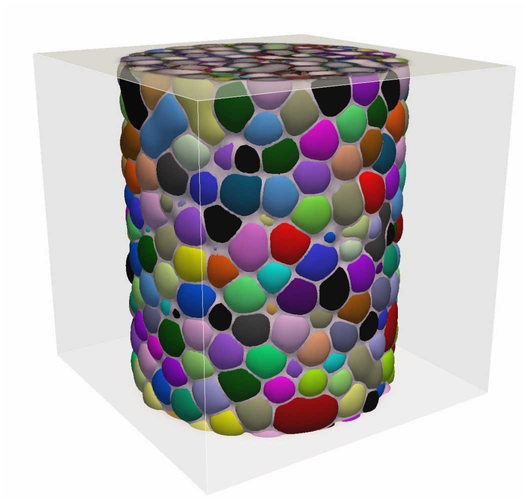
SAND2016-7598PE

Mesoscale Modeling of Grain Boundaries: From Segregation Phenomena to Faceting Instabilities

Fadi Abdeljawad
Materials Science and Engineering Center
Sandia National Laboratories, Albuquerque, NM, 87185 USA

Materials interfaces greatly influence the properties and performance of microstructures in applications ranging from structural and industrial to miniaturized devices for biomedical and electronics. In this talk, we begin with a brief introduction to mesoscale treatments of interfaces, which serve as a building block for the quantitative modeling of a wide range of materials phenomena, such as grain growth, coarsening, segregation and phase transitions. Herein, two problems involving materials microstructures will be discussed.

The first focuses on nanocrystalline (NC) alloys, where grain boundary (GB) solute segregation has been recently proposed as a route to thermally stabilize the grain structure of NC alloys. Through analytical and parametric studies, we quantitatively examine GB segregation and establish regimes, where the reduction in GB energy, due to segregation, can be large. Then we turn our attention to immiscible alloys, where the interplay between GB segregation and bulk phase separation determines the extent of solute partitioning between the grains and GBs, affecting the overall thermal stability of these systems.



The second deals with interface anisotropy, where cusps in the GB energy may exist as a function of GB inclination, defined by the plane normal. Therefore, an initially flat GB may facet resulting in a “zig-zag” structure with well-defined planes and corners/junctions connecting them. We investigate, through linear stability analysis and computational studies, GB faceting instability and highlight the role of junctions and their non-local interactions on facet coarsening dynamics and associated length scales.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.