi-energy processing. The deposition mechanism with and without the CO2 laser excitation was then discussed based on the OES spectral results.
Laser Resonant Vibrational Excitations of Precursor Molecules in Multi-Energy Processing for Diamond Synthesis

Z.Q. Xie
University of Nebraska
209N WSEC, Lincoln, 68588-0511, US
Phone: 402-472-8323, Email: ylu2@unl.edu

X.N. He
Y.S. Zhou
Y.F. Lu

Abstract:

Multi-energy processing (MEP) in material synthesis using lasers is very promising because it is capable of channeling energies directly to energy states of precursors and radicals. By coupling energy to desired vibrational or electronic states, reactions are controllable with high efficiency and high yield. How to couple laser energies into reactions is of extreme importance to the MEP. Carbon dioxide (CO2) laser has been widely applied in studies on vapor-phase reactions, in which laser energy is coupled into the reactions through vibrational resonance with reacting molecules. However, most CO2 lasers have only one fixed wavelength at 10.591 μm, which leads to several drawbacks. First, the fixed wavelength of the CO2 laser loses selectivity of excitations of different modes. Second, there is a variety of vibrational modes for the reaction molecules, most of which do not have wavelengths exactly at 10.591 μm. The mismatch of wavelengths between the CO2 laser and the molecular modes results in low efficiency of energy coupling.

In order to fulfill mode-selective excitations and have high efficiency of energy coupling, a wavelength-tunable CO2 laser (spectrum range from 9.2 to 10.9 μm) was applied. MEP in diamond synthesis using the combination of this CO2 laser and combustion flames was studied. There are two reasons why diamond synthesis was chosen for the study of MEP. First, diamond has only one element (carbon), making the process less complicated. Second, diamond has been avidly pursued because of its extraordinary properties, such as high hardness, high thermal conductivity, low friction coefficient, optical transparency and chemical inertness, and because of its wide range of applications. In this study, a premixed C2H4/C2H2/O2 gas mixture was used as precursors for synthesis of diamond. Laser energy is coupled into the reaction through resonances between the CO2 laser and the CH2 wagging mode (i7, 949.3 cm-1) of ethylene (C2H4) molecules. By resonantly exciting the CH2 wagging mode of ethylene molecules using the CO2 laser tuned at 10.532 μm, growth rate as well as crystal quality of the synthesized diamond were both increased. More importantly, high-quality diamond crystals were grown on silicon substrates with a high growth rate at ~ 139 μm/h. Diamond crystals with a length up to 5 mm and a diameter of 1 mm were grown in 36 h. Sharp Raman peaks at 1332 cm-1 with full width at half-maximum (FWHM) values around 4.5 cm-1 and distinct X-ray diffraction spectra demonstrated the high quality of the diamond crystals.
Laser Fabrication of Three-Dimensional Functional Photonic Structure: Holographic Approach and Laser Direct Writing

Kevin Chen
University of Pittsburgh
348 Benedum Hall, 3700 O'Hara Street, Pittsburgh, 15261, US
Phone: 724-6128935, Email: pec9@pitt.edu

Tong Chen
Department of Electrical and Computer Engineering, University of Pittsburgh, Pittsburgh, PA

Abstract:

In this paper, we discuss two complimentary laser fabrication approaches to produce three-dimensional photonic structures on-chip. A laser direct writing technique was used to fabricate high-quality and low-loss lightwave circuits in a wide array of transparent materials using high repetition rate femtosecond ultrafast lasers. The laser direct writing technique enables the fabrication of 3D optical circuits that allow lightwave circuits to be routed vertically and continuously in- and out-of a plane. This paper discusses waveguide qualities and optical characteristics fabricated in active glasses, sapphire, chalcogenide glasses, and nonlinear optical materials (LiNbO3 and LiTaO3). The three-dimensional device density, thermal stability, index profiles, optical loss, and minimal bending losses were characterized in telecommunication windows and in mid-IR wavelength range.

To produce three-dimensional periodic photonic structures, multi-layer near-field diffractive optical elements (e.g. phase masks) were developed and employed to construct 3D holographic patterns in photoresist. 3D periodic photonic structures such as diamond-like photonic crystals were fabricated by one optical element and one laser exposure process. In this paper, we detailed the fabrication of multi-layer diffractive optical elements to control phase, diffractive angles, and diffraction efficiency of laser beams for holographic fabrication. Their applications to produce 3D photonic crystals were demonstrated in SU8 photoresist. The multi-layer phase mask can be conveniently built into the existing multiple mask fabrication flow in optoelectronic integrated circuit manufacturing. This enables the monolithic integration of photonic crystal structures with other on-chip optical components.
Femtosecond Laser Fabrication of New Fiber Sensors

