

APS Workshop 2: Advancing Materials Research: Synergies in Large Scale Simulations and APS-U Imaging and Microscopy Techniques

Wednesday, May 7, Morning

- 8:30 – 9:00 Ross Harder and Jon Tischler (X-ray Science, Argonne National Laboratory)
Introduction and Opening Remarks
- 9:00 – 9:30 Anter El-Azab (School of Materials Engineering, Purdue University)
Machine Learning of Dislocation Microstructure from DAXM Data and a Theoretical Perspective from Mesoscale Theory of Crystal Defects
- 9:30 – 10:00 Felix Hofmann (Department of Engineering Science, University of Oxford)
Irradiation-induced Structure and Property Evolution in Metals: Combining Large-scale Atomistic Simulations and X-ray Observations
- 10:00 – 10:30 Break
- 10:30 – 11:00 Subramanian Sankaranarayanan (Center for Nanoscale Materials, Argonne National Laboratory)
Probing Defect Dynamics through Integrated Molecular Simulations, Imaging, and Machine Learning
- 11:00 – 11:30 Youping Chen (University of Florida)
Concurrent Atomistic-continuum Simulation of Materials and Heterostructures from Synthesis to Microstructure and Properties
- 11:30 – 12:00 Anthony Rollett (Department of Materials Science and Engineering, Carnegie Mellon University)
Synchrotron X-ray Microscopy Combined with Simulation and Machine Learning
- 12:00 – 1:30 Lunch Break

Wednesday, May 7, Afternoon

- 1:30 – 2:00 Henning Poulsen (The 3D Imaging Center, Technical University of Denmark)
Dark Field X-ray Microscopy and the Origin of Metal Plasticity
- 2:00 – 2:30 Leora Dresselhaus-Marais (Geballe Laboratory for Advanced Materials, Stanford University)
Subsurface Imaging of Multi-timescale Defect Dynamics
- 2:30 – 3:00 Stephan O. Hruszkewycz (Materials Science, Argonne National Laboratory)
Guiding High-energy Coherent Diffraction and HEDM Measurements with Mesoscale Crystal Plasticity Modeling

- 3:00 – 3:30 Break
- 3:30 – 4:00 Mathew J. Cherukara (X-ray Science, Argonne National Laboratory)
AI-enhanced X-ray Imaging: Bridging Length Scales to Visualize Materials Dynamics
- 4:00 – 4:30 Paul Evans (Materials Science and Engineering, University of Wisconsin-Madison)
Solid-phase Crystallization of Complex Oxides: Complementarity of X-ray Nanobeam Diffraction and Molecular Simulation
- 4:30 – 5:00 Workshop Organizers
Closing Discussion
- 5:00 Adjourn