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ARMS 1010

PETER VOORHEES

Frank C. Engelhart Professor Materials Science & Engineering & Professor of Engineering Sciences and Applied Mathematics (by courtesy)

Northwestern University

"Simulations of Microstructural Evolution at the Mesoscale"

Abstract: Simulations can be used to both measure materials parameters and predict the evolution of the morphology of interfaces in materials. Following an introduction to the phase field method, the central role of quantitative phase field simulations in mesoscale simulations will be illustrated by a rapid throughput method to determine grain boundary properties, and simulations of microstructural development during additive manufacturing. By comparing the evolution of experimentally determined three-dimensional grain structures to those derived from simulation, it is possible to measure the reduced mobilities of thousands of grain boundaries. Using a time step from these data an initial condition in a phase-field simulation, the computed structure is compared to that measured experimentally at a later time. An optimization technique is then used to find the reduced grain boundary mobilities of over 1300 grain boundaries in iron that yield the best match to the simulated microstructure. We find that the grain boundary mobilities are largely independent of the five macroscopic degrees of freedom given by the misorientation of the grains and the inclination of the grain boundary. A phase field model will be presented that follows the evolution of thousands of grains during additive manufacturing in three dimensions. The model is developed in the rapid solidification limit where there is no segregation in the solid. The advantage of the approach is that it captures the physics of the motion and rotation of the grain-boundary-solid-liquid-interface trijunctions that are responsible for the evolution of the grain morphology; it is not a rule-based model. A comparison between the grain shapes predicted by the simulations and those measured experimentally will be given.

Biography: Peter Voorhees is the Frank C. Engelhart Professor of Materials Science and Engineering at Northwestern University, and Professor of Engineering Sciences and Applied Mathematics (by courtesy). He is co-director of the Northwestern-Argonne Institute of Science and Engineering, director of the Center for Hierarchical Materials Design and is chair of the Department of Materials Science and Engineering. He received his Ph.D. in Materials Engineering from Rensselaer Polytechnic Institute and was a member of the Metallurgy Division at the National Institute for Standards and Technology until joining the Department of Materials Science and Engineering at Northwestern University. He has received numerous awards including the ASM International Materials Science Division Research Award (Silver Medal), the TMS Bruce Chalmers Award, the ASM J. Willard Gibbs Phase Equilibria Award, and the McCormick School of Engineering and Applied Science Award for Teaching Excellence. Professor Voorhees is a fellow of ASM International, the Minerals, Metals and Materials Society, and the American Physical Society. He is a member of the American Academy of Arts and Sciences. He has published over 300 papers in the area of the thermodynamics and kinetics of phase transformations.

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