



Mechanical and Civil Engineering Thesis Defense

Monday, June 15, 2015

2:30 p.m. in 101 Guggenheim (Lees-Kubota Hall)

“A general model for the energy and morphology of grain boundaries in crystalline materials”

Brandon Runnels

Graduate Student, Mechanical Engineering

• **Abstract** It has been well-established that interfaces in crystalline materials are key players in the mechanics of a variety of mesoscopic processes such as solidification, recrystallization, grain boundary migration, and severe plastic deformation. 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. Interfaces are a unique type of material defect in that they demonstrate a breadth of behavior and characteristics eluding simplified descriptions. Indeed, modeling the complex and diverse behavior of interfaces is still an active area of research, and to the author’s knowledge there are as yet no predictive models for the energy and morphology of interfaces with arbitrary character. The aim of this thesis is to develop a novel model for interface energy and morphology that i) provides accurate results (especially regarding “energy cusp” locations) for interfaces with arbitrary character, ii) depends on a small set of material parameters and iii) is fast enough to incorporate into large scale simulations.

• In the first half of the work, a model for planar, immiscible grain boundary is formulated. By building on the assumption that anisotropic grain boundary energetics are dominated by geometry and crystallography, a construction on lattice density functions (referred to as “covariance”) is introduced that provides a geometric measure of the order of an interface. Covariance forms the basis for a fully general model of the energy of a planar interface, 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 only three material parameters. It is observed that the planar constraint on the model is, in some cases, over-restrictive; this motivates an extension of the model.

• In the second half of the work, the theory of faceting in interfaces is developed and applied to the planar interface model for grain boundaries. Building on previous work in mathematics and materials science, an algorithm is formulated that returns the minimal possible energy attainable by relaxation and the corresponding relaxed morphology for a given planar energy model. It is shown that the relaxation significantly improves the energy results of the planar covariance model for FCC and BCC tilt and twist boundaries. The ability of the model to accurately predict faceting patterns is demonstrated by comparison to molecular dynamics energy data and experimental morphological observation for for asymmetric tilt grain boundaries. It is also demonstrated that by varying the temperature in the planar covariance model, it is possible to reproduce a priori the experimentally observed effects of temperature on facet formation.

• Finally the range and scope of the covariance and relaxation models having been demonstrated by means of extensive MD and experimental comparison, future applications and implementations of the model are explored.