Lan Jiang
Beijing Institute of Technology
Laser Micro/Nano Fabrication Laboratory, School of Mechanical Engineering, Beijing, 100081, CN
Phone: 86-01-6891-4517, Email: jianglan@bit.edu.cn

Lan Jiang
Beijing Institute of Technology, Beijing, Beijing

Sumei Wang
Beijing Institute of Technology, Beijing, Beijing

Xin Li
Beijing Institute of Technology, Beijing, Beijing

Abstract:

During new fiber sensor development experiments by femtosecond laser processing, a simple single-model structure on fibers is accidently discovered, which demonstrate surprising and exciting potentials in high-quality sensing of reflectivity-sensitive parameters such as temperature, concentration, humidity, pressure, stress and strain. The easy-to-be-fabricated simple novel sensing structure is first unintentionally obtained by chance when a 50fs 800nm 1kHz laser is used to make a trench that just overlaps the fiber core. The transmission loss difference of the novel structure is more than 25dB at resonance wavelengths with very high fabrication and sensing repeatability. The spacing of neighboring resonance wavelengths shortens as the trench length increases. But, the sensing mechanism remains unclear. According to the plasma model analysis developed by the authors, it may be due to reflectivity gradient within the 1-2\(\mu\)m surface formed by femtosecond laser processing, which in turn forms a gradient planar waveguide with gradient optical properties. Also, a quantum multiscale model is proposed to investigate the femtosecond pulse and fiber interaction, which consists of the first-principles calculation, molecular dynamics simulation, plasma model, and improved two-temperature model for free electron generation, electron-lattice heating and phase change mechanism. Theoretic predictions are in agreement with the experimental results in terms of threshold fluence, ablation depth, size and profile.
Multibeam Laser Processing for Nanoscale Direct-Writing

Craig Arnold
Princeton University
Department of Mechanical and Aerospace Engineering, Princeton, US

Abstract:

Near-field intensity enhancement enables laser modification of materials with feature sizes below the classical diffraction limit. Incorporating such effects into direct write techniques allows for the creation of arbitrary patterns with nanoscale resolution, but is typically limited by its serial nature, making it unsuitable for manufacturing operations. In this presentation, we review multibeam laser strategies with an eye toward increasing the throughput to enable more rapid processing. In particular, we examine the applicability of optical trapping to position near-field focusing elements near the substrates of interest. In this experiment, a CW laser is used to optically trap and position an array of liquid-dispersed microspheres near a substrate using 2-d Bessel beams. A second, pulsed laser is directed through the bead array and modifies the surface below. Both ablative and non-ablative transformations are possible and direct manipulation of the bead or substrate enables the accurate control of the feature placement. The constant optical scattering force in the propagation direction created by the Bessel beam on the microsphere is balanced by the net repulsive interaction near the surface thereby creating an equilibrium spacing between the two, regardless of large scale surface features. This effect enables nanoscale direct-write over rough or curved surfaces and the parallelization of the process using arrays of beads, each with identical spacing above the surface. In addition, the harmonic nature of the interaction potential and the liquid environment allows the microsphere to be displaced from its equilibrium position only to quickly return with large damping. This effect has important implications for ablative and chemically enhanced processes.
Multi-fluid Model of Early-stage Femtosecond Laser-induced Plasma: Progress and Limitations

Samuel Mao
Lawrence Berkeley National Laboratory, US

Abstract:

In this presentation, our on-going research to model initiation and development of femtosecond laser-induced plasma in an ambient gas will be summarized. We consider a 100 fs, 800 nm wavelength laser pulse irradiating a copper surface in 1 atm nitrogen environment. Electron and lattice temperature of laser-irradiated target were calculated based on a conventional two-temperature model, while surface electron emission and ion ejection under a built-in electric field were utilized as the boundary condition for plasma initiation. Plasma development above the target was calculated based on conservation laws for electrons, material ions, as well as atoms and ions of the ambient gas. Field-enhanced thermionic emission was found to be the dominant mechanism for the ejection of charged ions from laser-irradiated metal surface. Also presented will be our recent attempt to experimentally measure the electric field above laser-irradiated metal surface.
Opportunities for Multi-Energy Processing

Judith Todd
The Pennsylvania State University
Department of Engineering Science and Mechanics, 212 Earth-Engineering Sciences Building, University Park, PA 16802-6812
Phone: (814) 863-0771, Email: jtodd@psu.edu
Track 6

Nondestructive Evaluation of Materials
Infrastructural NDE and Structural Health Monitoring

ORGANIZERS:

Stephen Holland, Iowa State University

Halil Ceylan, Iowa State University
Developments in Testing and Health Monitoring for Civil Infrastructure Materials and Structures

John Popovics
University of Illinois
The University of Illinois at Urbana-Champaign, 205 N. Mathews MC-250, Urbana, 61801, US
Phone: 217.244.0843, Email: johnpop@illinois.edu

