Continuum modeling of grain boundary plasticity using dislocations and disconnections

Nikhil Chandra Admal

Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Illinois, USA

The macroscopic thermomechanical response of a polycrystalline material depends on its microstructure, which itself evolves. The focus of this talk is on the mesoscale modeling of the evolution of grain boundaries, which is a fundamental open problem relevant to technologically important processes such as additive manufacturing.

Traditionally, grain boundary (GB) evolution was modeled as motion by curvature (Mullins model [3]) which is a consequence of minimizing the GB energy. On the other hand, molecular dynamics simulations demonstrate that grain boundaries not only respond to stress but also plastically deform a material as they move resulting in a coupling between GB motion and deformation in phenomena such as stress-induced GB motion, and grain rotation. This observation, and the necessity to study large aggregates of grains motivate us to generalize the Mullins model.

In this talk, I will describe two approaches to model GB evolution and the accompanying plasticity. In the first approach [1], GBs are constructed using geometrically necessary dislocations (GNDs), and the GB energy is included in the constitutive law via the norm of the GB-GNDs. The simplicity of the model, and its ability to describe the coupled phenomena mentioned above are the highlights of the model. On the other hand, its major shortcoming arises from the non-uniqueness of GNDs to describe a grain boundary.

Next, motivated by the recent work of [2], I will describe our ongoing work on a second approach wherein GB evolution is modeled using continuum disconnections, which are dislocations with a step character. While the disconnections-based approach addresses the shortcomings of the GND-based approach, it is limited to specialized (Σ) grain boundaries. Finally, I will close with a proposal of a model that combines ideas from the two approaches and will enable us to model GB evolution in arbitrary polycrystals.

References

[1] N. C. Admal, G. Po, and J. Marian. "A unified framework for polycrystal plasticity with grain boundary evolution". *International Journal of Plasticity* 106 (2018), pp. 1–30.

[2] J. Han, S. L. Thomas, and D. J. Srolovitz. "Grain-boundary kinetics: A unified approach". *Progress in Materials Science* 98 (2018), pp. 386–476.

[3] W. W. Mullins. "Two-dimensional motion of idealized grain boundaries". *Journal of Applied Physics* 27.8 (1956), pp. 900–904.