



Kaushik Bhattacharya

Distinguished graduate of the University of Minnesota

Howell N. Tyson Senior Professor of Mechanics, Professor of Materials Science and Vice Provost for Research at Caltech

Visionary researcher and pioneer of the study of phase transformations, the shape memory effect and the behavior of functional materials.

Dedicated teacher, author and editor, and a mentor to a generation of students and postdoctoral fellows in solid mechanics.

EMERGING IDEAS IN MECHANICS AND MATERIALS SCIENCE

UNIVERSITY OF MINNESOTA



**A day of celebration on the
occasion of the conferral of the
Outstanding Achievement Award
to Kaushik Bhattacharya**

October 19, 2018

Program

Morning, 9:00-12:00 Akerman Hall 225

9:00-9:05 Introduction, Richard James

9:05-9:25 Paul Plucinsky, Postdoctoral Associate, AEM, “The designs and deformations of generalized Miura Origami”

9:25-9:45 Eduardo Vitral, Graduate Student, AEM, “Curvature driven evolution of a smectic liquid crystal interface out of thermodynamic equilibrium”

9:45-10:05 Ashley Bucsek, President’s Postdoctoral Associate, AEM, “Ferroelectric energy conversion using first-order phase transformations”

10:00-10:20 Coffee break

10:20-10:40 Mingjian Wen, Graduate Student, AEM, “Data-driven interatomic potentials for 2D heterostructures”

10:40-11:00 Fan Feng, Postdoctoral Associate, AEM, “Several concepts and results on phase transformation of helical structures

11:00-11:20 Kuan Zhang, Postdoctoral Associate, AEM, “Multiscale simulation of 2D heterostructures: Structural and electron diffraction scaling of twisted graphene bilayers”

Combining the crystallographic texture of an electrode with its Li-composition field

Ananya Renuka Balakrishna, Postdoctoral Associate, Aerospace Engineering and Mechanics

A polycrystalline electrode's crystallographic texture affects its properties. For example, grain boundaries and edge-dislocation defects in an electrode influence its fracture toughness and electrochemical potential. These crystallographic defects evolve during battery operation, and little is known about how they interact with the Li-composition field. In this talk, I will introduce a multi-scale phase-field model that couples the host electrode's crystallographic texture with the guest-Li composition field. This approach models individual lattice distortions in the host electrode as a function of the Li-composition field. The study provides insights into how interstitial Li-diffusion accelerates grain boundary migration in an electrode. Overall, the study demonstrates that the phase-field model could be used to crystallographically engineer microstructures with enhanced electrode properties.

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Multiscale simulation of 2D heterostructures: Structural and electron diffraction scaling of twisted graphene bilayers

Kuan Zhang, Postdoctoral Associate, Aerospace Engineering and Mechanics

Layered heterostructures formed by stacking two-dimensional (2D) materials are attracting considerable attention with remarkable properties. The registry-dependent nature of the van der Waals interactions between the layers can drive incommensurate to commensurate structural transitions, complicating the mechanical and electronic behavior. We have developed multiscale framework for simulating the mechanical response of 2D heterostructures. We use this method to study the structural relaxation in twisted graphene bilayers, which involves a localized rotation and shrinking of AA domains that scales in two regimes with the imposed twist. For small twisting angles, the localized rotation tends to a constant; for large twist, the rotation scales linearly with it. The results are validated experimentally through a simulated electron diffraction analysis of the relaxed structures. We predict a complex electron diffraction pattern involving the appearance of weak satellite peaks at small twist regime. The mechanism of this new phenomenon is found to be intimately tied to the scaling behavior, and explained by using an analytical model in which the relaxation kinematics are described as an exponentially-decaying (Gaussian) rotation field centered on the AA domains. Both the angle-dependent scaling and diffraction patterns are in quantitative agreement with experimental observations.

Program (cont.)

11:20-11:40 Ananya Renuka Balakrishna, Postdoctoral Associate, AEM, “Combining the crystallographic texture of an electrode with its Li-composition field”

11:40-12:00 Free-flowing discussion with Kaushik Bhattacharya about science, engineering and career

12:15-1:30 Lunch, **Dale Shepard Room, 4th Floor, Campus Club, Coffman Union**

Afternoon, **2:30-4:30, John T. Tate Hall, Room 105**

2:30-2:35 Dean Mos Kaveh, Remarks and introduction of President Kaler

2:35-2:45 President Eric Kaler, Conferral of the Outstanding Achievement Award

2:45-3:00 Break

3:00-3:15 Richard James, “Introduction to the technical and educational accomplishments of Kaushik Bhattacharya”

3:15-4:15 Kaushik Bhattacharya, “Getting stuck and breaking free: adhesion, friction, strength and toughness”

If you wish to join in the evening’s events, please contact Richard James, james@umn.edu

Abstracts of the Lectures

Getting stuck and breaking free: adhesion, friction, strength and toughness

Kaushik Bhattacharya

Professor and Vice Provost for Research

Outstanding Achievement Awardee, University of Minnesota

Many phenomena of scientific and technological interest are described by the evolution of free boundaries or free discontinuities. Examples include the peel front while peeling an adhesive tape, the rupture front of earthquakes, dislocations in solids and the crack set during fracture. This evolution takes place in a heterogeneous medium where the length-scale of the heterogeneities are much smaller than the length scale of the overall phenomena and we are interested in understanding the overall or effective behavior. This effective behavior is not characterized by averaging, but instead dominated by critical events. Thus, the effective behavior can be qualitatively different from the local behavior. This makes such problems difficult to study, but also offers opportunities for exploiting heterogeneities to dramatically affect material properties. This talk will discuss the underlying issues with examples drawn from fracture, friction, dislocation dynamics, phase boundary propagation and peeling of adhesive tape.