Invited Presentation

Abstract:

Recent research work on non-destructive testing and health monitoring for civil infrastructure materials and structures are described. Several different on-going efforts are described. First contactless sensing and imaging for concrete structures is demonstrated. Two applications are discussed: air-coupled bridge deck scanning using local seismic (vibration) measurements, and internal material reconstruction using ultrasonic tomography. The first application aims to locate and characterize shallow delamination defects within concrete bridge decks, and the second internal inclusions within concrete structural elements. Reconstructed images for both cases are presented and internal defects are identified. Next, ultrasonic reflection measurements are applied to monitor stiffening processes in early-age portland cement samples. The normal-incidence reflection factor for p-waves and s-waves are related to settlement, flocculation and percolation processes during the first hours after mixing. Reflection data are also related to cement shrinkage processes. Finally, a magnetic sensing approach to monitor in situ corrosion of metals is described. GMR magnetic field sensors are applied under ambient environment conditions to monitor the corrosion in steel and aluminum without direct electrical connection to the corroding metal. Measured magnetic field data are shown to be directly related to corrosion rate in the metals.
Detection of Corrosion Damage in Concrete Using Infrared Thermography

Glenn Washer
University of Missouri
Dept. Of Civil Engineering, E2509 Lafferre Hall, Columbia, 65211, US
Phone: (573)884-0320, Email: washerg@missouri.edu

Rilya Rumbayan
University of Missouri, Columbia, MO

Seth Nelson
University of Missouri, Columbia, MO

Abstract:

Infrared thermography has the potential to detect subsurface defects in concrete bridge elements and could be used as an effective tool to enhance the visual inspection of bridges. The technology has traditionally been applied to bridge decks, which are exposed to radiant heating from the sun. This solar loading helps develop thermal gradients in the concrete that are necessary to create thermal contrast at the surface of the concrete resulting from subsurface delaminations. The research reported herein explored the application of thermography for bridge soffits, which are not exposed to solar loading and hence must rely on ambient environmental temperature changes to induce the necessary thermal gradients through convective heat transfer. The capability of these diurnal temperature variations to induce the necessary thermal gradients in the concrete depends on not only the magnitude of temperature changes, but also the rate of temperature change and surrounding environmental conditions such as wind speed. To study these effects, experimental studies and field testing were conducted to develop recommendations regarding the necessary environmental conditions for practical application of the technology. The ability to image deterioration on the soffit areas of the bridge is significant to ensuring highway safety, as this deterioration has the potential to result in concrete falling into traffic below overpass bridges. This paper will also report on guidelines developed for this application of the technology that address the necessary environmental conditions to enable detection of damage in bridge soffit areas.
High Volume, Remote Sensing, Non-invasive & Repeatable Synchronized Multi-Discipline Bridge Investigations

Gary J. Weil
Entech Engineering, Inc.
228 Meadowbrook C. C. Way, Ballwin, 63011-1604, US
Phone: 636-207-0200, Email: gjweil@entechworld.com

Abstract:

In 1988 EnTech Engineering, Inc.’s engineers worked with ASTM to write the first bridge Remote Sensing inspection procedure, D4788. Since then it has performed over 600 bridge inspections throughout the world. Some as small as 20 feet long and others as long as 5,280 ft. In 2007, it developed its newest iteration; designated EnSITE VII Complete Bridge Investigation System, to specifically address the enormous bridge inspection needs of the 21st century. This system, with multiple sensors mounted on a helicopter, is designed to totally use remote sensing to: 1) Perform a complete structural 3D dimension investigation with accuracy of 2cm in 3D space; 2) Detect and map all previous deck pavement repairs and surface spalling; 3) Detect and map internal concrete and asphalt covered concrete deck pavement half-depth and full-depth delaminations and internal corrosion areas; 4) Develop full defect statistics in both spread sheet and image formats for easy interpretation and integration into Client GIS systems; 5) All data collection is totally repeatable, so when data collection is repeated every few years, trend analysis may be performed to determine when the most economical time to perform repairs or replacement is to be performed; 6) Data collection on up to 50 bridge structures can be performed per day or night; and because of the high volume 7) Total bridge inspection costs are up to half for data that is more accurate and timely than any other existing single or combination of techniques.

