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Using Atomistic Simulations to Inform Mesoscale Simulations of Microstrucuture Evolution

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Predicting and controlling the evolution of materials microstructure is one of the central challenges of materials science. The simulation of microstructural evolution requires a detailed knowledge of the properties, including energies and mobilities, of interfaces in the material. In this talk, the use of molecular dynamics simulations to determine these interfacial properties will be discussed as well as theoretical concepts required to incorporate this information into higher length scale simulations. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC0494AL85000.