

Final Report

Workshop on

“New frontiers of solid mechanics – from earthquakes to single molecules”

held at Providence, Rhode Island from June 1 to June 3 of 2011

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Supported by

U. S. National Science Foundation

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Summary

This is the final report of the NSF project of gathering and sharing information on possible Future Directions in Mechanics Research: “New Frontiers of Solid Mechanics - From Earthquakes to Single Molecules.” For this effort a workshop was organized and held at the Renaissance Providence Downtown Hotel, Providence, Rhode Island during June, 1 - 3, 2011. It was planned and organized with great help of the advisory committee composed of J. D. Achenbach of Northwestern University, R. J. Clifton of Brown University, J. W. Hutchinson of Harvard University, W. D. Nix of Stanford University, J. R. Rice of Harvard University and J. R. Willis of Cambridge University. In addition, the workshop leveraged the opportunities of reviewing past and ongoing research on solid mechanics by concurrently co-organizing the Freund Symposium supported by separate private organizations. Approximately seventy people of young as well as established researchers participated in the workshop, including graduate students and 51 registered senior researchers representing a variety of disciplines in engineering and science. As an outcome, many new ideas on possible future directions in mechanics research were shared across traditional disciplinary boundaries. The workshop was held successfully and has reached a conclusion that research is actively carried out, in the mechanics community, on solving problems in emerging new interdisciplinary fields as well as on new insights in unsolved challenging problems of traditional areas for both Intellectual merits and broad impacts. It is also noticed that hybrid approaches of experiments coupled with or guided by large scale computation is highly effective in discovering rich phenomena at various length and time scales. Some suggestions on the directions for research and education are described in this report.

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INTRODUCTION

A range of interesting lines of interdisciplinary research and education empowered by mechanics concepts has emerged over the past two to three decades in conjunction with modern technologies such as bio, information, nano, energy/environment technologies and other branches of engineering science such as geo-science and large scale computational science, etc. In particular, researchers have focused attention on bridging understandings in mechanical behavior of materials at broad length and time scales. As mechanics concepts are highly effective in understanding mechanical phenomena at broad scales, such conceptual tools have been applied not only to understand and describe scale dependent deformation processes but also to solve problems ranging from earthquakes to single molecules.

Regarding the large length scale phenomena, advancements in modeling and experiments have been steadily made in the field of geo-science including earthquake rupture dynamics, mechanics of glacial flow and ice fracture, and dynamics of tsunami, etc. which have strong relevance in mitigation of natural disasters. With respect to small length scale phenomena, advancement of computational science has provided the means to simulate materials on an atom-by-atom basis, while advanced experimental instrumentations have identified mechanisms for hard as well as soft material deformation and failure processes which are activated thermally or by stress.

These developments have an almost immediate impact on technology, and serious research efforts have been made, in engineering and science communities, in order to exploit them for various applications. In order to sustain and support these efforts, it is important for the mechanics community to become better informed on these developments, to coordinate efforts aimed at addressing the very challenging research problems which require mechanics input for their solutions, and to educate young people who can sustain and advance these important areas in the years ahead. Therefore, we have timely organized a workshop to gather and share information on possible Future Directions in Mechanics Research: “New Frontiers of Solid Mechanics - From Earthquakes to Single Molecules.”

The workshop was organized and held at the Renaissance Providence Downtown Hotel, Providence, Rhode Island during June, 1 - 3, 2011. The organizing committee composed of Huajian Gao and Kyung-Suk Kim of Brown University, and Ares Rosakis and Guruswami Ravichandran of California Institute of Technology planned and organized the workshop with help of the advisory committee. The workshop was concurrently co-organized with the Freund Symposium to leverage the opportunities of reviewing past and ongoing research on solid mechanics in the mechanics community. We invited representative active researchers who are currently working on solving problems in emerging new interdisciplinary fields or on new insights in unsolved challenging problems of traditional areas. The invitees came not only from various universities over the whole U.S. but also from abroad - Asia and Europe. The session titles and the topics of the presentations are listed as follows:

Dynamics of Solids in Broad Scales

- Earthquake rupture dynamics with strong thermal weakening
- The seismological wind tunnel: The unique ground shaking of supershear earthquakes and its effects on buildings
- Effective constitutive relations for waves in composites

Biomechanics in Broad Scales

- Tu(r)ning weakness to strength
- The greening of biology
- Understanding the mechanics of cells and biomolecules

Mechanics of Energy Materials

- Models for lithium-ion battery performance and damage
- Mechanics of quantum dots for intermediate band solar cells

New Insights in Nonlinear Mechanics of Solids

- Thermo-mechanics of shape-memory polymers
- Cavitation instabilities in soft solids: A defect-growth theory and applications to elastomers
- Chemomechanics of cell-material interactions: Pulling it all together

New Insights in Micromechanics of Structural Instabilities

- From wrinkles to creases in elastomers: The extreme imperfection-sensitivity of wrinkling
- Soft materials: Functionality through instabilities & deformations

Micromechanics of Stretchable Functional Materials

- Giant voltage-induced deformation in dielectric elastomers: Theory and experiment
- Mechanics of stretchable electronics

Advanced Molecular Mechanics of Solids

- Compatibility and hysteresis
- Brownian motion and elasticity in biological filaments & networks
- Interatomic potentials, Forces and the uniqueness of stress

New Insights in Experimental Dynamics of Solids

- Dynamic ductile failure in polycrystalline materials
- Converging shocks in solids using Mach waves

Mechanics of Nanostructures

- Deformation analysis of hierarchical carbon nanotube bundles under uniaxial compression
- Combinatorial nanocalorimetry of thin metallic films

As listed above, the area of active research ranges over mechanics problems in broad scales in diverse fields – geomechanics, biomechanics, mechanics of energy materials, mechanics of nanostructures such as nanotubes, nanowires and graphene, etc., and nano- and micro-mechanics of coupled multi-physical and multi-scale phenomena including molecular mechanics. The issues include dynamics of solids, nonlinear mechanics of soft materials and phase transformations, structural instabilities, micromechanics of stretchable functional materials, experimental dynamics of solids. Methodologies cover mathematical formalism for the description of molecular, thermomechanical or biomechanical motions in solids, large scale computational algorithms, and instrumentations for fast or small length scale motions.

The outcome of the workshop is described in the following sections; the Workshop Program, Participants and Abstracts are presented in the Appendices A, B and C correspondingly.

FINDINGS

Modeling Aspects

Three major efforts in modeling have been noticed. The first is to advance rigorous mathematical modeling, which include formulation of nonlinear dynamic constitutive relations of heterogeneous media, identification of mathematical invariance on incompatibilities at phase boundaries, mathematical modeling of rupture dynamics caused by thermal softening, mathematical modeling of large deformation instabilities in soft materials including imperfection sensitivities, uniqueness of the projection of atomistic force field to continuum stress field and mathematical formulation of statistical mechanics of Brownian motions under structural constraints, etc.

The second is the advancement of computational simulation methodologies. In this category, the advancement of simulation technologies will improve the probability of observing possible new phenomena in various length scales. It complements difficulties in certain accessibility of experimental observations and measurements. Especially for small length scale problems, much of the effort is focused on expanding the capabilities of the simulation for a large number of degree of freedom and for a long-time behavior of physical processes. One of the strategies in this field is to reduce redundant degree of freedom, in turn, to develop adaptive resolution refinement techniques. Another strategy is to advance parallel processing technology by identifying re-directed or reduced coordinate systems in the degree-of freedom space, that provide spatially and temporally independent physical processes.

The third is advancement of modeling technology focused on representative- physical-mechanism identifications at different length and time scales. This field has a great potential in developing broad scale-bridging technologies. Research in this area requires advancement of technologies in underlying-mechanism-aware field descriptions and system-integration-aware mechanism descriptions. Collective behavior of atoms, molecules and defects with short-range interactions in nano-meter scale leads to a transition from short-range-interaction cooperative processes to long-range-interaction cooperative processes. Technological advancement in this area is essential in developing reliable control of nano- and micro-structural evolution of materials to provide principles of self-organizing, (self-replicating and self-correcting) processes at various length and time scales.

Experimental Aspects

There are major experimental challenges in small length scale experiments, dynamic process experiments, multi-physical process (e.g. battery or bio) experiments and large deformation instability experiments. For example, experimental efforts in mechanics of materials at small length scales are focused on observing and characterizing material behavior at the nano-meter scale to provide understanding and quantitative control of manufacturing processes of nano- and micro-structures. Two different types of experimental approaches have been observed in characterizing of nano- and micro-mechanical behavior of materials. One is the load – response type experiment, which includes nano-indentation, nano-probe tribology experiments, optical-tweezers experiments for molecular deformation experiments, and deformation and fracture testing of MEMS devices. The other one is the field-based experiment. This includes material-behavior characterization based on microscopy and nano-metrology, such as HRTEM coupled with image processing metrology or interferometry, scanning probe imaging and deformation metrology or interferometry, and various spectroscopies such as fluorescence-based stress measurement and surface roughness evolution spectroscopy.

In any case, the experimental techniques need substantial improvement of resolution in the scale of length, strain, force, and time. Many innovative experimental techniques must be developed based on proper operating deformation-mechanisms at various length and time scale instead of simple reduction of conventional mean-field-concept testing methods. For example, nano-indentor testing needs tremendous modeling support if used as a material characterizing experiment; continuum mean-field approximation breaks down quite often in the nano-meter length scale. Challenging experiments include HRTEM coupled with in-situ MEMS testing, nano-tribology testing of scale-bridging experiments and roughness evolution of solid surfaces and interfaces, bio-molecular testing of high spatial and temporal resolution.

RECOMMENDATIONS

Research

The success of the field can be achieved by advancing capabilities of modeling and experimentation in various length and time scales. In modeling, it is necessary to develop reliable computational schemes for the study of coupled processes involving multiple length and/or time scales which are mathematically rigorous. In experimentation and laboratory observation, diverse experimental techniques must be developed which go beyond the simple size or time scaling of present standard testing techniques; new test methods must be developed which lend themselves to the evaluation of material behavior at the specific length and time scales. Technologically rich problems must be actively researched by studying the broad scale mechanics of coupled phenomena. For these tasks, cross-disciplinary research and education must be continuously cultivated.

It is further noticed that hybrid approaches of experiments coupled with or guided by large scale computation will be highly effective in discovering rich phenomena at various length and time scales, and use of such hybrid method is strongly recommended.