This paper will present a description of the technologies developed for this new inspection system along with a case study of it used on the I270 ‘Chain of Rocks Bridge’ 5,200-foot long x 4 lanes wide bridge over the Mississippi River.
The Use of Nondestructive Technologies to Determine Load Ratings of Existing and Historic Bridges

Donald Harvey
Atkinson-Noland & Associates
2619 Spruce St, Boulder, 80302, US
Phone: 303-444-3620, Email: dharvey@ana-usa.com

Shan Wo
Atkinson Noland & Associates, Boulder, CO

Scott Aschermann
Bridge Diagnositics, Inc., Boulder, CO

Abstract:

Structural information about existing or historic bridge structures is often needed in order to determine a load rating for present day conditions. However, creating accurate models of existing structures can be complicated by unknown subsurface conditions and deterioration. Nondestructive evaluation techniques such as ground penetrating radar (GPR) and covermeter metal detection can help determine subsurface as-built conditions. This information along with data from small probes and visual observations can be used to create a structural model of the existing bridge. An instrumented quasi-static load test can be used to measure stresses, strains, and deflections that provide response data to refine the bridge model. The model can then be used to determine the bridge rating and to analyze various load cases. Instrumentation used in testing can then be left in place or modified to create an effective structural health monitoring system. Case studies of this approach applied to different types of bridges such as cast in place concrete, prestressed concrete, concrete tee beam, and stone will be discussed along with the advantages and limitations of these methods.
Development and Application of Magnetostrictive NDE Technique for the Integrity Assessment of the Steel Strand Embedded in the Concrete Grout

Zhong Soo Lim
Research Institute of Industrial Science and Technology
San 32, Hyojadong, Namku, Pohang, 790-330, KR
Phone: +82 54 279 6661, Email: zslim@rist.re.kr

Taek ryong Seong
Research Institute of Industrial Science and Technology, Kihung, Kyunggido

Kyu sik Park
Research Institute of Industrial Science and Technology, Kihung, Kyunggido

Abstract:

The bridge is subject to a harsh environmental conditions for corrosion and breaking under varying stress. The assessment of the integrity of the prestressed multi wire steel strands embedded in the concrete grout is not an easy job until now and no particular method has been successfully developed. The magnetostrictive sensor can be used to generate the guided wave into the multi-core steel strand traveling along the axial direction. But the spatial restriction at the end section of the embedded concrete structure for multi strands layout makes it difficult to apply the magnetostrictive sensor technology therefore it has been restricted only to the stayed cable section. And the background noise from the embedded concrete structure makes it difficult to identify the flaw from the noise. We are focusing on the possibility of the application of the magnetostrictive sensor technology for the nondestructive inspection of the prestressed multi strands with multi core steel cable based on our self-developed electronics and custom software. The conventional heavy magnet is replaced by Ni-based strip using the remanent magnetic force as the bias magnetic field. The spatial restriction from the multi strand layout can be overcome by using the strip method which was developed for the pipe inspection. We has wrapped the multi-core steel strand with Ni-strip band which has been wound with Cu coil. And the band can be tightly fixed on the steel strand by a proper method. The electronics for the magnetostrictive sensor can be easily driven for the frequency scan and the frequency spectrogram is used for the defect assessment. The conventional rf waveform is susceptible to the noise from the embedded structure and a diversity of signal processing techniques has been developed to enhance the signal to noise ration. We can see directly the defect feature from the frequency spectrogram. But since the noise is still prominent we need further study to identify the defect information from the measurements. In this paper we will report the possibility of the magnetostrictive sensor technology for the defect assessment of the prestressed multi-core steel strand embedded in the concrete deck.
Monitoring of Longitudinal Stress Using Diffuse Ultrasonic Backscatter

Christopher Kube
University of Nebraska at Lincoln
317.4 W.Nebraska Hall, Lincoln, 68588, US
Phone: 3083701160, Email: ckube@huskers.unl.edu

Joseph A. Turner
University of Nebraska at Lincoln, Lincoln, NE

Goutam Ghoshal
University of Illinois at Urbana/Champaign, Urbana, IL

Abstract:

Monitoring stress in structures is very important for a variety of safety reasons. One of the challenging problems is to quantify stress non-destructively in structural components as a function of loading conditions so that accurate maintenance can be performed before failure. In this presentation, the influence of material stress on the scattering of ultrasound in polycrystalline materials is discussed. Ultrasonic backscatter results from the multitude of reflections and refractions that occur at the grain boundaries due to variation of the single-crystal elastic moduli. First, the theoretical framework is outlined in which the scattering of ultrasound is related to applied stresses through the single-crystal acoustoelastic response. The covariance of the elastic moduli is calculated in closed-form for statistically isotropic distributions of grains. The impact of applied stress on the longitudinal and shear scattering is then discussed with a focus on measurement configurations of interest. Next, experimental laboratory results are presented that highlight the dependence of scattering on applied stress. Both normal incidence (longitudinal) and oblique incidence (shear) measurements are shown to vary with applied stress, although the degree of variation is a function of several parameters. This work has led to the development of a portable device for field monitoring of structures. This device magnetically attaches to a structure and provides ultrasonic scattering data using longitudinal and shear wave scattering. Finally, future prospects and applications of this work are discussed. [Work supported by FRA]
A Performance Measure for Ceramic Armor Integrity

