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Ab-initio investigation of metallic dopant segregation and embrittlement in molybdenum grain boundaries

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Mo is widely used as a refractory material due to its excellent high temperature properties, but a critical limitation is its room temperature brittleness resulting from its ductile-to-brittle transition temperature (DBTT). Doping the grain boundaries (GBs) of Mo with metals such as Zr, Re or Al have previously been demonstrated as a promising approach to remedy this limitation, whereas other alloy elements are known to exacerbate it. In this work we investigated the segregation and strengthening/embrittling effects of 29 metallic dopants at the Σ5(310) tilt and Σ5(100) twist Mo GBs using density functional theory (DFT) calculations. We show that GB segregation for most dopants is independent of the type of GB. Based on previous works for other metals, we also developed a model that uses radius and cohesive energy of the dopants relative to that of Mo as a good predictor of the strengthening/embrittling effect. However, when comparing our values to previous empirical continuum models, we find that dopant chemistry for elements such as Ni also plays a significant role in affecting segregation behavior at GBs, particularly in driving the formation of intermetallic precipitates or 2-D interfacial phases (complexions). We also show that the site preference of a dopant in the GB can lead to strengthening effects that deviate from those predicted using simple bond-breaking arguments. Under a fast cleavage model of fracture, Ta, Re, Os and W are predicted to have a weak strengthening effect on Mo for the Σ5(310) tilt GB.

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