Grain Boundary Mobility Tensor and Topological Phase Transitions

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Abstract:
The GB mobility relates the GB velocity to the driving force. While the GB velocity is normally associated with motion of the GB normal to the GB plane, there is often a tangential motion of one grain with respect to the other across a GB; i.e., the GB velocity is a vector. Grain boundary motion can be driven by a chemical potential jumps across a GB or by shear applied parallel to the GB plane; the driving force has three components. Hence, the GB mobility must be a tensor (the off-diagonal components indicate shear coupling). Recent Molecular Dynamics (MD) and experimental studies show that the GB mobility may abruptly jump, smoothly increase, decrease, remain constant or show multiple peaks with increasing temperature. Performing MD simulations on symmetric tilt GBs in copper, we demonstrate that all six components of the GB mobility tensor are non-zero (the mobility tensor is symmetric, as required by Onsager). We demonstrate that some of these mobility components increase with temperature, while, surprisingly, others decrease.
We develop a disconnection dynamics-based statistical model that suggests that GB mobilities follow an Arrhenius relation with respect to temperature T below a critical temperature T_c and decrease as 1/T above it. T_c is related to the operative disconnection modes and their energetics. We implement this model in a kinetic Monte Carlo (kMC); the results capture all of these observed temperature dependencies and are shown to be in quantitative agreement with each other and direct MD simulations of GB migration for a set of specific grain boundaries. We demonstrate that the abrupt change in grain boundary mobility results from a Kosterlitz-Thouless (KT) topological phase transition. This phase transition corresponds to the screening of the long-range interactions between (and unbinding of) disconnections. This phase transition also leads to abrupt change in GB sliding and roughening. We analyze this KT transition through mean-field theory, renormalization group methods, and kMC simulation. Finally, we examine the impact of the generalization of the mobility and KT transition for grain growth and superplasticity.