COLLEGE OF ENGINEERING
MECHANICAL ENGINEERING
UNIVERSITY OF MICHIGAN

Diffuse Interface Methods for Modeling Materials: Concepts and Applications

Katsuyo Thornton

L.H. and V.E. Van Vlack Professor of Materials Science & Engineering
University of Michigan

Tuesday, September 3rd, 2024
4:00 PM to 5:00 PM
Room 2540 GGB

ME Seminar Link
Passcode: 421395

Add ME Seminar to Google Calendar

Abstract:
Controlling microstructures in multiphase/composite materials is one of the primary routes for improving the properties and performance of materials. However, material microstructures are typically complex, with irregularly shaped phase boundaries that can evolve, necessitating simulations to understand and predict their effects on properties. Traditional interface tracking is numerically difficult because the boundary mesh can become entangled or otherwise become unsuitable for solution convergence. In this talk, I present two diffuse interface approaches: the

phase-field modeling, which is well established in predicting microstructure evolution, and the Smoothed Boundary Method, which is a generic method for setting boundary conditions within a computational domain. I will first provide an overview of these approaches and various applications. I will then present a few insights gained through simulations enabled by these methods, including the modeling of electrochemical dynamics in battery electrodes, which combines both of these methodologies. I will also describe the activities within the Software Innovation Center, PRISMS, which are facilitating advances in simulation-based material science and engineering.

Bio:

Professor Thornton is the L.H. and F.E. Van Vlack Professor of Materials Science & Engineering. She received her B.S. degree in Physics with Honors from Iowa State University and her M.S. and Ph.D. degrees in Astronomy and Astrophysics from the University of Chicago. Following appointments at Northwestern University and MIT, she joined the faculty at the University of Michigan. Her research focuses on computational modeling of materials based on the thermodynamics and kinetics of materials, as well as electrochemical reactions and other processes that alter material behavior. She harnesses the growing high-performance-computing resources to elucidate the complex interplay between thermodynamics and kinetics of materials, as well as mechanics and electrochemistry. She has nearly 150 publications in journals and books, including Nature, Nature Materials, Science Advances, Proceedings of the National Academy of Sciences, Applied Physics Letters, Physical Review Letters, and Advanced Materials. Her work has been recognized through the TMS Julia and Johannes Weertman Educator Award, TMS Brimacombe Medal, the TMS MPMD Distinguished Service Award, the TMS Early Career Faculty Fellow Award, the NSF CAREER Award, the Jon R. and Beverly S. Holt Award for Excellence in Teaching, and the Carl Sagan Excellence in Teaching Award. She is a Fellow of the ASM International.