Derrick Rollins
Iowa State University, Department of Chemical and Biological Engineering, 1033 Sweeney Hall, Ames
Phone: 515-294-5516, Email: drollins@iastate.edu

Cory Stiehl
Iowa State University, Ames, IA

Lucas Beverlin
Iowa State University, Ames, IA

Kaylee Kotz
Iowa State University, Ames, IA

Abstract:
Composite/ceramic laminate armor, where ceramic tiles are sandwiched between fiber-reinforced composites, can provide good ballistic protection and is a good choice for some applications. Ceramics are attractive for armor applications because they are lighter weight than the traditionally used metallic materials and have other properties that make them efficient, such as low density, high hardness, high compressive strength, and high elastic modulus. Currently, there is interest in studying the effect of defects in the armor. Development of inspection approaches for both production quality assurance and detection of field induced damage has been identified as a need. Ultrasound is a powerful tool for examining the interfaces in a composite material, since the wave propagation characteristics depend strongly on the boundary conditions at the interfaces within the composite. A disbond within the composite material can slow down the speed of the sound wave, thus making it possible to detect defects within the material.

Principal Component Analysis (PCA) has been applied to thru-transmission ultrasound data taken on ceramic composite armor. PCA will help find and accentuate differences within the armor, making it easier to find defects. First, thru-transmission ultrasound data was taken and analyzed for a number of samples, some with known defects. As the ultrasound transducer moves along the surface of the sample, the signal from the sound wave is measured as it reaches the receiver, giving a time signal at each location on the sample. The transducer moves back and forth across the sample, creating a matrix of time signals. The information from each time signal is dissected into segments, and a signal characteristic, such as maximum peak value in our case, is measured within each segment, or gate. This gives a vector of measurements associated with each location on the sample. An image can be produced for each of the gate measurements, thus enabling researchers to visually inspect the sample. While a visual inspection can provide valuable information, it is often difficult to determine whether or not the inconsistencies found represent a flaw that will impact the integrity of the armor. To get around this problem, it would be desirable to have a single quantitative measure, or performance measure, that would summarize the results of the ultrasound analysis and also correlate well to the ballistics tests that were later performed on the samples. In an attempt to achieve this goal, PCA was applied to the ultrasound data for a number of samples, and a performance measure was developed from the loading information. When this performance measure was compared to the results of the ballistics tests, it was found that the performance measure correlated well to the penetration velocities found from the ballistics tests.
Abstract:

Ultrasonic testing techniques allow for the non-destructive monitoring of a variety of issues, including material cleanliness, delamination in composites, and crack propagation in many materials to name a few. Implementation of ultrasonic methods requires that metrics and standards be identified to make results from ultrasonic testing comparable across a range of samples, whether identically dimensioned or completely different designs. The work presented here focuses on bearing steel cleanliness, and shows how ultrasonic scanning can be implemented in an effective fashion for everyday production and engineering practice. Previous published work by the authors has estimated steel cleanliness qualitatively from ultrasonic C-Scan images of entire bearing cups or cones and identified ‘good’ or ‘bad’ locations in the bearing sample. The first part of the work presented here expands on this by investigating the geometric properties of the inclusions through the use of post-processing software including quantities such as the total inclusion area, total inclusion volume, and the maximum size of any individual inclusion in the inspected volume. The ultrasonic scanning includes both through thickness (bulk) material scanning and surface wave scanning results used in identifying near surface defects, which can potentially be the most detrimental due to rolling contact fatigue based on previous analysis by Murakami. In the second part of this work, the geometric inclusion information from the ultrasonic C-Scan images is used in conjunction with the Murakami model to allow predictions to be made of the bearing fatigue life. In addition, applications of these techniques are used in conjunction with extreme value methods, i.e. the extreme deviation from the median in a given probability distribution in a bulk material, and their use for predicting steel cleanliness in bulk materials. The work can be implemented to reduce the likelihood of premature failure, or as a method of steel supplier verification and quality control. These results are anticipated to impact ultrasonic non-destructive evaluation of bearing steel products. [Work supported by Amsted Rail]
Probing Acoustic Nonlinearity using Mixing Waves

Minghe Liu
Northwestern University
2145 Sheridan Road, Tech A 236, Evanston, 60208, US
Phone: 8474915164, Email: m-liu@u.northwestern.edu

Guangxin Tang
Department of Mechanical Engineering, Northwestern University, Evanston, IL

Laurence Jacobs
School of Civil and Environmental Engineering, Georgia Tech, Atlanta, GA

Jianmin Qu
Department of Civil and Environmental Engineering, Northwestern University, Evanston, IL

Abstract:

The measurement of acoustic nonlinearity parameter beta is very important in nondestructive evaluation due to its correlation to fatigue damage in metallic materials. In this investigation, we demonstrate the possibility of using collinear mixing waves to measure material nonlinearity beta. Compare to conventional nonlinear ultrasonic harmonic generation technique, this method is potentially more interesting for its lower sensitivity to background nonlinearity and higher spatial sensitivity to material nonlinearity, which could further lead identifying the source location of nonlinearity possible. In this paper, a longitudinal wave and a shear wave were used as the incident waves. Under certain conditions, the nonlinear interaction of incident waves generates a third shear resonance wave with comparatively high amplitude at the difference frequency. The relationship between the resonance wave amplitude and material nonlinearity was obtained analytically through asymptotic solution of nonlinear wave equation. Numerical simulations were also performed using a finite difference method to predict the generation of resonance shear wave, and it was experimentally measured on samples made of aluminum and steel, respectively. Results from numerical simulations and experimental measurement show good agreement and the measured beta values are also consistent with those given in the literature.
Probing Inhomogeneous Media

ORGANIZERS:

Stephen Holland, Iowa State University

Lester Schmerr, Iowa State University
Ultrasonics of Periodic Structures

Nico Declercq
Georgia Tech Lorraine
Office 224, GT-Lorraine Building, 2 rue Marconi, Metz-Technopole, 57070, France
Email: nico.declercq@me.gatech.edu

Invited Presentation

Abstract:
Wave Propagation in Elastic Media with Non-uniform Quadratic Nonlinearity

Guangxin Tang
Department of Mechanical Engineering, Northwestern University, Evanston, IL
2145 Sheridan Road, Tech A156, Mechanical Engineering, Evanston, 60208, US
Phone: 8474915164, Email: g-tang@u.northwestern.edu

Laurence J. Jacobs
School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA

Jianmin Qu
Department of Mechanical Engineering, Department of Civil and Environmental Engineering, Northwestern University, Evanston, IL

Abstract:
The propagation of the one-dimensional fundamental sinusoidal wave in elastic media with non-uniform quadratic nonlinearity is considered. Second harmonics will be generated when a fundamental wave interacts with material nonlinearity. The explicit results of second harmonic generation are obtained for a half-space where the displacement is prescribed on the surface of the half-space. It is found that the backscattering second harmonic will be generated because of the heterogeneous nonlinearity. The combination of the forward and backward second harmonic will generate a standing wave at the surface of the half-space in steady-state wave motion. Another problem considered here is the reflection and transmission through a finite nonlinear layer with heterogeneous quadratic nonlinearity embedded in an otherwise linear medium with infinite extent. The results show that the transmission of second harmonic is simply proportional to the spatial average of the nonlinearity across the nonlinear layer and does not depend on the distribution of the nonlinearity. On the other hand, the reflected second harmonic depends on a weighted average of the nonlinearity and the weight function is related to the spatial distribution of nonlinearity, which makes the reflection of second harmonic depends on the spatial distribution of the nonlinearity. Finally, the paper ends up with some discussion about the case when the nonlinearity distribution is a stochastic function.
Nanoscale Interfacial Probing of Rubbery Interphase In Polymer Grafted SiO2/epoxy Nanocomposites

Jianing Gao
Rensselaer Polytechnic Institute
RM233 MRC RPI, Troy, 12180, US
Phone: 518-698-3288, Email: gloragster@gmail.com

Abstract:

Silica nanoparticles with block copolymers grafted from the surface were used to improve the ductility of epoxy. The grafted copolymer consists of an inner block of hexylmethacrylate monomers (HMA) and an outer block of mixed hexylmethacrylate monomers and glycidylmethacrylate monomers (GMA). The inner block has a glass transition temperature below room temperature, and thus works as a rubbery region between the particles and the matrix. The outer block consists of poly-GMA, which has epoxy side groups at the end and can make the grafted copolymer layer compatible and reactive with the epoxy matrix. Preliminary result showed that the strain-to-break value from the tensile test of the neat epoxy was doubled by adding less than 0.1 wt% of highly grafted (0.7 chains/nm²) copolymer-silica, consisting of a rubbery inner block with a molar mass of 30,000 g/mol and of an epoxy compatible block with a molar mass of 68,000 g/mol. No decrease in the Young's modulus and tensile strength was observed in the nanocomposites compared to the neat epoxy. It is hypothesized that the interphase between the nanoparticles and the matrix promote plastic deformation in the matrix, similar to rubber inclusions. To study the mechanical properties at the interphase, samples were microtomed followed by FIB (focused ion beam) etching to ensure reproducible and consistent data. NanoDMA and modulus mapping using a North Star 40nm cube corner tip was applied to measure the viscoelastic properties at the interfaces. Local variations in glass transition temperatures were investigated by performing nanoDMA frequency sweeps at elevated temperatures. AFM tapping mode with tip of 1 nm radius was used to resolve the thickness of the interfaces. AFM force modulation with tip of 10 nm radius was performed to measure the hardness at the interfaces.
Fundamental Limits of Active Thermography