Education

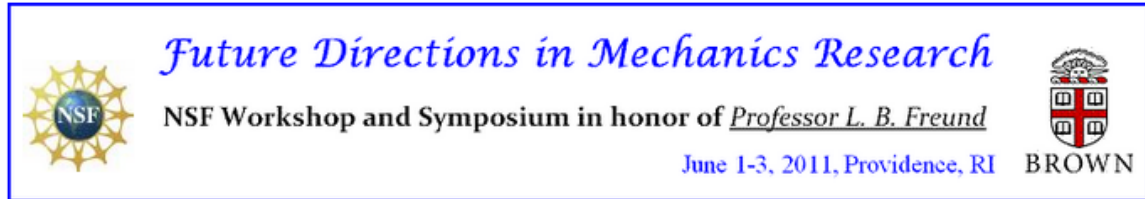
A critically important aspect of the commitment required for broad impact is in education, that is, the preparation of young people for contributing roles in an area of research that will be changing continuously. This will require that decisions on content of graduate programs in mechanics within universities should be guided to some extent by broad national research needs, and that the tools of mechanics which result from research must be made more readily accessible to those nonspecialists who can benefit from their application.

Cross-disciplinary education characterized by neighbor-field-aware in-depth education is required to handle broad-scale multi-physics problems.

ACKNOWLEDGMENT

It is gratefully acknowledged the participation of Workshop Administrators – Patricia Capece, Angely Saldana, Rich Minogue, Estelle Lang, and Help Desk Students – Mazen Diab, Chien-Kai Wang, Hsiao-Mei Wu and Dibakar Datta.

Appendix A. Workshop Program



Introduction

Welcome to the NSF workshop and Freund symposium to be held near Brown University campus, Renaissance Providence Downtown Hotel, to celebrate pioneering contributions of Professor L. B. Freund on mechanics research. The theme of the NSF workshop and Freund symposium is “New Frontiers of Solid Mechanics - From Earthquakes to Single Molecules.”

Organization

Advisory Board

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J. W. Hutchinson	hutchinson@husm.harvard.edu
W. D. Nix	nix@stanford.edu
J. R. Rice	rice@seas.harvard.edu
J. R. Willis	j.r.willis@damtp.cam.ac.uk

Organizing Committee

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Kyung-Suk Kim	kyung-suk_kim@brown.edu
G. Ravichandran	ravi@caltech.edu
Ares J. Rosakis	rosakis@aero.caltech.edu

Symposium Schedule

Wednesday, June 1: Renaissance Providence Downtown Hotel

05:00-07:00pm: Reception

Thursday, June 2: Renaissance Providence Downtown Hotel

07:00-08:00 am: Continental Breakfast

08:00-08:30 am: Opening Ceremony

08:30-10:00 am: Session 1 - Dynamics of Solids in Broad Scales
(Chair: M. Zhou, A. Bower)

J. R. Rice: Earthquake rupture dynamics with strong thermal weakening
A. J. Rosakis: The seismological wind tunnel: The unique ground shaking of
supershear earthquakes and its effects on buildings
J. R. Willis: Effective constitutive relations for waves in composites

10:00-10:30 am: Coffee Break/Posters

10:30-12:00 pm: Session 2 - Biomechanics in Broad Scales
(Chair: Y. Lin, J. Tang)

M. J. Buehler: Tu(r)ning weakness to strength
R. Phillips: The greening of biology
G. Bao: Understanding the mechanics of cells and biomolecules

12:00-01:30 pm: Lunch/Posters

01:30-02:30 pm: Session 3 - Mechanics of Energy Materials
(Chair: J. W. Kysar, W. A. Curtin)

R. M. McMeeking: Models for lithium-ion battery performance and damage
H. Johnson: Mechanics of quantum dots for intermediate band solar cells

02:30-03:30 pm: Panel Discussion - Frontiers in mechanics derived from applications in broad scales
J. L. Bassani
K. J. Hsia
B. W. Sheldon

03:30-04:00 pm: Coffee Break/Posters

04:00-05:30 pm: Session 4 - New Insights in Nonlinear Mechanics of Solids
(Chair: Y. W. Zhang, P. Guduru)

L. Anand: Thermo-mechanics of shape-memory polymers
O. Lopez - Pames: Cavitation instabilities in soft solids:
A defect-growth theory and applications to elastomers
K. Van Vliet: Chemomechanics of cell-material interactions:
Pulling it all together (This talk is continued from Session 2.)

05:30-07:00 pm: Posters/Cocktail Reception

07:00-09:00 pm: Banquet, Renaissance Providence Downtown Hotel

Friday, June 3: Renaissance Providence Downtown Hotel

07:00-08:00 am: Continental Breakfast/Posters

08:00-09:00 am: Session 5 - New Insights in Micromechanics of Structural Instabilities
(Chair: S. Mandre, E. Chason)

J. Hutchinson: From wrinkles to creases in elastomers: The extreme
imperfection-sensitivity of wrinkling

K. Bertoldi: Soft materials: Functionality through instabilities & deformations

09:00-10:00 am: Session 6 - Micromechanics of Stretchable Functional Materials
(Chair: R. Huang, C. Franck)

Z. Suo: Giant voltage-induced deformation in dielectric elastomers: Theory and experiment

Y. Huang: Mechanics of stretchable electronics

10:00-10:30 am: Coffee Break/Posters

10:30-12:00 pm: Session 7 - Advanced Molecular Mechanics of Solids
(Chair: J. Freund, V. B. Shenoy)

R. James: Compatibility and hysteresis

P. Purohit: Brownian motion and elasticity in biological filaments & networks

N. C. Admal and E. B. Tadmor: Interatomic potentials, Forces and the uniqueness of stress

12:00-01:30 pm: Lunch/Posters

01:30-02:30 pm: Session 8 - New Insights in Experimental Dynamics of Solids
(Chair: X. Markenscoff, J. Blume)

K. Ravi-Chandar: Dynamic ductile failure in polycrystalline materials

G. Ravichandran: Converging shocks in solids using Mach waves

02:30-03:30 pm: Session 9 - Mechanics of Nanostructures
(Chair: N. Sottos, S. Kumar)

S. B. Hutchens, A. Needleman, and J. Greer: Deformation analysis of hierarchical carbon nanotube
bundles under uniaxial compression

J. J. Vlassak: Combinatorial nanocalorimetry of thin metallic films

03:30-04:00 pm: Coffee Break/Posters

04:00-05:00 pm: Panel Discussion - Frontiers in mechanics derived from response mechanisms of
materials

D. M. Parks

T. Nakamura

Y. Gao

05:00-05:30 pm: Closing Lecture by L. B. Freund (Chair: H. Gao)

07:00-09:00 pm: Closing Lobster Dinner, DeWolf Tavern, Bristol, RI

Symposium Brochure

L. B. Freund

National Academy of Science
Election Year: 1997

NAS Citation

"Freund's contributions have shaped the field of dynamic fracture mechanics. His mathematical techniques and physical insight have been instrumental in bringing the field to its current state of maturity. In the area of microelectronic devices he has made pioneering contributions to the mechanics of dislocations and stress effects in thin films."

Dynamics Fracture Mechanics

is the first book to present a comprehensive survey of research in the field, much of which has been carried out by the author and others over the past twenty years.

Thin Film Materials

coauthored with Subra Suresh is the book to provide comprehensive coverage of the major issues of stress in thin films and its consequences, including defect formation and surface evolution.

"*Dynamic Fracture Mechanics*" was written just before Ben's 50th birthday, while "*Thin Film Materials*" was written around his 60th birthday. Continuing on this trend, we anticipate another monograph in molecular and cellular biomechanics from Ben for his 70th birthday.

Workshop and Symposium Schedule

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5 Avenue of the Arts, Providence, RI 02903 (tel: 401-919-5000)

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Future Directions in Mechanics Research

NSF Workshop and Symposium in honor of Professor L. B. Freund

June 1-3, 2011, Providence, RI BROWN



Advisory Board

J. D. Achenbach Northwestern
R. J. Clifton Brown
J. W. Hutchinson Harvard
W. D. Nix Stanford
J. R. Rice Harvard
J. R. Willis Cambridge

Organizing Committee

Huajian Gao Brown
Kyung-Suk Kim Brown
G. Ravichandran Caltech
A. J. Rosakis Caltech

Symposium Administrators

Help Desk

Mazen Diab Brown
Chien-Kai Wang Brown
Hsiao-Mei Wu Brown
Dibakar Datta Brown
Patricia Capece Brown
Angely Saldana Brown
Rich Minogue Brown
Estelle Lang Brown
Cheryl Carvalho Brown

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T. Nakamura

Y. Gao

05:00-05:30 pm: Closing Lecture by L. B. Freund (Chair: H. Gao)

07:00-09:00 pm: Closing Lobster Dinner, DeWolf Tavern, 259 Thames Street, Bristol, RI 02809 (tel: 401-254-2005)

Appendix B. [Participants](#)

Registered Attendees

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50	John	Hutchinson	Harvard University	hutchinson@husm.harvard.edu
51	James	Rice	Harvard University	rice@seas.harvard.edu

Poster Presenters

Board No.	Name	Affiliation
1	Nikhil Chandra Admal	University of Minnesota Minneapolis
	<i>Interatomic Potentials Forces and the Uniqueness of Stress</i>	
2	Eric Buchovecky	Brown University
	<i>Numerical Modeling of Stress Generation and Whisker Growth in Thin Sn Films on Cu</i>	
3	Peng Chen	Brown University
	<i>Strain Stiffening Induced by Molecular Motors in Active Crosslinked Biopolymer Networks</i>	
4	Huck Beng Chew	Brown University
	<i>Nanoplasticity in FCC Metals during Ion Bombardment</i>	
5	Viswanath Chinthapenta	Brown University
	<i>Numerical Simulations of Intergranular Strain Evolution during Deformation of Nanocrystalline Materials</i>	
6	Michael Chon	Brown University
	<i>Mechanics of Energy Storage Materials</i>	
7	David E. Cipoletti	Brown University
	<i>A Microstructure based Model of the Deformation Mechanisms and Flow Stress during Elevated Temperature Straining of a Magnesium Alloy</i>	