Several concepts and results on phase transformation of helical structures

Fan Feng, Postdoctoral Associate, Aerospace Engineering and Mechanics

An important way of doing research is to make generalization and analogy to previous methods. In the 1990s, Kaushik and Dick developed the martensitic phase transformation theory based on geometrical compatibility in crystalline solids with translation symmetry. The theory was validated experimentally later, in successfully predicting microstructures, shape memory effect, and hysteresis during phase transformation.

In this talk, I will present a similar idea of phase transformation in helical structures with helical symmetry. To do this, several key concepts in martensitic phase transformation of crystalline solids as well as helical structures will be presented, including continuous deformation, compatibility condition, Cauchy-Born rule, point groups, variants, and energy wells. Though the analogy is not perfect, the results of compatible interfaces, average super compatibility, and self-accommodation are promising in helical structures. We conjecture that some similar phenomena such as microstructures and low-hysteresis effect will also exist in helical structures, by satisfying the conditions we derived.

Data-driven interatomic potentials for 2D heterostructures

Mingjian Wen, Graduate Student, Aerospace Engineering and Mechanics

Two-dimensional (2D) heterostructures created by stacking 2D materials have remarkable properties that enable a host of innovative nanotechnological devices. To understand 2D heterostructures and accelerate their development and application, molecular simulations with highly-accurate interatomic potentials are needed. Using state-of-the-art data analytics and machine learning techniques, we are developing interatomic potentials for 2D heterostructures. In this talk, I will present a potential for multilayer graphene systems, which employs an artificial neural network to describe the short-range interactions and a Lennard-Jones potential to capture the long-range van der Waals forces. This potential can accurately predict structural, elastic, and thermal properties of multilayer graphene systems. Additionally, I will show that a neural network potential trained with the dropout technique is equivalent to a Bayesian neural network, thus allowing uncertainty quantification and propagation in molecular simulations

The designs and deformations of generalized Miura Origami

Paul Plucinsky, Postdoctoral Associate, Aerospace Engineering and Mechanics

The Japanese art of paper folding (Origami) is now being exploited in engineering applications—from small-scale MEMs and NEMs devices with complex surface morphologies, to large deployable space structures—due to the dramatic change of shape and reconfigurability achievable through systematic folding. In this talk, we address two general questions of reconfigurability: 1) What are all quadrilateral mesh origami that can be folded from flat to folded flat, and 2) how do we efficiently compute their designs and deformations? Our key idea is a rigidity theorem characterizing the designs of 3×3 flat-foldable, quadrilateral mesh Origami. With this rigidity theorem, we then develop an explicit algorithm for the designs and deformations of any generalized Miura Origami (i.e., flat-foldable, quadrilateral mesh Origami). Finally, we highlight a few examples enabled by this algorithm, which show that the design landscape for these systems is quite rich.

Curvature driven evolution of a smectic liquid crystal interface out of thermodynamic equilibrium

Eduardo Vitral, Graduate Student, Aerospace Engineering and Mechanics

We introduce a mesoscale model of a complex fluid to study the two phase interface separating a layered phase of uniaxial symmetry from an isotropic phase. The model is used to derive capillary and elastic contributions to local equilibrium conditions at deformed interfaces (generalized Gibbs-Thomson relations), extra stresses and their contribution to flow, and the nonequilibrium equations governing interfacial motion. Particular attention is paid to often neglected surface isometric invariants such as the Gaussian curvature, and its role in driving changes of topology of the interface during its evolution. The methodology also lends itself to large scale computational analysis, with a parallel implemented pseudo-spectral approach. Our study is motivated by recent experiments on surface instabilities of toroidal focal conic domains in smectic films, and out of equilibrium numerical results are shown to match some of the experimentally observed morphologies. Through the derived equations for the interface, we discuss how the curvature induced evaporation and the alignment of the smectic planes explain the formation of these nonequilibrium structures.

Ferroelectric energy conversion using first-order phase transformations

Ashley Bucsek, President's Postdoctoral Associate, Aerospace Engineering and Mechanics

The discovery of new methods of generating energy without adversely affecting the environment is the most compelling scientific problem of our time. Due to continuously rising societal needs, energy is being both consumed and wasted in increasing quantities. Roughly 60% of unrecovered waste heat is considered "low grade" because of the difficulty of converting small temperature differences to electric or mechanical energy using conventional technologies. Yet, the abundance of natural and industrial waste heat at small temperature differences is a growing and drastically underutilized stockpile of convertible energy. We present a novel energy conversion device that converts small temperature differences to electricity using ferroelectric capacitors. Ferroelectrics undergo a first-order phase transformation between a phase that is strongly polarized and a phase that is not polarized. We use analogies between the ferroelectric phase transformation and the first-order phase transformation utilized in steam engines to discuss thermodynamic efficiencies and power densities. We also demonstrate the conversion capabilities of such a device, present a theoretical framework to model the circuit parameters, and discuss using phase engineering to achieve extreme cyclic repeatability.