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THE ROLE OF GRAIN BOUNDARY METASTABILITY IN SOLUTE SEGREGATION ENERGETICS: AN ATOMISTIC SIMULATION STUDY

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Most functional materials are polycrystalline systems. Their microstructures are comprised of crystalline grains that are joined at internal interfaces, termed grain boundaries (GBs). In general, the GB geometry is defined by five macroscopic degrees of freedom (DOF); three for misorientation and two for the GB plane normal. Further, three microscopic DOF (so called metastable states) are needed to describe rigid body translations of the two abutting crystals parallel and normal to the GB plane. Doping GBs with alloys greatly influences many interface phenomena in polycrystalline solids, including curvature-driven GB motion, which is responsible for grain growth in these systems. In is study, we explore solute segregation in a wide range of metastable GBs in a model Al-Mg alloy using atomistic simulations. Realizations of atomistic bicrystal geometries with metastable GBs are obtained along with their corresponding lowest energy ones. Atomistic simulations are used to obtain segregation energies (i.e., bi-crystal free energy difference when Mg in host lattice compared to one in GB) at 0K for the metastable GB structures. Simulation results and detailed analysis of Al GB structures indicate that preferential sites for Mg segregation are strongly correlated with the local atomic environments, which we characterize using Voronoi cells, coordination number, and free volume. Our results indicate that to a first order the dependence of segregation energy on GB metastability is captured by the local free volume. Future scope of work includes using machine learning techniques to find higher order parameters defining segregation energy for a more accurate prediction of the favorable sites.

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