Ricky Reusser
Iowa State University Center for NDE
111 Applied Sciences Complex II, 1915 Scholl Road, Ames, 50011-3042, US
Phone: 608-216-6197, Email: rreusser@iastate.edu

Stephen D. Holland
Iowa State University Center for NDE, Ames, IA

Abstract:
Active thermography is an NDE technique that uses the flow of heat resulting from energy input to find flaws, material properties, and internal discontinuities. Probing deeply is difficult because of the diffusive nature of heat. This presentation focuses on fundamental limits of active thermography methods that rely on direct thermal excitation. The excitation may be a pulse or flash, a step, or even cyclic or swept-frequency heating. All of these techniques probe the same physics and are subject to the same fundamental limits imposed by infrared camera sensitivity and convective losses. We discuss these limits in the context of different forms of excitation, and how they impact the penetration depth and detection capability of each method.
Laser Ultrasonic Thermometry for In-Situ Characterization of Semiconductor Material

Steve Suh
Texas A&M University
Mechanical Engineering Dept., 3123TAMU, College Station, 77843, US
Phone: 979-845-1417, Email: ssuh@tamu.edu

Abstract:

Laser Induced Stress Wave Thermometry (LISWT) is a non-contact thermal diagnostic technique for the rapid thermal annealing of single crystalline silicon wafers using laser-generated, ultrasonic, Lamb waveguide modes. The required knowledge base for establishing LISWT as a viable alternative to current pyrometric and ellipsometric techniques for temperature measurement up to 1,000°C with ±1°C resolution is presented. A comprehensive elasto-viscoplastic wave model is explored for correlating wave characteristics from being elastic to viscoplastic with annealing temperatures ranging from room temperature to exceeding 1,000°C. The model is a system of 9 coupled first-order hyperbolic equations formulated based on the kinematics of elasto-plastic deformation, conversion of linear momentum and a temperature-dependent viscoplastic constitutive law for single crystalline silicon material. Physical validation is performed using a Thermo-Acousto-Photonic Nondestructive Evaluation (TAP-NDE) setup on wafers of different thicknesses to determine the maximum possible resolution towards temperature sensitivity and to demonstrate the ability to differentiate between wafers of different deposition layer thickness at temperatures up to 600°C. Temperature resolution is demonstrated for ±10°C resolution and for ±5°C resolution; while thickness differentiation is carried out with wafers carrying 4000Å and 8000Å of aluminum deposition layer. The group velocity of the frequency components and their corresponding changes with respect to temperature for different thicknesses are investigated. It is shown both theoretically and experimentally that there exists a correlation for differentiating thickness variation as a function of varying group velocities for different frequencies at different temperatures, thus establishing the groundwork for the optically generated Lamb wave thermometric methodology for silicon wafer.
Depth Profiling of Temperature in Heated Materials Using Ultrasonic Technique Combined with Finite Different Calculation

Ikuo Ihara
Nagaoka University of Technology
1603-1 Kamitomioka, Nagaoka, 940-2188, JP
Phone: +81-258-47-9720, Email: ihara@mech.nagaokaut.ac.jp

Manabu Takahashi
Sendai National College of Technology, Natori, Miyagi

Abstract:

In the fields of materials science and processing, there are high demands for monitoring internal temperature and its distribution in a heated material. This is basically because temperature is one of the most important factors that dominate the material properties and behavior. In particular, it is strongly required to monitor the temperature profile and its transient variation of the material being processed at high temperatures because such temperature profile during the process often influences the quality and productivity of final products.

In this work, a new ultrasonic method for monitoring temperature gradient of a material being heated or cooled is presented. The method provides non-invasive monitoring of internal temperature gradient of materials during heating or cooling. The principle of the method is based on the temperature dependence of the velocity of ultrasonic wave propagating through a material. An effective analysis method coupled with a finite difference calculation is developed to determine one-dimensional temperature distributions along the direction of ultrasound propagation in material. The advantage of the proposed method is that no boundary condition at the heating or the cooling surface is needed. To verify the practical feasibility of the method, some experiments have been demonstrated for industrial materials such as steel, aluminum and ceramics. A single side of a specimen of 30 mm thickness is heated up to 200 degree C by contacting with a heater and subsequently cooled down by contacting with water or ice. Ultrasonic pulse-echo measurements are then performed for the specimen and the measured transit time of ultrasound across the specimen is used for the analysis to determine temperature gradient in the specimen. The temperature gradient and its transient variation determined by the ultrasonic method almost agree with those obtained using thermocouples or an infrared radiation camera. It has been shown that the ultrasonic method can monitor the transient variation in temperature gradient during heating and cooling in which conventional thermocouples may not be available due to its relatively slow time response. Furthermore, the ultrasonic method is applied to a metal casting process to monitor both internal temperature gradients of a mold and solidified metal during the casting. It is demonstrated that the ultrasonic method has a high potential for on-line or in-situ monitoring of temperature gradients in heated materials.
Physics-based Analysis of Infrared Images of Pulsed Buried Heat Sources

