Atomistic and Mesoscale Modeling of Grain Boundary Segregation in Nanocrystalline Alloys

Fadi Abdeljawad
Department of Mechanical Engineering
Clemson University, Clemson, SC USA 29634

Owing to their small crystalline grain size, nanocrystalline (NC) materials exhibit a unique combination of properties that are not commonly observed in their coarse-grained counterparts. The high density of grain boundaries (GBs) in NC materials, however, renders them highly susceptible to grain growth even at low service temperatures; there exists a large driving force for grain coarsening in order to reduce their total GB area and attain lower energy states. Recently, GB solute segregation has been proposed as a route to mitigate grain growth in NC metals and thermally stabilize their grain structures. Herein, based on atomistic and phase field modeling treatments, we present quantitative analysis of GB segregation and its impact on grain growth dynamics. First, analytical treatments are presented, which establish regimes where the reduction in GB energy, and thus the driving force for grain growth, is large. Then we turn our attention to immiscible NC alloys, where the interplay between GB segregation and bulk precipitation determines the extent of solute partitioning between the grains and GBs, affecting the overall thermal stability of these systems. Finally, we highlight several features and limitations of the modeling framework and discuss further extensions aimed at incorporating anisotropy into the segregation behavior.