- 8 Mazen Diab Brown University
Folding Wrinkles of a Stiff Thin Layer on a Soft Substrate
- 9 Alexander K Epstein Harvard University
Bioinspired Actuable Surface Nanostructures with Arbitrary Geometry and Stiffness
- 10 Yanfei Gao University of Tennessee/Oak Ridge National Laboratory
Scale and Stochastic Effects on Incipient Plasticity in Confined Volumes at Small Scales
- 11 Rassin Grantab Brown University
Anomalous Strength Characteristics of Tilt Grain Boundaries in Graphene
- 12 Julia R. Greer California Institute of Technology
General Activity of Greer Group at CalTech
- 13 Tong Jiao Brown University
High Frequency Measurements of Viscoelastic Properties to Qualify Human Tissue Engineered Heart Valves
- 14 Sung Hoon Kang Harvard University
Self-assembly of Nanofibers with Controlled Hierarchy & Shape by Adhesion Mediated Elastocapillary
- 15 A. Lazarus Massachusetts Institute of Technology
Geometry Induced Rigidity in Pressurized Elastic Shells
- 16 Qunyang Li University of Pennsylvania
On the Origins of Rate and State Friction: Frictional Ageing of Rock Materials Explored via Single-asperity Experiments
- 17 Xiaoyan Li Brown University
Dislocation Nucleation Govern Softening and Maximum Strength in Nanotwinned Metals
- 18 Yinfeng Li Brown University
Computer Simulation of Molecule-coated Nanoparticles Translocation across Lipid Membrane
- 19 Bin Liu Brown University
Force-free Swimming of a Model Helical Flagellum in Viscoelastic Fluids
- 20 Thao D Nguyen Johns Hopkins University
The Thermoviscoelastic Mechanisms of Shape Memory Polymers
- 21 Gregory J. Rizza Brown University
Plane Deformations Generating a Prescribed Finite Rotation Field

- 22 Jongmin Shim Harvard University
Buckling-induced Pattern Transformation of Structured Elastic Shells
- 23 Pavel Trapper Harvard University
Confined Cylinders: from Sinusoidal to Helical Buckling
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Poster Awards

<i>First Place</i>	(15) A. Lazarus	Massachusetts Institute of Technology
<i>Second Place</i>	(2) Eric Buchovecky	Brown University
<i>Second Place</i>	(14) Sung Hoon Kang	Harvard University
<i>Third Place</i>	(6) Michael Chon	Brown University
<i>Third Place</i>	(16) Qunyang Li	University of Pennsylvania
<i>Third Place</i>	(26) Lifeng Wang	Massachusetts Institute of Technology



From left to right: V. B. Shenoy, R. J. Clifton, G. Ravichandran, A. J. Rosakis, L. B. Freund, H. Gao, K.-S. Kim, A. F. Bower



Appendix C. [Abstracts](#)

Earthquake rupture dynamics with strong thermal weakening

James R. Rice

School of Engineering and Applied Science, and
Department of Earth and Planetary Sciences,
Harvard University, Cambridge, MA

Field observations of maturely slipped faults show that despite a generally broad zone of damage by cracking and granulation, large shear deformation, and therefore heat generation, in individual earthquakes takes place with extreme localization to a zone of order 1 mm or less width within a finely granulated fault core. Relevant fault weakening processes during large crustal events are therefore likely to be thermal, although a constraint to be met is that melting within fault zones seems relatively rare, at least in the upper crust. Further, given the porosity of damage zones, it seems reasonable to assume groundwater presence.

It is suggested that two primary dynamic weakening mechanisms, expected to be active in at least the early phases of nearly all crustal events, are (1) flash heating at highly stressed frictional micro-contacts, and (2) thermal pressurization of native fault-zone pore fluid. Other weakening processes, prior to bulk melting, may also become active at large enough temperature rise. E.g., endothermic decomposition reactions may occur which release pore fluid at high pore pressure as CO₂ from carbonate rocks or H₂O from clays or serpentines, and leave nanometer scale grains of solid product which have as yet little- understood weakening features of their own.

Spontaneous dynamic rupture modeling, an area to which landmark contributions were made by L. Ben Freund, has been developed using procedures that embody mechanisms (1) and (2). The results show how faults can be statically strong yet dynamically weak, and operate under low overall driving stress, in a manner that generates negligible heat and meets major seismic constraints on slip, stress drop, and self-healing rupture mode.

The presentation summarizes studies done collaboratively in recent years with Nicolas Brantut (ENS/Paris), Eric Dunham (Stanford), Nadia Lapusta (Caltech), Hiroyuki Noda (Caltech), John Platt (Harvard), Alan Rempel (Univ. Oregon) and John Rudnicki (Northwestern).

Effective constitutive relations for waves in composites

John Willis

Centre for Mathematical Sciences
University of Cambridge

Recent work has established a general form for effective constitutive relations for the dynamics of composites (Willis, 2011). It applies to a variety of wave types, including electromagnetic and (visco-)elastodynamic. The composite is taken to have random microgeometry (including, as a special case, perfectly periodic geometry except that the placing of one period cell is considered to be random). In the context of visco-elastodynamics, the effective relations give the ensemble mean stress $\langle \sigma \rangle$ and ensemble mean momentum density $\langle p \rangle$ in terms of the strain and velocity associated with a weighted ensemble mean $\langle wu \rangle$ of displacement u . The effective relations are non-local in space and time, and are non-unique because effective strain and effective velocity are both derived from $\langle wu \rangle$. They become unique, however, if an independent “transformation strain” is introduced. A general expression for the non-local operators that participate in these relations was given in terms of the medium’s Green’s function by Willis (2011). In practice, it is likely that calculations will be performed relative to a “comparison medium”. The corresponding formula is developed here. No “self-adjointness” property of the medium is assumed but, when the medium has this property, it is transferred up to the effective relations. In this case, both the original problem and the “effective medium” problem have variational formulations, and the latter can be derived directly from the former. Some illustrative results will be presented.

Selected References:

[1] J.R. Willis “Effective constitutive relations for waves in composites and metamaterials”, *Proc. R. Soc. A*. doi: 10.1098/rspa2010.0620 (2011).

Tu(r)ning weakness to strength

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MIT

Biology efficiently creates hierarchical structures, where initiated at nano scales, are exhibited in macro or physiological multifunctional materials to provide a variety of functional properties that include: structural support, force generation, catalytic properties, or energy conversion. This is exemplified in a broad range of biological materials such as hair, skin, bone, spider silk or cells. For instance, despite its simple building blocks spider silk is one of the strongest, most extensible and toughest biological materials known, exceeding the properties of many engineered materials including steel. This is particularly puzzling since despite its great strength, spider silk is made of some of the weakest chemical bonds known, H-bonds. Using a bottom-up computational approach that spans all the scales from nano (protein) to macro (spider web) we have discovered that the great strength and extensibility of spider silk can be explained based on its particular structural makeup, which involves several hierarchical levels. Thereby, the structural confinement of H-bonds into ultra-small beta-sheet nanocrystals with dimensions of only a few nanometers is a key aspect to overcome the intrinsic limitations of H-bonds, creating mechanically strong, tough and resilient cross-linking domains between a semi-amorphous phase composed of 31 protein helices (Keten, Buehler et al., *Nature Materials*, 2010). This work unveils a material design strategy that enables silks to achieve superior material properties despite its simple and structurally inferior material constituents. Exploiting this concept could lead to a novel materials design paradigm, where enhanced functionality is not achieved using complex building blocks but rather through the utilization of universal repetitive constitutive elements arranged in hierarchical structures. We discuss analogies with other protein materials such as collagen and intermediate filaments, and present approaches towards the design of adaptable, mutable and active materials that rely on simple, abundant and cheap building blocks to realize highly functional materials. Applications specifically to the design of materials from mechanically inferior materials such as silica and silica as found in diatoms or sea sponges are discussed, and opportunities for de novo materials design are outlined. Such applications are critical for the development of new infrastructure materials via the application of a multiscale material design paradigm that integrates the concepts of structure and materials. This talk will also contain a review the broader field of multiscale mechanics of biological materials and give an outlook to future challenges and opportunities.

The Greening of Biology

R. Phillips

We are living through a time of explosive growth in the study of the living world that in many ways parallels advances in astronomy after the invention of the telescope. One of the powerful lenses through which these biological advances are being viewed is that of mechanics. In this talk, I will give a personal view of how our understanding of living matter can be colored by appealing to ideas from mechanics with special reference to unusual ways in which Green functions can be used to explore these questions. In particular, this talk will describe several key examples from cell biology which focus on how cells decide what to eat and where to go.

Understanding the Mechanics of Cells and Biomolecules

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It is well established that mechanical forces and deformations play an important role in almost all major aspects of a living cell, including the regulation of cell behavior and functions. However, it is necessary to establish a better understanding of mechanics at the cellular and molecular levels, especially force-sensing, force-bearing, force-generation and mechanotransduction in living cells.

In this talk I will first discuss mechanosensing and mechanotransduction in cells, and the recent discovery that the HuR gene in human umbilical vein endothelial cells may constitute a critical link between applied mechanical stress and the inflammatory response by being regulated by shear stress as well as regulating other stress-sensitive genes such as Kruppel-like factor 2 (Klf2), endothelial nitric oxide synthase (eNOS) and bone morphogenic protein 4 (BMP-4). As the second example, I will discuss the recent development of a novel mechanical nanodevice driven by the F1-ATPase motor. We systematically characterized the performance of the nanodevice, including ATP-dependent rotation, torque generation, and the controllability of the motor. Potential application of this nanodevice is also discussed. These examples help illustrate the richness and potential of the mechanics of cells and biomolecules.

Models for lithium-ion battery performance and damage

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Models are developed for the transport of Li ions in the electrolyte of lithium ion batteries, their diffusion through storage electrode particles, and their kinetics through the surface of the particles between the electrolyte and the particles. As a consequence of the Li ion intercalating in the storage particles, their lattice swells, leading to elastic stress when the concentration of Li ions in the particles is not uniform. The models of transport are based on standard concepts for multi-component diffusion in liquids and solids, but are not restricted to dilute solutions, or to small changes in the concentration of the diffusing species. In addition, phase changes are permitted during mass transport as the concentration of lithium varies from the almost depleted state of the storage particle to one where the material is saturated with its ions. The elastic swelling and shrinkage may involve very large dilatations, which are allowed for in the formulation of the model. Thus, the models are suitable for storage particle, where the amount of Li can vary by large amounts depending on the state of charge, for staging as observed in the storage process in graphite, for the enormous swelling that takes place when silicon is used for storage, and for electrolytes in which the concentration of Li ions is high. The model is used to compute the processes of charging and discharging the battery to assess the parameters that influence the development of stress in the storage particles, and to deduce the likelihood of fracture of the storage particle material. The objective is to assess designs of porous electrode microstructures that permit rapid charging and discharging, but obviate the likelihood of fracture and other mechanical damage that limit the performance and reliability of the battery.

