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A Variational Approach to Crystalline Interfaces: A New Method for Predicting Interface Energy and Morphology

Brandon Runnels
Computational Solid Mechanics Group, California Institute of Technology
E-mail: lwlin@me.berkeley.edu

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Abstract:

Interfaces in crystalline materials are at the forefront of research in micromechanics and multiscale modeling. In particular, interfaces with complex morphologies have been observed to play a crucial role in many micromechanical phenomena such as grain boundary migration, stability, and twinning. However, the complex and diverse behavior of interfaces is still an active area of research, and it appears that there are no predictive models for the energy and morphology of interfaces with arbitrary character. In my talk, I introduce a new model for predicting the energy of an interface of arbitrary character between crystalline materials of arbitrary structure. Building on this general interface energy model, I propose a method for predicting the relaxed energy and morphology of interfaces. I formulate a variational principle for interface energy, and show that the interface energy functional is in most cases nonconvex. Because of this, the functional lacks lower semicontinuity and consequently the the infimum is not attained in general. Following the usual approach for treating nonconvexity in mechanics, I propose a faceting construction that recovers the convexification of the interface energy functional, making the problem well-posed. I then formulate the model in a computationally convenient manner and introduce an algorithm for computing the relaxed energy and structure with an arbitrary interface energy model. I then discuss our implementation of the convexification method together with the general interface energy model, and provide results for several examples in various face-centered cubic (FCC) grain boundaries. For symmetric tilt boundaries, it is concluded that the relaxation construction greatly improves the energy calculation from the unrelaxed model. For asymmetric tilt and symmetric twist boundaries, it is determined that the convexification gives good results for the energy and morphology of the interfaces.

Biographical Sketch

Brandon Runnels is currently a graduate student at the California Institute of Technology in the Computational Solid Mechanics group, working with Professor Michael Ortiz. He earned his B.S. in Mechanical Engineering from New Mexico Tech in 2011; his M.S. in Mechanical Engineering from Caltech in 2012, and will graduate from Caltech with his PhD in Mechanical Engineering this Spring. In addition to his studies at the university, he has worked for 9 summers at Los Alamos National Lab, most recently as a fellow at the LANL Seaborg Institute.