An atomistic perspective on interface diffusion and migration mechanisms

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How do atoms move during interface diffusion and migration? The most detailed answers to these questions currently come from atomistic simulations. Although these simulations are limited with respect to both time and length scales, they give valuable insights into how interface diffusion and migration mechanisms vary with crystallography, composition and temperature. In this talk, I will discuss our recent efforts to characterize grain boundary migration mechanisms in FCC metals and interface diffusion mechanisms in pure Al grain boundaries and Al-Si composites. Collective mechanisms which involve the correlated motion of many atoms are found to be ubiquitous during both interface diffusion and migration. I will review two types of methods which have been useful for the analysis of collective mechanisms: 1) geometric lattice matching methods in the dichromatic pattern and 2) statistical methods to quantify dynamical heterogeneity.