UNIVERSITY OF CALIFORNIA, IRVINE THE DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

Is Proud to Host a Seminar by:

## ASSISTANT PROFESSOR AMANDA R. KRAUSE

Department of Materials Science and Engineering Carnegie Mellon University



CAPTURING GRAIN BOUNDARY MIGRATION IN 3D POLYCRYSTALS

> DATE: Thursday, May 30, 2024 TIME: 2:00 - 3:20 PM LOCATION: McDonnell Douglas Engineering Auditorium

Abstract: Curvature is considered the common local driving force for grain boundary motion in all polycrystals. However, models and simulations derived from curvature-based motion cannot predict irregular, albeit commonly observed, grain growth behavior. To build better predictive models, we need to employ new tools to understand what governs microstructure evolution. This talk will highlight two of these tools: high energy x-ray diffraction microscopy (HEDM) and machine learning. HEDM is a non-destructive method that maps the full microstructure, providing an opportunity to observe grain growth in real 3D polycrystalline systems. In this talk, I will compare experimental observations of growth in strontium titanate and alumina with Monte Carlo Potts simulations to interrogate the role of curvature and grain boundary energy in microstructure evolution. Then, I will then describe how machine learning models can capture the underlying behavior of an evolving Markov decision process and "teach" it to maximize the "rewards" regarding the agreement between prediction and experimental observations. To demonstrate the feasibility of this approach, we built a deep reinforcement model that emulates grain growth by training on Monte Carlo Potts grain growth simulations. The accuracy of our short and long-term predictions will be evaluated. Then, I will discuss how HEDM and our machine learning model can be combined to understand how anisotropic grain boundaries migrate in 3D polycrystals.

**Bio:** Dr. Amanda R. Krause is an Assistant Professor in the Materials Science and Engineering Department at Carnegie Mellon University. She received her B.S. and M.S. in Materials Science and Engineering from Virginia Tech, and her Ph.D. in Materials Science from Brown University. Before joining Carnegie Mellon University in 2022, she was an Assistant Professor at University of Florida (2019-2022) and a post-doctoral research associate at Lehigh University. Her research focus is engineering grain boundaries and microstructures for improving the mechanical performance and degradation response of ceramics used in extreme environments. She is a recipient of the NSF CAREER award (2022) and the Wimmer Faculty Fellowship (2023) from CMU's Eberly Center for Teaching Excellence & Educational Innovation.