Cavitation instabilities in soft solids: A defect-growth theory and applications to elastomers

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It is by now well established that loading conditions with sufficiently large triaxialities can induce the sudden appearance of internal cavities within elastomeric (and other soft) solids. The occurrence of such instabilities, commonly referred to as cavitation, can be attributed to the growth of pre-existing defects into finite sizes.

This work introduces a new theory to study the phenomenon of cavitation in soft solids that, contrary to existing approaches, simultaneously: (i) allows to consider general 3D loading conditions with arbitrary triaxiality, (ii) applies to large (including compressible and anisotropic) classes of nonlinear elastic solids, and (iii) incorporates direct information on the initial shape, spatial distribution, and mechanical properties of the underlying defects at which cavitation can initiate. The basic idea is to first cast cavitation in elastomeric solids as the homogenization problem of nonlinear elastic materials containing random distributions of zero-volume cavities, or defects. Then, by means of a novel iterated homogenization procedure, exact solutions are constructed for such a problem. These include solutions for the change in size of the underlying cavities as a function of the applied loading conditions, from which the onset of cavitation — corresponding to the event when the initially infinitesimal cavities suddenly grow into finite sizes — can be readily determined. In spite of the generality of the proposed approach, the relevant calculations amount to solving tractable Hamilton-Jacobi equations, in which the initial size of the cavities plays the role of “time” and the applied load plays the role of “space”. An application of the theory to the case of isotropic solids containing a random isotropic distribution of vacuous defects will be presented.

Selected Reference:

[1] O. Lopez-Pamies, M. Idiart, T. Nakamura 2011, “Cavitation in elastomeric solids: I—A defect-growth theory.” *Journal of the Mechanics and Physics of Solids* [doi:10.1016/j.jmps.2011.04.015](https://doi.org/10.1016/j.jmps.2011.04.015).

[2] O. Lopez-Pamies, T. Nakamura, M. Idiart 2011, “Cavitation in elastomeric solids: II—Onset-of-cavitation surfaces for Neo-Hookean materials.” *Journal of the Mechanics and Physics of Solids* [doi:10.1016/j.jmps.2011.04.016](https://doi.org/10.1016/j.jmps.2011.04.016) .

From Wrinkles to Creases in Elastomers: The Extreme Imperfection-sensitivity of Wrinkling

John W. Hutchinson

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The stability of the wrinkling experienced by a compressed half-space of neo-Hookean material is investigated using both an analytical initial post-bifurcation approach and a numerical method. It is shown that wrinkling is highly unstable due to the nonlinear interaction among the multiple modes associated with the critical compressive state. Concomitantly, wrinkling is sensitive to exceedingly small initial imperfections that significantly reduce the compressive strain at which the instability occurs. The imperfection-sensitivity is revealed through asymptotic analytical results and detailed numerical calculations. The study connects wrinkling with an alternative surface instability mode, the finite amplitude crease, or sulcus. The shape of the critical combination of wrinkling modes is crease-like, and a tiny initial imperfection can trigger a wrinkling instability which evolves into a crease.

The co-author of this work is Yanping Cao of the Engineering Mechanics Department of Tsinghua University.

Giant voltage-induced deformation in dielectric elastomers: theory and experiment

Zhigang Suo

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I first learned of electromechanical coupling at a small ONR workshop, held at Brown University, in late 1980s, in a talk given by Ben Freund. I was graduate student at Harvard. John Hutchinson drove several of us from Cambridge to Providence. The workshop made a lasting impression on me. Ben Freund has since been an inspiring role model for me to explore mechanics in emerging technologies. This talk describes recent work on giant voltage-induced deformation. Subject to a voltage, a membrane of a dielectric elastomer reduces its thickness and expands its area. Dielectric elastomer transducers are being developed for diverse applications, such as soft robots, adaptive optics, Braille displays, and energy harvesting. Desirable attributes include large deformation, low-cost, lightweight, and noiseless. Voltage-induced deformation in an elastomer is often limited by a type of electromechanical instability, commonly known as the pull-in instability. Our recent theory and experiment show that the same electromechanical instability can be harnessed to achieve giant voltage-induced deformation. For example, for a membrane inflated by a gas in a chamber of an intermediate size, an application of voltage can cause the membrane to expand its area by 1692%, far beyond the values reported in the literature. Implications for the design of materials and devices are discussed.

Mechanics of Stretchable Electronics

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Recent advances in mechanics and materials provide routes to integrated circuits that can offer the electrical properties of conventional, rigid wafer-based technologies but with the ability to be stretched, compressed, twisted, bent and deformed into arbitrary shapes. Inorganic electronic materials in micro/nanostructured forms, intimately integrated with elastomeric substrates offer particularly attractive characteristics in such systems, with realistic pathways to sophisticated embodiments. Mechanics plays a key role in this development by identifying the underlying mechanism and providing analytical solutions to guide design and fabrication. Mechanics models for the enabling technologies (e.g., transfer printing [1], reversible adhesion [2]) and materials (e.g., stretchable silicon [3-6]) are presented, as well as their applications to stretchable and foldable circuits [7,8], electronic-eye camera [9] and tunable eye camera [10], flexible solar cell [11], semi-transparent and flexible LED display [12,13] and its application to medicine [14], neural [15] and cardiac sensors [16], and cardiac ablation therapy [17]. Commentary and review of stretchable electronics have recently published [18,19].

Selected Reference:

- [1] Meitl et al., 2006, *Nature Materials*, **Vol. 5**, p 33 (cover article). [2] Kim et al., 2010, *PNAS*, **Vol. 107**, p 17095.
- [3] Khang et al., 2006, *Science*, **Vol. 311**, p 208.
- [4] Sun et al., 2006, *Nature Nanotechnology*, **Vol. 1**, p 201. [5] Jiang et al., 2007, *PNAS*, **Vol. 104**, p 15607.
- [6] Jiang et al., 2008, *JMPS*, **Vol. 56**, p. 2585.
- [7] Kim et al., 2008, *Science*, **Vol. 320**, p 507 (inner cover article). [8] Kim et al., 2008, *PNAS*, **Vol. 105**, p 18675 (cover article).
- [9] Ko et al., 2008, *Nature*, **Vol. 454**, p 748 (cover article). [10] Jung et al., 2011, *PNAS*, **Vol. 108**, p 1788 (cover article).
- [11] Yoon et al., 2008, *Nature Materials*, **Vol. 7**, p 907 (cover article). [12] Park et al., 2009, *Science*, **Vol. 325**, p 977.
- [13] Kim et al., 2011, "Unusual strategies for using InGaN grown on silicon (111) for solid state lighting," *PNAS* (in press).
- [14] Kim et al., 2010, *Nature Materials*, **Vol. 9**, p .929.
- [15] Kim et al., 2010, *Nature Materials*, **Vol. 9**, p 511 (cover article).
- [16] Viventi et al., 2010, *Science Translational Medicine*, **Vol. 2**, 24ra22, 2010 (cover article).
- [17] Kim et al., 2011, "Materials for multifunctional ballon catheters with capabilities in cardiac electrophysiological mapping and ablation therapy," *Nature Materials* (in press).
- [18] Rogers and Huang, 2009, *PNAS*, **Vol. 106**, p 10875.
- [19] Rogers et al., 2010, *Science*, **Vol. 327**, p 1603.

Compatibility and hysteresis

Richard James

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Big first order phase transformations in solids can still be highly reversible, if the lattice parameters are “tuned” to satisfy certain relations that promote the compatibility between phases. We present some recent measurements of hysteresis in martensitic materials resulting from this kind of tuning. The data has some fascinating features, including an apparent singularity. We re-examine the origins of hysteresis in light of these measurements. We conclude that a certain energy barrier, not pinning or thermal activation, is primarily responsible for hysteresis in martensitic phase transformations. We combine this kind of tuning, together with the lattice parameter sensitivity of magnetic properties, to find some interesting new multiferroic materials. These alloys can be used for the direct conversion of heat to electricity, and provide interesting possible ways to recover the vast amounts of energy stored on earth at small temperature difference.

Brownian motion and elasticity in biological filaments and networks

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It is well known that biofilaments at thermodynamic equilibrium under the action of forces and moments fluctuate around their minimum energy configuration due to Brownian motion. This remains true of filaments in networks and gels such as those of actin, spectrin, fibrin or other biopolymers. The thermal motion of these filaments at the microscopic scales manifests itself as entropic elasticity at the macroscopic scales. In this talk we present a theory to efficiently calculate the thermo-mechanical properties of fluctuating heterogeneous filaments and networks. The central problem is to evaluate the partition function and free energy of heterogeneous filaments and networks under the assumption that their energy can be expressed as a quadratic function in the kinematic variables. We analyze the effects of various types of boundary conditions on the fluctuations of filaments and show that our results are in agreement with recent work on homogeneous rods as well as experiments and simulations. We apply similar ideas to filament networks and calculate the area expansion modulus and shear modulus for hexagonal networks. We also apply our methods to study partially unfolded proteins and the consequences of unfolding on the macroscopic behavior of fibrin networks.

Selected References:

- [1] P.K. Purohit, R.I. Litvinov, A.E.X. Brown, D.E. Discher, J.W. Weisel, 2011, "Protein unfolding accounts for the unusual mechanical behavior of fibrin networks", *Acta Biomaterialia*, In press.
- [2] M.E. Arsenault, P.K. Purohit, Y.E. Goldman, H. Shuman, H.H. Bau, 2010, "Comparison of Brownian-dynamics-based estimates of polymer tension with direct force measurements", *Phys. Rev. E.*, **Vol. 82**, pp. 051923.
- [3] T. Su, P.K. Purohit, 2010, "Thermomechanics of a heterogeneous fluctuating chain," *J. Mech. Phys. Solids*, **Vol. 58**, pp. 164-186.
- [4] T. Su, P.K. Purohit, 2009, "Mechanics of forced unfolding of proteins," *Acta Biomaterialia*, **Vol. 5**, pp. 1855-1863.
- [5] A.E.X. Brown, R.I. Litvinov, D.E. Disher, P.K. Purohit, J.W. Weisel, 2009. "Multiscale mechanics of fibrin polymer: Gel stretching with protein unfolding and loss of water," *Science*, **Vol. 325**, pp. 741-744.

