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Grain boundary segregation in phase separating nanocrystalline alloys[1] FADI ABDELJAWAD, PING LU, NICOLAS ARGIBAY, STEPHEN FOILES, Sandia National Laboratories — Grain boundary (GB) solute segregation has been proposed as a route to mitigate grain growth in nanocrystalline (NC) metals and stabilize their structures. Based on a diffuse interface model, we examine grain growth dynamics in immiscible NC alloys, where an interesting effect emerges due to GB segregation and bulk phase separation processes. Analytical treatments identify regimes, where the reduction in GB energy is significant. Simulation results reveal that the stability and solute partitioning between bulk and GB regions are a manifestation of the competing effects of GB segregation and alloy phase separation. More specifically, in systems with low GB segregation, precipitation of solute-rich domains and associated GB pinning effects lead to sluggish grain growth rates. In contrast, GB solute segregation plays a more pronounced role as the heat of segregation increases in comparison with bulk heat of mixing. In broader terms, our treatment provides a framework to examine both bulk alloy and interfacial effects and their roles on the stability of NC metals.

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