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ABSTRACT:

Mesoscale Modeling of Grain Boundary Solute Drag in Multicomponent Alloys

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Grain boundary (GB) solute segregation has been proposed as a design strategy to control the processing pathways of polycrystalline materials. Of particular interest is GB solute drag, wherein segregated solute atoms impose a resistive force that impedes GB migration. However, a mechanistic understanding of GB migration kinetics in doped, multicomponent alloys remains limited, as most existing frameworks are restricted to binary systems. In this work, we develop a combined theoretical and computational framework to model GB solute drag in multicomponent alloys. Our results demonstrate that solute–solute interactions among various alloying species give rise to complex segregation trends, including synergistic cosegregation and induced desegregation, which strongly influence GB migration rates. Notably, simulation results reveal that, in multicomponent systems, solute desegregation can be as effective as segregation in generating significant solute drag. It is found that GB solute drag exhibits a non-monotonic dependence on alloy concentration, driven by solute-solute interactions within both the bulk and GB regions. More broadly, the predictive capability of the proposed framework provides new insights into the migration kinetics of chemically complex interfaces and offers guidance for the design of advanced alloys with tailored microstructures and properties.