Interatomic Potentials, Forces and the Uniqueness of Stress

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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 and heat flux, 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 [1,2], 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 and differential geometry play an important role in the derivation and point to the existence of a unique stress tensor. The theoretical framework as well as numerical results will be presented.

Selected Reference:

- [1] N. C. Admal and E. B. Tadmor, 2010, "A Unified Interpretation of Stress in Molecular Systems," *J. Elast*, Vol. 100, pp. 63-143.
- [2] N. C. Admal and E. B. Tadmor, 2011, "Stress and heat flux for arbitrary multi-body potentials: A unified framework", *J. Chem. Phys.*, Vol. 134,

Deformation Analysis of Hierarchical Carbon Nanotube Bundles Under Uniaxial Compression

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Vertically aligned carbon nanotubes (VACNTs) serve as integral components in a variety of applications including MEMS devices, energy absorbing materials, dry adhesives, light absorbing coatings, and electron emitters, all of which require structural robustness. Understanding of the VACNT structures' mechanical properties and constitutive stress-strain relationship is central to the rational design of many of these applications. We demonstrate results of in-situ uniaxial compression experiments of 50 micron diameter cylindrical bundles of these complex, hierarchical materials as they undergo unusual deformation behavior. Most notably they deform via a series of localized folding events, originating near the bundle base, which propagate laterally and collapse sequentially from bottom to top. This deformation mechanism accompanies an overall foam-like stress-strain response having elastic, plateau, and densification regimes with the addition of undulations in the stress throughout the plateau regime that correspond to the sequential folding events. Microstructural observations indicate the presence of a strength gradient, due to a gradient in both tube density and alignment along the bundle height, which plays a key role in both the sequential deformation process and the overall stress-strain response. We capture the sequential buckling phenomena and strength gradient effect through application of a finite element model based on a viscoplastic solid in which the flow stress relation contains an initial peak, followed by strong softening and successive hardening. Through this combination of experimental and modeling approaches, we discuss the particular mechanisms governing non-trivial energy absorption via the sequential formation of localized buckles in the VACNT bundles.

Selected References:

[1] S. B. Hutchens, L. J. Hall, and J. R. Greer "In situ Mechanical Testing Reveals Periodic Buckle Nucleation and Propagation in Carbon Nanotube Bundles" *Adv. Funct. Mater.*, **20**, 1-9 (2010)

[2] S.B.Hutchens, A. Needleman, and J.R. Greer "Analysis of uniaxial compression of vertically aligned carbon nanotubes" *J Mech Phys Solids* (in review, 2011).

Combinatorial nanocalorimetry of metallic thin films

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The parallel nano-scanning calorimeter (PnSC) is a silicon-based micromachined device for calorimetric measurement of nanoscale materials in a high-throughput methodology. The device contains an array of calorimetric sensors, each one of which consists of a silicon nitride membrane and a tungsten heating element that also serves as a temperature gauge. The small mass of the individual sensors enables measurements on samples as small as a few hundred nanograms at heating rates up to 10^4 K/s. The sensitivity of the device is demonstrated through the analysis of the melting transformation of a 25-nm indium film. To demonstrate the combinatorial capabilities, the device is used to analyze a thin-film Ni–Ti–Zr sample library. As-deposited amorphous samples are crystallized by local heating in a process that lasts just tens of milliseconds. The calorimetry scans reveal the glass transition of the amorphous alloys, as well as a multi-stage crystallization process. The martensite–austenite transformation in the crystallized Ni–Ti–Zr samples is analyzed and the dependence of transformation temperature on composition is revealed. The transformation temperature is depressed compared to bulk shape memory alloys because of the very fine microstructure of the samples.

Interatomic Potentials, Forces and the Uniqueness of Stress

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Minneapolis, MN 55455

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 and heat flux, 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 [1,2], 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 and differential geometry play an important role in the derivation and point to the existence of a unique stress tensor. The theoretical framework as well as numerical results will be presented.

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[1] N. C. Admal and E. B. Tadmor, 2010, "A Unified Interpretation of Stress in Molecular Systems," *J. Elast*, **Vol. 100**, pp. 63-143.

[2] N. C. Admal and E. B. Tadmor, 2011, "Stress and heat flux for arbitrary multi-body potentials: A unified framework", *J. Chem. Phys.*, in press.

Numerical Modeling of Stress Generation and Whisker Growth in Thin Sn Films on Cu

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The spontaneous growth of long, filamentary whiskers from the surface of Sn-plated Cu conductors poses a serious threat to the reliability of electronic components. While it is generally accepted that whiskers form to relax compressive stress generated by the localized growth of Cu_6Sn_5 intermetallic compound (IMC), the mechanisms are not fully understood. In this work, finite element analysis (FEA) is used to quantitatively assess the interactions among parallel mechanisms of stress generation and relaxation, and determine how they control whisker growth. The FEA model includes growth of an IMC phase, elastic and plastic deformation within the Sn grains, and stress-driven diffusion along grain boundaries, all of which are indicated by experimental evidence. FEA results reveal that plastic yield within Sn grains coupled with stress-driven grain boundary diffusion effectively transmits stress through the Sn and, significantly, can account for the experimentally measured stress evolution without relaxation due to whisker growth. In addition, the columnar microstructure of the Sn, presence of surface oxide and non-planar IMC morphology are all found to be necessary for stress build-up, suggesting that processing or treatment that disrupts these features will reduce the stress level in the Sn.

Modeling also indicates previously unrecognized kinetic relations governing whisker growth, including the emergence of two kinetic regimes controlled by the balance between strain generation and relaxation. In one regime whiskers dominate relaxation and whisker velocity scales directly with IMC growth rate, in the other, multiple competing mechanisms relax strain and whisker velocity varies weakly with IMC growth rate. A mathematical model is presented to describe these kinetic relations.

Strain stiffening induced by molecular motors in active crosslinked biopolymer networks

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Recent experiments on networks that consist of actin filaments crosslinked by filamin A (FLNa) and bipolar filaments of muscle myosin II show that in the absence of any applied loads, the motors stiffen the network by about two orders of magnitude. The degree of stiffening was found to increase with increasing density of myosin motors. Another key observation from this study relates to the magnitude of stiffening caused by compliant and in compliant crosslinks. Interestingly, it was found that in distinct contrast to the flexible FLNa, rigid scruin does not promote active stiffening of F-actin networks upon addition of myosin. Why do compliant crosslinks in active networks lead to large strain stiffening while no significant increase in stiffness is observed in the case of in compliant crosslinks? To answer this question and to quantitatively study the interplay of internal strains generated by molecular motors and external loads, we study the elastic response of actin networks with both compliant and rigid crosslinks by modeling molecular motors as force dipoles. Our finite element simulations show that for compliant crosslinkers such as filamin A, the network can be stiffened by two orders of magnitude while stiffening achieved with in compliant linkers such as scruin is significantly smaller, typically a factor of two, in excellent agreement with recent experiments. We show that the differences arise from the fact that the motors are able to stretch the compliant crosslinks to the fullest possible extent, which in turn causes to the deformation of the filaments. With increasing applied strain, the filaments further deform leading to a stiffened elastic response. When the crosslinks are in compliant, the contractile forces due to motors do not alter the network morphology in a significant manner and hence only small stiffening is observed.

Nanoplasticity in FCC metals during ion bombardment

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Prismatic dislocation loops, pure or composite, are conventionally immobile under uniform applied stress, and can glide only under pressure-gradient or grow by thermally activated diffusion of atoms. Here, we uncover a new stress-driven motion mechanism of shear-normal composite prismatic loops, in which the loop glides and grows at the same time in an interstitial-rich environment. Such composite prismatic loops are also able to switch their direction of travel once they reach a critical size. Using molecular dynamics simulations, we show that this unique loop motion mechanism is abundantly activated during the low energy ion beam irradiation of a large class of fcc metals. Near-sonic irradiation of ions with lattice-incompatibility generates a self-interstitial-rich subsurface layer where the compressive stress is accrued. In this layer, stress-driven composite prismatic dislocation loops glide and grow, soaking in interstitials until the loops reach a critical size at which they shoot to the surface and relax the compressive stresses. This dislocation-assisted subsurface atomic transport mechanism clarifies previously unexplainable experimental observations of nanometer-scale morphology evolution on ion-irradiated aluminium surfaces, and of near-surface stress relaxation associated with such morphology evolution. In addition, such non-conservative prismatic loop motion has important implications in the annealing of point defects caused by radiation damage in nuclear materials.

Numerical simulations of intergranular strain evolution during deformation of nanocrystalline materials

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It is well known that grain boundary phenomena such as dislocation emission/annihilation, grain-boundary (GB) sliding, and GB diffusion dominate the deformation behavior of nanocrystalline materials. As a result, their mechanical behavior differs substantially from that of their coarse-grained counterparts. To probe the microstructure-level mechanisms of deformation in nanocrystalline materials, recent studies [1] have used synchrotron x-ray and neutron diffraction techniques to determine the evolution of intergranular strain during straining in both nanocrystalline and bulk materials. These studies show that intergranular stresses in nanocrystalline materials are substantially lower than those in bulk materials, despite the large increase in flow stress in nanocrystalline specimens. It has been suggested that this behavior is a result of a transition in deformation mechanism from dislocation dominated behavior to grain boundary dominated behavior. To this end, we have used the microstructure-based nanocrystal model developed by [2] to compute the evolution of intergranular strain in copper as functions of strain rate and grain size at room temperature. Our results for nano-copper show that inter-granular strain decreases with the decrease in the applied strain-rate and grain size (in the inverse Hall-Petch regime), which are in qualitative agreement with the in situ synchrotron x-ray measurements in nanocrystalline metals [1].

Keywords: nanocrystalline, grain boundary sliding and diffusion, intergranular strain

Selected Reference:

[1] S. Cheng, A.D. Stoica, X.-L. Wang, Y. Ren, J. Almer, J.A. Horton, C.T. Liu, B. Clausen, D.W. Brown, P.K. Liaw, L. Zuo, "Deformation crossover: from nano- to mesoscale," *PRL* 103, 035502 (2009)

[2] Y. Wei, A.F. Bower, H. Gao, "Enhanced strain-rate sensitivity in fcc nanocrystals due to grain-boundary diffusion and sliding," *Acta Mater.* 56, 1741-1752 (2008).

