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Temperature-dependent modeling of grain boundary energy anisotropy and applications to interface morphology

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Grain boundaries (GBs) in polycrystalline materials are unique defects that exhibit a strong energetic dependence on relative crystallographic orientation. This behavior, referred to as grain boundary anisotropy, dominates many mesoscopic mechanisms such as solidification, recrystallization, grain boundary migration, and severe plastic deformation. To this end, it is of great importance to understand and predictively model grain boundary energy. An analytical model is presented in this work that computes GB energy quickly and predictively for a wide range of materials and crystal structures for all GB configurations in the five-dimensional space of crystallographic orientation pairs. This forms the basis for a fully general, temperature-dependent energetic grain boundary energy model, and it is demonstrated by comparison with a wide selection of molecular dynamics energy data for FCC and BCC tilt and twist boundaries that the model accurately reproduces the energy landscape using a consistent set of three material parameters. By the application of a relaxation method, it is then demonstrated that the model can be extended from planar GBs to GBs with complex morphology. Application of this method shows that GB facet patterns arise as energy minimizers in a wide range of orientations, and the model predictions are validated by MD and experimental observations. Additionally, it is shown that the model captures the temperature-dependence of the GB energy by reproducing experimentally observed temperature-dependent faceting transitions. The talk concludes with a brief discussion of current challenges, future directions, and direct applications of the model.