

Workshop II: Atomistic and Mesoscale Modeling of Materials Defects

Monday October 22, 2012

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome and Opening Remarks*
- 9:00–9:50 **Dallas Trinkle** (University of Illinois at Urbana-Champaign)
Dislocation cores and defect interactions from first principles: Current state of the art and new challenges
- 10:00–10:15 *Break*
- 10:15–11:05 **Wei Cai** (Stanford University)
Entropic Effect On the Rate of Dislocation Nucleation
- 11:15–11:30 *Break*
- 11:30–12:20 **Kristen Fichthorn** (Pennsylvania State University)
Accelerating Rare-Event Simulations by Solving the Small-Barrier Problem
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Ken Elder** (Oakland University)
Patterning of Heteroepitaxial Overlayers from Nano to Micron Scales
- 3:30–4:00 *Break*
- 4:00–4:50 **Steve Wise** (University of Tennessee)
- 5:00–7:00 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 23, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Mark Asta** (University of California, Berkeley (UC Berkeley))
Insights into Grain-Boundary Motion through Coupling of In-Situ Electron Microscopy and Molecular Dynamics Simulations
- 10:00–10:15 *Break*
- 10:15–11:05 **Danny Perez** (Los Alamos National Laboratory)
Vibrational contributions to kinetics in the solid state
- 11:15–11:30 *Break*

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- 11:30–12:20 **Abhijit Chatterjee** (Indian Institute of Technology Kanpur)
Building an Error Measure for a Kinetic Monte Carlo Model
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Christoph Ortner** (University of Warwick)
Optimising Multiscale Defect Simulations
- 3:30–4:00 *Break*
- 4:00–4:50 **Marisol Koslowski** (Purdue University)
Effect of microstructural uncertainty on the mechanical response of nanocrystalline materials

Wednesday October 24, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Irene Beyerlein** (Los Alamos National Laboratory)
Interface-driven microstructure evolution in two-phase nanocomposites
- 10:00–10:15 *Break*
- 10:15–11:05 **Anthony Rollett** (Carnegie-Mellon University)
Hot Spots in Viscoplastic Deformation of Polycrystals
- 11:15–11:30 *Break*
- 11:30–12:20 **Abdelkader Kara** (University of Central Florida)
Self-Learning Kinetic Monte Carlo: From 2D on-lattice to 3D off-lattice and beyond
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Alexander Stukowski** (Technische Universität Darmstadt)
Large-Scale Atomistic Simulations of Crystals: Defect Identification and Indexing Methods
- 3:30–4:00 *Break*
- 4:00–4:50 **John Lowengrub** (University of California, Irvine (UCI))
Bijels: Stabilizing Fluid-fluid Interfaces by Colloidal Particles - A Navier-Stokes-Cahn-Hilliard-Phase-Field-Crystal Approach

Thursday October 25, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Talat Rahman** (University of Central Florida)
*The extended Self Learning Kinetic Monte Carlo Method: now lurking into 3D**
- 10:00–10:15 *Break*

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- 10:15–11:05 **David Rodney** (Institut National Polytechnique de Grenoble (INPG))
Understanding the thermally activated glide of dislocations from the atomic scale
- 11:15–11:30 *Break*
- 11:30–12:20 **Arvind Baskaran** (University of California, Irvine (UCI))
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Shaun Hendy** (Victoria University of Wellington)
Effective rate constants for nanostructured heterogeneous catalysts
- 3:30–4:00 *Break*
- 4:00–4:50 **Brian Laird** (University of Kansas)
Atomistic simulations of chemically heterogeneous metal interfaces

Friday October 26, 2012

- 8:00–9:00 *Continental Breakfast*
- 9:00–9:50 **Jim Evans** (Iowa State University)
Self-assembly and directed-assembly of multi-component metal nanoclusters
- 10:00–10:15 *Break*
- 10:15–11:05 **Xanthippi Markenscoff** (University of California, San Diego (UCSD))
Driving forces on moving defects: dislocations and phase boundaries (with inertia effects)
- 11:15–11:30 *Break*
- 11:30–12:20 **Jeremy Mason** (Lawrence Livermore National Laboratory)
Rigorous quantification of the grain growth microstructure in two and three dimensions
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Tim Schulze** (University of Tennessee)
Off-lattice KMC simulation of quantum dot formation