Mechanics of Energy Storage Materials

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Developing high energy density battery systems has emerged as a major challenge in recent years. Silicon is considered to be a promising anode material for future lithium ion batteries that can increase the energy density by as much as 30%. Since silicon undergoes large compositional strains during charge-discharge cycling, managing the stress and deformation fields in it is the central challenge in designing silicon-based electrodes. This work examines the basic mechanical behavior of silicon and the coupling between stress and electrochemical performance of the material. The stress field associated with the crystalline to amorphous phase transformation in silicon is measured and its contribution to damage evolution is examined.

A microstructure based model of the deformation mechanisms and flow stress during elevated temperature straining of a magnesium alloy

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We show that the variation of flow stress with strain rate and grain size in magnesium alloy AZ31 deformed at a constant strain rate and 450°C can be predicted by a crystal plasticity model that includes an explicit description of grain boundary sliding and diffusion. The model also predicts the grain size dependence of the critical strain rate that will cause a transition in deformation mechanism from dislocation creep to grain boundary sliding, and yields estimates for grain boundary fluidity and diffusivity in the magnesium alloy. Grain boundary sliding is found to be significantly faster in magnesium alloys than in aluminum alloys with comparable grain size, and simulations suggest that there is no threshold stress for grain boundary sliding in magnesium.

Selected Reference:

D.E. Cipoletti, A.F. Bower, and P.E. Krajewski, *Scripta Materialia* **64** (2001) 931-934.

Folding wrinkles of a thin stiff layer on a soft substrate

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We present mechanics of folding surface-layer wrinkles on a soft substrate, i.e. inter-touching of neighboring wrinkle surfaces without forming a cusp. Upon laterally compressing a stiff layer attached on a finite-elastic substrate, certain material nonlinearities trigger a number of bifurcation processes to form multi-mode wrinkle clusters. Some of these clusters eventually develop into folded wrinkles. The first bifurcation of the multi-mode wrinkles is investigated by a perturbation analysis of the surface-layer buckling on a pre-stretched neo-Hookean substrate. The post-buckling equilibrium configurations of the wrinkles are then trailed experimentally and computationally until the wrinkles are folded. The folding process is observed at various stages of wrinkling, by sectioning 20–80nm thick gold films deposited on a PDMS substrate at its stretch ratio of 2.1. Comparison between the experimental observation and the finite element analysis shows that the Ogden model deformation of the substrate coupled with asymmetric bending of the film predicts the folding process closely. In contrast, if the bending stiffness of the film is symmetric or the substrate follows the neo-Hookean behavior, the wrinkles are hardly folded. The wrinkle folding is applicable to construction of long parallel nano/micro channels and control of exposing functional surface areas.

Bioinspired Actuable Surface Nanostructures with Arbitrary Geometry and Stiffness

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Biology abounds with examples of functional structures, whose superior mechanical, optical, adhesive, self-cleaning, actuation and sensing properties are unmatched in today's smart synthetic materials. Notably, the common feature of the many largely unrelated natural designs is a use of fibers and high-aspect-ratio nano- and micro-structures. However the difficulty of systematically and conveniently varying the geometries of synthetic versions of these structures has significantly limited their function-specific design and optimization. We have been developing an integrated low-cost platform for producing bio-inspired arbitrarily-designed actuable surfaces with high-aspect-ratio (HAR) nanostructures that are themselves responsive to a variety of stimuli and exhibit finely-tuned mechanical properties. In our approach, we adapt and significantly extend the soft lithography technique into a double-casting method to enable nanostructure fabrication in a choice of metals, ceramics, or polymers. The effective stiffness and thus sensitivity of these stable, HAR features can be varied by several orders of magnitude through tailoring the final material—as we demonstrate by varying polymer ratios—and the 3-D geometry of the nanostructures. [1,2] We show how anisotropic cross-sections and 2-D arrays are proportionally created by specific strain combinations of the PDMS mold, thus transcending one-to-one replication constraints. Furthermore, we introduce a new high-throughput benchtop method that enables a HAR array to be reshaped with nanoscale precision by electrodeposition of conductive polymers. The method—named STEPS (structural transformation by electrodeposition on patterned substrates)—makes it possible to proportionally increase the dimensions of original features, to merge or mechanically reinforce isolated features for robustness, and to transform a simple parent two dimensional nanostructure array into new 3-D patterned structures with nontrivial tapered, tilted, anisotropic, or overhanging geometries that would be expensive or infeasible via conventional lithography.[2] As we continue modeling and measuring the mechanical responses of these arrays of nanostructures, the resulting bio-inspired surfaces will offer multifunctional characteristics that include superhydrophobicity, actuation under e-beam, hydrogel, and other stimuli, as well as field-sensing capabilities.

Selected References:

- [1] “Fabrication of Bio-Inspired Actuated Nanostructures with Arbitrary Geometry and Stiffness”, B. Pokroy, A. K. Epstein, M. C. M. Persson-Gulda, J. Aizenberg, *Adv. Mater.*, **2009**, *21*, 463-469.
- [2] “Biomimetic Nanostructured Surfaces with Designer Mechanics and Geometry for Broad Applications”, A.K. Epstein and J. Aizenberg. In: *Biosurfaces and Biointerfaces*, edited by J.A. Garrido, E. Johnston, C. Werner, T. Boland (Mater. Res. Soc. Symp. Proc. Volume 1236E, Warrendale, PA, **2010**) Paper# 1236-SS09-07
- [3] “STEPS: Structural Transformation by Electrodeposition on Patterned Substrates.” P. Kim, A.K. Epstein, M. Khan, L.D. Zarzar, D.J. Lipomi, G.M. Whitesides and Joanna Aizenberg, *Nano Lett.*, **DOI**: 10.1021/nl200426g.

Scale and Stochastic Effects on Incipient Plasticity in Confined Volumes at Small Scales

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Nanoindentation pop-in may correspond to a homogeneous dislocation nucleation event when the applied resolved shear stress approaches the theoretical strength of a defect-free single crystal, as shown by Mo and NiAl experiments [1,2]. The statistical fluctuations of the measured pop-in loads are a consequence of the stress-assisted, thermally-activated process of homogeneous dislocation nucleation. Yet pop-in can result from defect-assisted processes, such as a sudden and unstable change of existing dislocation network (e.g., dislocation bowing out as in the Frank-Read model), which dominates when the indenter radius increases or the pre-existing dislocation density increases [2]. The statistical fluctuations of the measured pop-in loads, as illustrated by the cumulative probability, thus contain convoluted information from the homogeneous dislocation nucleation and heterogeneous dislocation nucleation. A unified model that addresses both thermal and spatial effects predicts the dependence of incipient plasticity on temperature, indenter size, defect density, material anisotropy, and crystallography. Implications on other related experiments will be discussed.

Selected Reference:

[1] H. Bei, Y.F. Gao, S. Shim, E.P. George and G.M. Pharr, 2008, "Strength Differences Arising from Homogeneous versus Heterogeneous Dislocation Nucleation," *Physical Review B*, **Vol. 77**, 060103(R).

[2] T.L. Li, Y.F. Gao, H. Bei and E.P. George, 2011, "Indentation Schmid factor and orientation dependence of nanoindentation pop-in behavior of NiAl single crystals," *Journal of the Mechanics and Physics of Solids*, in press.

Anomalous strength characteristics of tilt grain boundaries in graphene

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Graphene in its pristine form is one of the strongest materials tested, but defects influence its strength. Using atomistic calculations, we find that, counter to standard reasoning, graphene sheets with large-angle tilt boundaries that have a high density of defects are as strong as the pristine material and, unexpectedly, are much stronger than those with low-angle boundaries having fewer defects. We show that this trend is not explained by continuum fracture models but can be understood by considering the critical bonds in the strained seven-membered carbon rings that lead to failure; the large-angle boundaries are stronger because they are able to better accommodate these strained rings. Our results provide guidelines for designing growth methods to obtain sheets with strengths close to that of pristine graphene.

Self-Assembly of Nanofibers with Controlled Hierarchy and Shape by Adhesion Mediated Elastocapillary Interaction

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Recently there has been a growing interest in studying evaporative self-assembly of soft fibers to generate biomimetic hierarchical structures for a range of applications including drug delivery, adhesives, and structural color. Here we show that unique helical patterns with structural hierarchy can be formed from arrays of polymeric nanofibers assembling in an evaporating liquid, and demonstrate that balancing the mechanical (geometry and modulus) with the surface (wetting and adhesion) properties of the fibers provides a simple way to control the size, chirality, and anisotropy of the final assembly pattern [1-2]. While evaporative self-assembly of fibers has been modeled as a competition between capillary and elastic forces, we found that adhesion forces play a key role in controlling the appearance of helicity as well as the final assembly size. In particular, the dynamic interplay between adhesion and elasticity determines how many hierarchical stages will be preserved and the propensity of fibers to twist around each other. Our findings provide insight into how multiple parameters work together to control the self-assembly of nanofibers and provide a diverse set of options for fabricating a variety of self-assembled nanostructures. Finally, we present results showing the potential for using the dynamic assembly process for particle trapping and release and for biomimetic adhesives.

Selected References:

- [1] B. Pokroy, S. H. Kang, L. Mahadevan, J. Aizenberg, *Science* **323**, 237-240, 2009.
- [2] S. H. Kang, B. Pokroy, L. Mahadevan, J. Aizenberg, *ACS Nano* **4**, 6323-6331, 2010.

Geometry induced rigidity in pressurized elastic shells

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We study the mechanical response of thin elastic shells subject to point or plate load and in different mechanical environments (with or without an in-out pressure difference). The geometry and material properties of the ellipsoidal shells used in our experiments can be accurately controlled using digital fabrication techniques. The mechanical response of the shells is quantified through load-displacement compression tests and the differential pressure is regulated through pressure sensors with feedback loop control. We focus here on the linear regime to explore the geometry-induced rigidity of shells with different shapes. We found that the effective stiffness of an elastic shell is dependent on its Gauss curvature around the indentation zone. Taking into account this local Gauss curvature in a classical theory of shells, we develop a theoretical framework to predict the geometry-induced rigidity of ellipsoidal shells with or without an in-out pressure difference. Whereas this project focused on proof of concept at the centimeter length scale, the scale independence of geometrical properties should enable the predictive scaling of the mechanics down towards micro- or nano-meter applications with Atomic Force Microscopy of living cells or upwards for larger scale for design of shell type structures in Civil Engineering.

