MSE SEMINAR

Materials Science and Engineering
Michigan Technological University

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3:00 pm – 4:00 pm
Room 610, M&M Building

Combined Simulation and Experimental Approaches to Understanding Growth and Coarsening Processes

John & Virginia Towers Distinguished Lecture Series

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Abstract

Increasing computational power is allowing simulation to become an important tool for materials scientists and engineers in understanding and optimizing material behavior and performance. In this talk, I will show two examples of how phase-field simulations, closely coupled with experiments and theory, have given new insights into growth and coarsening processes. In the first example, the evolution of a dendritic microstructure in an Al-Cu alloy was studied during coarsening as a solid-liquid mixture. The microstructure was captured in real time using 4D X-ray tomography and the time evolution was compared with phase-field simulations, which allowed the calculation of the diffusion coefficient of solute in the liquid phase. The simulation results were used to inform a theoretical prediction of the rate of pinching of liquid and solid rods during coarsening, which is applicable to phenomena such as the detachment of dendrite secondary arms during casting and directional solidification. In the second example, the growth of GaN quantum dots and GaN/InGaN heterostructures by selective area epitaxy was studied for applications in hot carrier solar cells. A model was developed to simulate kinetically limited growth of GaN by metallorganic chemical vapor deposition, where the growth rate is a function of crystallographic orientation. By comparing simulations with experiments, the relative importance of deposition pathways was determined, and this information was used to predict the optical properties of InGaN active layers embedded in the quantum dots. A parametric study was also performed to predict growth conditions leading to improved optical properties.

Biography: Dr. Larry Aagesen is currently a postdoctoral research fellow in the Department of Materials Science and Engineering at the University of Michigan. His research interests are in the application of theoretical and computational techniques to study the evolution of microstructures and nanostructures during crystal growth, phase transformations, coarsening, and exposure to extreme environments, and how this evolution affects material properties. Current projects at Michigan focus on the growth of semiconductor quantum dots for high-efficiency third-generation solar cell designs and corrosion of zirconium for nuclear power applications. Larry received a B.A. in physics from the University of California Berkeley. He served as an officer in the U.S. Navy's nuclear power program for several years prior to graduate school, which sparked an interest in materials for energy applications. He received M.S. and Ph.D. degrees in materials science and engineering from Northwestern University, where his research focused on phase-field simulation and analysis of dendritic microstructures formed during solidification of metal alloys.

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