

USACM Thematic Workshop
Recent Advances in the Modeling and Simulation of the Mechanics of
Nanoscale Materials

Glandt Forum, Singh Center for Nanotechnology, 3rd Floor

Wednesday, August 21

8:15-8:45am Registration and light breakfast

8:45-9:00am Welcome and opening remarks

Session 1: First Principle Calculations and Quantum Properties

9:00-9:30am **Vikram Gavini.** Large-scale real-space electronic structure calculations

9:30-10:00am **Amartya Banarjee.** Symmetry, deformations and the search for unprecedented materials from first principles

10:00-10:30am **Mauricio Ponga.** How defects affect quantum mechanical properties in crystalline materials.

10:30-11:00am Refreshment Break

Session 2: Plasticity

11:00-11:30am **David Rodney.** Physical foundation of non-Schmid yield criterion in BCC metals

11:30-12:00pm **Eugen Rabkin.** The microstructural origins of size effect in strength of metal nanoparticles

12:00-12:30pm **John Bassani.** Non-associative plastic flow: insights from multiscale simulations

12:30-1:45pm Lunch

Session 3: Defects I

1:45-2:15pm **David McDowell.** Some challenges in length and time scaling for modeling dislocations

2:15-2:45pm **Michael Ortiz.** Atomistic simulation of hydrogen storage in Pd nanoparticles

2:45-3:15pm **Emmanuel Clouet.** Secondary slip of screw dislocations in hcp zirconium

3:15-3:45pm Refreshment Break

Session 4: Defects II

- 3:45-4:15pm **Jaime Marian.** Simulating dynamic strain aging in body-centered cubic metals on diffusive timescales
- 4:15-4:45pm **Anter El-Azab:** A continuum theory for defects and microstructure evolution in irradiated crystalline solids
- 5:00-6:30pm Poster Session (3rd Floor)

Thursday, August 22

- 8:00-8:30am Light Breakfast

Session 5: Grain Boundaries and Interfaces

- 8:30-9:00am **Yas Kulkarnee.** Mechanistic insights into crystalline interfaces via thermal fluctuations
- 9:00-9:30am **Nikhil Admal.** Polycrystal plasticity with anisotropic grain boundary evolution
- 9:30-10:00am **Brandon Runnels.** Unifying mechanisms of grain boundary migration through a continuum thermodynamic framework
- 10:00-10:30am Refreshment Break

Session 6: Mechanics of Materials I

- 10:30-11:00am **Garritt Tucker.** Implementing higher-order descriptors to unravel competing deformation effects at an atomic scale
- 11:00-11:30am **Tim Rupert.** Probing nanoscale complexion transformations with computational techniques that complement experiments
- 11:30-12:00pm **Jun Lou.** Quantitative in-situ nanomechanical study of low dimensional materials
- 12:00-12:30pm **Mitra Taheri.** Toward the tailoring materials properties far from equilibrium: Convergence of microscopy, data science, and theory
- 12:30-1:45pm Lunch

Session 7: Mechanics of Materials II

- 1:45-2:15pm **Ryan Elliott.** A framework for the interpretation of modulated martensites in shape memory alloys
- 2:15-2:45pm **Prashant Purohit.** Interactions and assembly of inclusions on lipid membranes
- 2:45-3:15pm **Andrej Kosmrlj.** Statistical mechanics of microscopically thin thermalized structures
- 3:15-3:45pm Refreshment Break

Session 8: Mechanics of Materials III

- 3:45-4:15pm **Pradeep Sharma.** Flexoelectricity and Electrets
4:15-4:45pm **Kaushik Dayal.** Electromechanics and statistical mechanics of dielectric elastomers
4:45-5:15pm **Pedro Ponte-Castañeda.** Macroscopic instabilities and domain formation in elastomeric composites
7:30pm Dinner; White Dog Cafe

Friday, August 23

- 8:00-8:30am Light Breakfast

Session 9: Phase Field Models

- 8:30-9:00am **Peter Voorhees.** The morphology and topology of nanoporous metals
9:00-9:30am **Katsuyo Thornton.** Nanoscale simulations using phase-field- crystal models
9:30-10:00am **Martin Diehl.** TBA
10:00-10:30am Refreshment Break

Session 10: Scale Bridging I

- 10:30-11:00am **Jarek Knap.** Accelerating Scale Bridging via Surrogate Modeling
11:00-11:30am **Yuri Mishin.** Physically-informed artificial neural networks for atomistic modeling of materials
11:30-12:00pm **Xin Yan.** Time-Scaling in atomistics and the rate-dependent mechanical behavior of nanostructures
12:00-1:15pm Lunch

Session 11: Scale bridging II

- 1:15-1:45pm **Dan Mordehai.** Calculating the activation parameters of thermally activated dislocation mechanisms
1:45-2:15pm **Andrea Liu.** Exploiting the malleability of disorder to design biologically-inspired function