On the origins of rate and state friction: Frictional ageing of rock materials explored via single-asperity experiments

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This poster presents the first nanoscale, single-asperity experiments to address the issue of frictional ageing of rock materials, *i.e.*, the growth of static friction with time when they are held in stationary contact. This behavior is critical for understanding earthquake phenomenon, specifically the “evolution effect” long discussed in the phenomenological (but highly successful) model of *rate and state* friction [1,2,3]. Understanding the mechanism underlying the evolution effect would allow formulation of more physically-based frictional constitutive laws, allowing more confident extrapolation to natural faults for understanding earthquakes and other time-dependent friction phenomena in general. Despite its importance, the physical mechanism(s) that cause frictional ageing is not well understood. A prevailing view is that ageing results from increases in the real area of contact due to plastic creep of the contacting asperities. However, our experiments [4] show that at relatively low contact stresses in a well-defined, nanoscale, single-asperity contact, ageing is caused by changes in chemical bonding. Moreover, it has a much larger magnitude than observed in macroscopic studies. While this appears to be inconsistent with the macroscopic measurements, we demonstrate with mechanics modeling that the large magnitude is in fact required to reconcile single-asperity behavior with ageing in macroscopic, multi-asperity interfaces.

Selected References:

- [1] Dieterich, J.H.: Modeling of rock friction. 1. Experimental results and constitutive equations. *Journal of Geophysical Research*, **84**(NB5), 2161-2168 (1979)
- [2] Ruina, A.: Slip instability and state variable friction laws. *Journal of Geophysical Research*, **88**(NB12), 359-370 (1983)
- [3] Rice, J.R., Ruina, A.L.: Stability of steady frictional slipping. *J. Appl. Mech.-Trans. ASME*, **50**(2), 343-349 (1983)
- [4] Li, Q., Tullis, T.E., Goldsby, D., Carpick, R.W.: On the origins of rate and state friction: Frictional ageing from interfacial bonding. (Under review)

Dislocation nucleation govern softening and maximum strength in nanotwinned metals

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Conventionally, the metal strengths are controlled by dislocation interactions with grain boundaries and other obstacles. For nanostructured materials, in contrast, dislocation multiplication is severely confined by the nanometre-scale geometries so that continued plasticity can be expected to be source-controlled. Nanograined polycrystalline materials were found to be strong but brittle, because both nucleation and motion of dislocations are effectively suppressed by the nanoscale crystallites. Here we presented a dislocation-nucleation-controlled mechanism in nano-twinned metals in which there are plenty of dislocation nucleation sites but dislocation motion is not confined. We show that dislocation nucleation governs the strength of such materials, resulting in their softening below a critical twin-boundary spacing. Large-scale molecular dynamics simulations in nano-twinned metals show that there exists a transition in deformation mechanism, occurring at a critical twin-boundary spacing for which strength is maximized. At this point, the classical Hall–Petch type of strengthening due to dislocation pile-up and cutting through twin planes switches to a dislocation-nucleation-controlled softening mechanism with twin-boundary migration resulting from nucleation and motion of partial dislocations parallel to the twin planes. The simulations indicate that the critical twin-boundary spacing for the onset of softening in nano-twinned copper and the maximum strength depend on the grain size: the smaller the grain size, the smaller the critical twin boundary spacing, and the higher the maximum strength of the material. Based on the insights provided by atomistic simulations, we developed a kinetic model to describe the proposed dislocation nucleation governed softening mechanism. The predictions from the kinetic model are in good agreements with results from experiments and molecular dynamics simulations.

Computer simulation of molecule-coated nanoparticles translocation across lipid membrane

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Nanoparticle interaction with lipid membrane depends on the surface characterization as well as the arrangement of coating ligands on the nanoparticle surface. The dynamics of forced translocation of molecule-coated nanoparticle with different surface patterning across a lipid bilayer membrane has been studied by dissipative particle dynamics approach. Thermodynamic integration method is applied to estimate the free energy change associated with the penetration of nanoparticles. By comparing nanoparticle ‘isomers’ covered with similar amphiphilic composition, the penetration ability of alternating hydrophilic and hydrophobic groups is better, and the free energy change of penetration is smaller. The penetrate orientation can complicate the penetration behavior due to the anisotropic property caused by surface patterning. These findings may be helpful in understanding the current and future delivery of drug-loaded nanoparticle technologies.

Force-free swimming of a model helical flagellum in viscoelastic fluids

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Bacteria achieve motility by eluding the constraints of kinematic reversibility, for instance, by rotating a helical flagellum. We study experimentally the motility of the flagellum with a scaled-up model system, a motorized helical coil that rotates along its axial direction. The rotating helix is tethered on a linear stage that advances at prescribed speeds along the axial direction. A free-swimming speed is obtained when the net force on the helix is zero. In the Newtonian case, the free-swimming speed of the helix agrees well with the predictions from the available theories and computational tools. When the helix is immersed in a viscoelastic (Boger) fluid, we find an increase in the force-free swimming speed which is maximized at a Deborah number of approximately one, and whose magnitude depends on both the elasticity of the fluid and the geometry of the helix.

The Thermoviscoelastic Mechanisms of Shape Memory Polymers

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This work investigated the influence of stress and structural relaxation mechanisms on the recovery performance of amorphous shape memory polymers by developing a multiprocess thermoviscoelastic model capable of spanning the glass transition. The model incorporated the time-dependent mechanisms of stress and structural relaxation and viscoplastic flow to describe the glass transition of the material from a soft viscoelastic rubber to a hard viscoplastic glass. The model captured many important features of the free strain recovery response and of the stress hysteresis observed in the constrained recovery response. The study revealed that viscoelasticity was the underlying mechanism of the free strain recovery response. The onset temperature of the recovery rate was determined by the onset temperature of the glass transition, while the recovery rate was determined by the temperature breadth of the glass transition. The constrained recovery response was also strongly influenced by the relaxation mechanisms and also by thermal expansion. The peak recovery stress scaled nearly linearly with the glassy coefficient of thermal expansion. The free and constrained recovery response was also sensitive to the cooling rate of the programming stage and the heating rate of the recovery stage, which further supports the importance of thermoviscoelastic mechanisms.

Plane deformations generating a prescribed finite rotation field

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Compatibility conditions for various strain measures are well known in both small and finite strain kinematics. For many problems, such conditions enable boundary value problems to be formulated using strains, stresses, or a generating potential function, as the fundamental dependent variable(s). These methods are effective, as most strain fields fully determine the generating deformations up to an arbitrary rigid deformation. Our research is concerned with the compatibility issue for the rotation field. Although it is not a direct measure of the distortion in a deformation, the rotation associated with a deformation and its variation from point to point within a body turns out to carry quite a bit of information about the actual deformation. For the case of plane deformation, we have been able to show that any suitably smooth plane proper orthogonal tensor field may serve as a finite rotation tensor for a generating deformation. We have developed several examples demonstrating this relationship between material deformation and rotation fields. Our results demonstrate in the case of plane deformation, any skew-symmetric two-dimensional tensor field can serve as a plane rotation field. The relation between the position-dependence of a rotation field and generating deformation information has implications in both mechanical twinning and shear banding.

Keywords: Rotation field, non-linear elastic deformation, mechanical twinning, shear banding, finite strain kinematics

Buckling-Induced Pattern Transformation of Structured Elastic Shells

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We present a class of continuum shell structures which undergo a structural transformation induced by buckling under pressure loading. The geometry of the buckliball comprises a spherical shell patterned with a regular array of circular voids. Moreover, we show that the buckling-induced pattern transformation is possible only with five specific hole arrangements. These voids are covered with a thin membrane, thereby making the ball air tight. Beyond a critical internal pressure, the thin ligaments between the voids buckle leading to a cooperative buckling cascade of the skeleton of the ball. Both precision desktop-scale experiments and finite element simulations are used to explore the underlying mechanics in detail and proof of concept of the proposed structures. We find excellent qualitative and quantitative agreement between experiments and simulations. This pattern transformation induced by a mechanical instability opens the possibility for reversible encapsulation, over a wide range of length scales.

Confined cylinders: from sinusoidal to helical buckling

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Structural behavior of constrained cylinders under axial compression is of great interest in oil and natural gas industry, where coiled tubing is used to service wells. More recently, contractors have begun increase the angle at which boreholes are drilled in order to access oil and gas deposits more efficiently. In horizontal wells the motion of the coiled tubing is resisted by friction forces from contact with the borehole, which grow with the length of penetration. As a result, at certain point the coiled tubing buckles into sinusoidal shape and with further penetration and axial load growth it transforms to the helical shape. At this point the friction force between the coiled tubing and the borehole increases dramatically and the maximum penetration is rapidly reached. Further insertion attempts may result in the coiled tubing damaging which is highly undesirable. Computational tools to define the critical “lock-up” loads are badly needed. We use constrained minimization techniques for elastic energy in order to solve equilibrium and investigate structural behavior of confined cylinders under axial compression. We demonstrate our model on example of constrained elastic rod with frictionless possible contact to confining cylinder supported at both ends. We compare numerical results to experiments. Our numerical results are in a good qualitative agreement with experiments. Quantitatively, some deviation is observed due to absence of friction forces in our computational model between the inner rod and confining cylinder.

Fabrication and testing of nano scaled fiber reinforced ceramic coating

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A carbon composite consisting of nano-crystalline diamond (NCD) and carbon nano-tubes (CNTs) is envisaged to be a promising wear resistant coating for a variety of applications in tools, biosensors conformal coatings in MEMs for instance. Fabricating the composite coating can pose problems for it is known that CNTs act as a potential source for diamond growth. A delicate balance between the simultaneous etching of nano-tubes and growth of NCD to fill in as the matrix for the composite is preeminent. An approach for engineering such a nano-scaled composite on Si substrates is reported in this work. Furthermore, determining the fracture toughness of such coatings using the traditional indentation method on the coating itself is cautioned against, for reasons of unaccountability of coating de-lamination. Based on earlier work[1] performed by others in the group, an alternate approach is outlined.

Selected Reference:

[1] Z. Xia, W.A. Curtin, and B.W. Sheldon, 2004, "A new method to evaluate the fracture toughness of thin films", *Acta. Mater.* **52**, pp. 3507-17 (2004)

Nanomechanics of Grain Boundary Embrittlement in FCC Metals

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A nonlinear field projection method has been developed to study nanometer scale mechanical properties of grain boundaries in nanocrystalline FCC metals [1]. The nonlinear field projection is based on the principle of virtual work, for virtual variations of atomic positions in equilibrium through nonlocal interatomic interactions such as EAM potential interaction, to get field-projected subatomic-resolution traction distributions on various grain boundaries. The analyses show that the field projected traction produces periodic concentrated compression sites on the grain boundary, which act as crack trapping or dislocation nucleation sites. The field projection was also used to assess the nanometer scale failure processes of Cu $\Sigma 5$ and $\Sigma 9$ grain boundaries doped with Pb. It was revealed that the most significant atomic rearrangement is dislocation emission which requires local GB slip, and some Pb locks the local GB slip and in turn, embrittles the GB.

