Mesoscale Modeling of Grain Boundaries: From Inter-diffusion Processes to Alloy Segregation

F. Abdeljawad, P. Kotula, S. Prasad, S. M. Foiles

Material, Physical, and Chemical Sciences Center

Sandia National Laboratories, Albuquerque, NM, 87185 USA

The response of materials to a wide range of stimuli is a direct manifestation of their characteristic microstructural features. Thus, it is of great importance to understand microstructure in order to predict its role on the macroscopic properties of materials, and ultimately develop innovative ones with increased functionality. In this presentation, we cover the development of mesoscopic models aimed at examining the role of grain boundaries (GBs) in processes ranging from inter-diffusion and Kirkendall effect in thin films to alloy segregation in nanocrystalline (NC) materials. We first start by examining inter-diffusion processes in binary metallic alloys. A modeling framework is developed based on the smooth boundary method [1], which explicitly tracks vacancies and accounts for GBs as efficient sources/sinks for vacancies. Analytical and simulation results highlight the role of GB-vacancy interactions on the diffusive transport in binary alloys and formation of Kirkendall voids. The second part of the talk is focused on nanocrystalline (NC) materials and their instability against grain growth processes even at low service temperatures, an effect that hinders their use in extreme environments [2]. Grain boundary (GB) solute segregation has been recently proposed as a route to thermally stabilize the grain structures of NC materials [3]. With the aid of a mesoscale model [4], we examine GB solute segregation and its role on the stabilization of NC alloys. Simulation results identify regimes, where the reduction in GB energy, and thus the driving force for grain growth, is significant [5].

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