Steve Holland
Iowa State University
2331 Howe Hall, Iowa State University, Ames, 50011, US
Phone: 515-294-8659, Email: sdh4@iastate.edu

Abstract:

Modern infrared thermal cameras allow real time quantitative imaging of heat flow. Vibrothermography is a method of nondestructive evaluation that involves finding cracks from the heat they give off in response to vibration. Finding cracks in vibrothermography requires identifying and localizing pulsed surface and subsurface heat sources from a time-series of infrared images. We present an algorithm that uses a-priori knowledge of heat conduction to constrain curve fits of the temperature-time profile of the heating at each image pixel. The curve fitting process simultaneously compresses the time-series into a single image, improves sensitivity to faint indications, and estimates the source depth or distance. The critical parameters of fit quality, heating amplitude, and distance are combined into a single hybrid false-color image. This algorithm provides a means to transform the complicated sequence of images from a vibrothermography experiment directly into a single, easy to interpret summary. Examples of how this processing has the potential to improve industrial practice will be discussed.
Identification of Correlative Excitations in High Frequency Based on SEA

Shilin Xie
Xi'an Jiaotong University
MOE Key Laboratory for Strength and Vibration, Xi'an, 710049, CN
Phone: 86-29-82668483, Email: slxie@mail.xjtu.edu.cn

Xinong Zhang
MOE Key Laboratory for Strength and Vibration, Xi'an Jiaotong University, Xi'an, Shaanxi Prov.

Abstract:

High frequency excitations are difficult to be identified using the existing identification methods because the dynamic models of structural systems in high frequency domain are generally of poor accuracy. It is known that Statistical Energy Analysis (SEA) theory provides a powerful tool for the response prediction of system subjected to high frequency excitations. This is because that SEA model of system can produce an satisfactory description on dynamic behaviour in high frequency.

An identification method of high frequency excitation based on SEA is proposed in the paper. Under the frame of SEA theory, the input power values of high frequency excitations can be resolved from the SEA model of structural system according to the measured energies of subsystems. Moreover, the power spectrums of high frequency excitations can also be determined from the corresponding input power values. The above identification methodology is straightforward when the system is conservative, weakly coupling and subjected to a group of uncorrelated excitations.

However, it is frequently encountered in practical situations that the excitations applied on subsystems are correlated with each other. The classical statistical energy analysis approach is unapplicable in these cases. As a result, the present identification method has to take the effects of correlative excitations into account. On the basis of power flow analysis between two coupling oscillators subjected to two correlative excitations, the power balance equation of system under correlative excitations is derived in the paper. It is shown from the equation that the input power terms of subsystems in the case of correlative excitations are different from those in the case of uncorrelated excitations, while the left side of equation remains unchanged. Consequently, the real input power can be obtained from the given formulas when the above identification method is applied.

To validate the presented identification method, an experimental rig was built, which contains two rectangular plates jointed together through bolts. The SEA model of experimental system is firstly set up using power injection method. The average transfer mobility between two subsystems is also determined experimentally. Here, two proportionally correlative excitations are exerted on two subsystems respectively for simplicity. The real input powers are then identified based on measured subsystem energies using the modified input power expressions. The identified input powers are compared with measured ones obtained by two impedance heads. The results show that the former has a good agreement with the latter. The work provides a feasible way for identification of correlative excitations in high frequency.
Acoustic Characteristics Measurements on Nanoscale Surface with Ultrasonic AFM

Ik Keun Park
Seoul National Univ. of Technology
172 Gongneungdong, Nowon-gu, Seoul, 139-743, KR
Phone: 2-970-6332, Email: ikpark@snut.ac.kr

Chiaki Miyasaka
Penn State Univ., State College, PA

Abstract:

Nondestructive surface imaging of elastic characteristic and mechanical property have been studied on nanoscale surface with ultrasonic AFM. Resonance-frequency variation of cantilever is theoretically analyzed with respect to contact mechanics as well as experimentally measured. The contact-resonance frequency calculated theoretically using the spring-mass and Herzian model in accordance with the resonance frequency of UAFM cantilever measured experimentally. Consequently, the topography and amplitude images could obtain successfully and the elastic characteristic at the nanoscale surface was evaluated qualitatively by amplitude signals.