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Challenges in Modeling Polycrystalline Materials

Polycrystalline materials, such as steel, aluminum and copper, are ubiquitous in most technological applications. Their use can be found in small devices such as smartphones, as well as in much larger machines; cars, ships and airplanes. These materials exhibit complex response to thermal and mechanical loading that is mostly due to defects, their nucleation and evolution. Changes in defect content affect material response to further loading and is the source of nonlinear behavior. Understanding the variety of defects and their interactions is essential for accurate prediction at the macroscopic scale.

In this talk we discuss measure theoretic approach for modeling such materials and we focus on dislocations and twinning. We propose a variational formulation in new spaces of parameterized measures, allowing for a natural description of microstructures at small scales. Entropy plays an important role in this formulation. Evolution equations are obtained by minimizing free energy of the system in an appropriate metric.