ABSTRACT

Fundamental Insights into Grain Boundary Segregation and Solute Drag in Multicomponent Alloys

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High entropy alloys (HEAs) are a class of materials systems that are composed of multiple elemental species in equiatomic or near equiatomic compositions. Recent experimental studies revealed sluggish grain coarsening rates in HEAs during various processing treatments. These studies attributed the observed slow growth rates to segregation of elemental species to grain boundaries (GBs) and accompanying solute drag processes. GB dynamic solute drag results when segregated solutes exert a resistive force hindering boundary migration. However, GB solute drag in multicomponent alloys remains largely unexplored. The challenge here is that GB dynamics in HEAs involves a strong coupling between chemical driving forces, solute-solute interactions of all alloying elements, and various diffusive processes in both the bulk and interface regions. Herein, we present a model of GB segregation and solute drag [1,2] in HEAs that accounts for bulk and GB thermodynamics and it captures various mass transport mechanisms. Analytical and computational studies reveal a plethora of segregation profiles, including, for example, synergistic co-segregation and induced de-segregation, that are sensitively dependent on alloy-alloy interactions and diffusion processes within the GB. We perform parametric studies to quantify the role of the GB diffusion coefficients on solute drag values. Our approach provides avenues to employ GB segregation as a strategy to design HEAs with tailored microstructures and chemistries.

[1] M. Alkayyali, M. Taghizadeh, and F. Abdeljawad, Acta Mater., 275, 120037 (2024).
[2] M. Alkayyali and F. Abdeljawad, Phys. Rev. Lett., 127, 175503 (2021).