ME Seminar

Microstructure evolution in polycrystalline metals: from optimal transportation to phase field disconnections

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ABSTRACT

Grain boundary (GB) migration is a key mechanism underlying such phenomena as deformation twinning, recrystallization, solidification, and many others. While GB migration has received a great deal of attention at the atomistic level (both experimentally and computationally), the mesoscale picture of GBs has remained relatively unexplored. Consequently, mesoscale models of GBs have tended to be overly simplistic, failing to capture some of the key mechanisms of interest in microstructure evolution. The overarching goal of this work is to develop a comprehensive and predictive mesoscale treatment of GB migration. The contributions of this presentation are threefold: The first contribution of this work is the development of a rigorous continuum thermodynamic framework for GB migration. GBs are known to exhibit a wide range of migration behavior that is highly dependent on GB character, temperature, and loading conditions. In this work we show that shear-coupled GB migration is analogous to crystal plasticity (CP), and admits a corresponding formulation using the principle of minimum dissipation potential. It is shown that this general principle, when specialized to a number of different boundaries, is able to accurately reproduce the observed shear coupling behavior. The second contribution of this work is the demonstration that the mechanism of disconnection-mediated GB migration is, in fact, a natural consequence of (i) GB energy anisotropy and (ii) the minimum dissipation potential governing GB migration. Disconnections may be thought of as "facets" resulting from strong orientation dependence. These facets then create stress concentrations, which in turn produce strong driving forces localized at the facet corners. A phase field implementation of this model is developed, and results for several boundaries undergoing shear coupling are presented. The third contribution of this work is the development of a novel nucleation model that is used to introduce thermal dependence into the phase field disconnection framework. Just as with real disconnections, phase field disconnections require nucleation in order to propagate. We present a general algorithm that is able to consistently generate disconnections at the GB in a temperature-dependent manner. This model makes it possible to explore the effects of temperature and GB size on GB mobility from a continuum perspective.

ABOUT THE SPEAKER

Dr. Brandon Runnels received his PhD from the California Institute of Technology (Caltech) in June 2015 after receiving his B.S. and M.S. in Mechanical Engineering from New Mexico Tech (2011) and Caltech (2012), respectively, while working summers as a research asssistant at Los Alamos National Laboratory. In August 2015 he joined the Mechanical & Aerospace Engineering faculty at the University of Colorado in Colorado Springs, CO. Dr. Runnels' interests are focused on multiscale materials modeling of the behavior of solids from the atomistic to continuum scales, and developing the computational techniques needed to accelerate materials simulation. He leads a research group involved with projects ranging from designing solid rocket propellant to analytic multiscale models for microstructure evolution.

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