Abstract Submitted
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First-principles Co database: Energetics of binary Co alloys and compounds[1] SHAHAB NAGHAVI, VINAY HEGDE, CHRIS WOLVERTON, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA — The field of superalloys has received a recent spike in interest with the discovery of metastable γ'−Co_3(Al,W) precipitates with the $L1_2$ structures. We present density functional calculations for the first and second nearest-neighbor solute-vacancy binding energies of 27 substitutional solutes in fcc-cobalt. As by-products, we also calculate the dilute mixing energy, dilute volume of mixing, and solubility enthalpy. A modest correlation between the solute size and its binding to an accompanying vacancy has been found. Our calculations reveal that a vacancy not only relieves the strain associated with large solutes, but also mediates a weak bonding between the large solute and its next nearest-neighbor atoms, resulting in high solute-vacancy binding energies. We also find that the solute-vacancy binding energy is minimized for a half-filled d-band, in the middle of a transition metal series, and varies parabolically with the d-band filling. In general, $4d$ and their counterpart $5d$ transition metals have nearly similar solute-vacancy binding energies, but much larger than those of $3d$ transition metals, and the deviation increase by moving away from a half-filled band.

[1]Center for Hierarchical Materials Design (CHiMaD)

Shahab Naghavi
Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA

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