Selected Reference:

[1] C.-K. Wang, H. B. Chew and K.-S. Kim, 2011, "Nanometer Scale Mechanical Behavior of Grain Boundaries," *MRS Proceedings*, **Vol. 1297**. (published online)

Co-Continuous Periodic Composites for Stiffness, Strength, Energy Dissipation, and Damage Tolerance

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Natural and synthetic composite materials consisting of two or more different materials are a major avenue for achieving materials with enhanced properties and combination of properties. The combination of hard and soft materials enables outstanding combination of mechanical performance properties including stiffness, strength, impact resistance, toughness, and energy dissipation. In this work, we demonstrate the potential to achieve materials with enhancements in stiffness, strength and energy dissipation. We investigate the macroscopic mechanical response of 3D periodic glassy polymer/elastomer co-continuous composites with different geometric arrangements of the constituents through simulations and experiments. We have shown that 3D periodic co-continuous composites can have enhanced mechanical performance achieving a unique combination of stiffness, strength and energy absorption as compared to the conventional particle-reinforced composites, fiber-reinforced composites, and lamellar composites. This design concept can be extended to other material combinations such as polymer/ceramic and polymer/metal in co-continuous composites, which potentially provide a much higher stiffness and strength. Of particular note, the mutual constraints between two phases of the co-continuous structure enable enhanced dissipation by spreading of the plastic deformation and by containing cracking leading to a multitude of non-catastrophic dissipative events, which also provides damage tolerance of the co-continuous composites. These results provide guidelines for engineering and tailoring the nonlinear mechanical behavior and energy absorption of co-continuous composites for a wide range of applications.

Nanobearings in Nature

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The sandfish can quickly burrow into the sand and move through it for significant distances without hurting its skin. Its skin is well adapted to preventing scratches while it quickly dives in and out of desert sand. From SEM images, the nano-threshold structures were found in the skin every 6 to 8 μm . We also found that in nature the distribution of sand particles is smaller than 50 nm , or larger than 300 μm . To prove the phenomena of the sand binarization, the commercial finite element analysis software, ABAQUS, has been used to simulate the touching mechanism of sandwiching a small spherical sand particle with two large spherical sand particles. We believe that the configuration of the skin of a sandfish and the binarized distribution of sand particles in nature play important roles in providing the flawless mechanisms for the skin of a sandfish while it burrows into the desert sands. The application of the biomechanical phenomena is able to be further used for preventing the frictional damages of piston in the engines under back and forth motion.

Frequency- and Temperature-Invariant Dissipative Behaviors of Randomly Entangled Carbon Nanotube Networks under Cyclic Loading

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Recent experiments have shown that entangled networks of carbon nanotubes exhibit temperature- and frequency-invariant dissipative behaviors under cyclic loading. Here we perform coarse-grained molecular dynamics simulations to show that this intriguing phenomenon can be attributed to the dry adhesion/friction in the system induced by van der Waals interactions between individual CNTs. We show that this behavior can be described by a triboelastic constitutive model. The present study highlights the promise of carbon nanomaterials for energy absorption and dissipation under extreme conditions.

Mechanics Modeling and Simulation of the Nanomaterial-cell Interactions

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Recent in-vitro and in-vivo experiments show that mechanical parameters of nanomaterials, such as size, shape, and elasticity, can affect their cellular uptake. A thorough understanding of such phenomenon can assist in the design of nanomaterials for various applications such as cancer therapy, drug delivery, and enhanced bioimaging. In this poster, we show some of our work in which the quantitative mechanics modeling of a variety of cell-nanomaterial interaction problems were investigated using analytical and numerical methods. From our research, fundamental understandings and important findings have been achieved which have broad implications in biomedical engineering.

Deformation Mechanisms, Length Scales and Optimizing the Mechanical Properties of Nanotwinned Metals

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Optimizing the strength of metallic materials is often achieved through microstructure manipulation. Unfortunately, increase in metal strength is often accompanied by a concomitant decrease in ductility. Interestingly, it was demonstrated recently that in pure, nanotwinned Cu, the yield strength exhibits a maximum strength at a small, finite twin spacing. In addition, it was found that while the strength goes through a maximum at a critical twin spacing, the strain hardening and ductility increase monotonically with decreasing twin spacing. So far, the underlying mechanisms responsible for these interesting behaviors have not been fully understood.

We study the plastic deformation of polycrystalline nanotwinned copper through large-scale molecular dynamics simulations. It is found that three mechanisms are present in creating the plasticity deformation: 1) emission of full screw dislocations from grain boundaries and then cutting through twin boundaries, 2) emission of dislocations from grain boundaries and further moving parallel to the twin boundaries; 3) emission of 600 full dislocations from grain boundaries and moving across twin boundaries. For the last one, our simulations using various twin spacings show that a transition in the dominant deformation mechanism occurs at a small critical twin spacing. While at large twin spacing, cross-slip and dissociation of the Lomer dislocations create dislocation locks which restrict and block dislocation motion and thus enhance strength, at twin spacing below the critical size, cross-slip does not occur, steps on the twin boundaries form and deformation is much more planar. These twin steps can migrate and serve as dislocation nucleation sites, thus softening the material. Based on these mechanistic observations, a simple, analytical model for the critical twin spacing is proposed and the predicted critical twin spacing is shown to be in excellent agreement both with respect to the atomistic simulations and experimental observation. We further conducted calculations using nudged elastic band method to obtain the activation volume of the third mechanism and showed that its value is comparable with that of the first mechanism. All these suggest the dislocation mechanism transition reported here is a cause of the observed transition in nanotwinned Cu strength.

3D Modeling of the Growth of Alloy Quantum Dots Considering Morphological and Compositional Coupling

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Fabrication of quantum dots (QDs) with high density may be realized by self-assembly via heteroepitaxial growth of thin films. Since the electronic and optoelectronic properties of QDs are sensitive to size, morphology, mismatch strain and especially composition [1,2], it is of great importance to control their composition profiles and morphology, and engineer the strain in them. Since the growth is a dynamic process, which carries out via surface diffusion driven primarily by strain relaxation and chemical intermixing/segregation, the strong coupling between morphological and composition evolutions during this process leads to a rather complex dynamics, which has not been fully understood. In the present work, a three-dimensional finite element model is developed, which is capable of modeling the formation, self-assembly and coarsening of hetero-epitaxial alloy islands by considering the coupling of morphological and compositional evolution. Several interesting experimental observations, such as fast coarsening kinetics; asymmetries in composition profile and island shape; lateral motion of alloy islands have been observed in our simulations. Our finite element model predictions have painted a rather complete picture for the entire dynamic evolution during the growth of nanoscale heteroepitaxial islands.

Advanced Nanoindentation of Viscoelastic Properties in Soft Biomaterials

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Understanding the mechanical behavior of soft biomaterials is essential to the development of these materials and the devices in which they are used. In recent years, investigating these systems at a degree beyond the traditionally available macroscopic methods has become a great focus. Various methods are currently used to characterize the mechanical behaviour of biomaterials, commonly either dynamic tests or quasi-static tests (such as creep or stress relaxation tests). Such methods have major drawbacks: (i) the sample often needs to be of a specific shape and (ii) sample fixation can be problematic, especially for materials with high viscoelasticity. Nanoindentation is particularly appropriate because it is unaffected by these two limitations and allows the characterization of very small material volumes. However, the main drawback of nanoindentation tests is linked to the low thermal stability of most instruments. These instabilities introduce an uncontrollable penetration drift which, when coupled with the viscoelastic deformation of the sample, produces a composite response which is a mixture of that of the instrument and that of the sample. For many biomaterials, such limitations induce significant error in the measured mechanical properties. This paper presents alternative methods of performing nanoindentation in order to gain quantitative and meaningful data on such materials.

Chemo-mechanics of Alloy-Based Electrodes for Lithium Ion Batteries

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Although recent developments of nano-sized structures have significantly improved the cyclability, performance, reliability and cost competitiveness of Li-Si electrodes, challenges remain in the commercialization of such electrodes. For these nanostructures, large permanent shape changes, cavitations, and surface roughening are the dominant mechanisms causing the degradation in performance over charge-discharge cycles. These failure mechanisms are in sharp contrast to fracture and pulverization observed in Li-Si electrodes at the millimeter scale. Currently, the coupled chemo-mechanical-transport processes associated with the performance degradation are poorly understood, primarily because of the complicated interactions among the multiphysics mechanisms. Here, we focus on two issues. The first issue is the coupling between diffusion-induced stress development and stress-enhanced diffusion. Key factors considered are stress development, Li-host inter-diffusion and inelastic flow. The results show significant contribution of stress gradient to the driving force for Li/host inter-diffusion. For alloys with non-negligible host diffusivity, this effect can lead to significant relaxation of stresses even when the stress levels are well below the threshold for the onset of plastic flow. On one hand, the strength of the volumetric relaxation is controlled by the magnitude of the thermodynamic factor. On the other hand, the time scale is controlled by the ratio between the diffusivities of the host and Li atoms. The second issue analyzed is the formation of nano-voids in Li-Si NWs¹ upon cycling. The process is associated with large inelastic deformations and mass transport. Sethuraman et al.² showed that plastic (or viscoplastic) flow is an important mechanism that cannot be neglected. We present a model for the growth of nano-voids based on the balance of stress work rate and the rate of surface energy change. This theory is applied to anodes with core-shell structures to estimate the likelihood of cavitations in the silicon shell, yielding a critical void size above which a void nucleus would grow into a nano-pore and below which the nucleus would heal spontaneously. This critical void size is found to depend on the yield strength, state of charge, surface energy and local stress triaxiality.

- 1 Choi, J. W. *et al.* Stepwise Nanopore Evolution in One-Dimensional Nanostructures. *Nano Letters* **10**, 1409-1413 (2010).
- 2 Sethuraman, V. A., Chon, M. J., Shimshak, M., Srinivasan, V. & Guduru, P. R. In situ measurements of stress evolution in silicon thin films during electrochemical lithiation and delithiation. *Journal of Power Sources* **195**, 5062-5066.