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First-principles Co Database: Energetics of Binary Co Alloys and Compounds.

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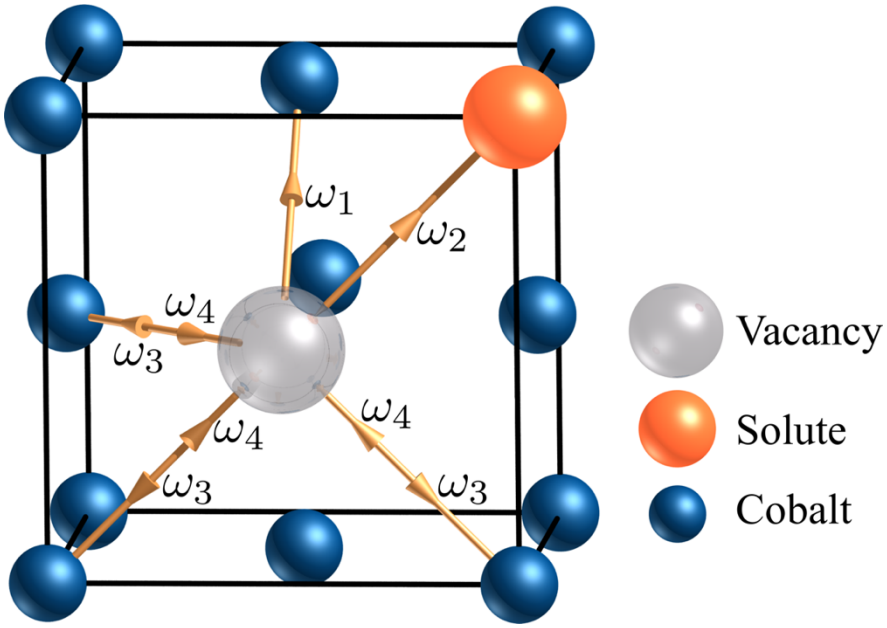

Caption: *Vacancy jumps in fcc cobalt near an impurity. The orange ball is the impurity and empty gray ball indicates the vacancy. ω_0: vacancy-host exchange rate. ω_1: rotation rate of impurity-vacancy. ω_2: impurity-vacancy exchange rate. ω_3: dissociation rate of impurity-vacancy pair. ω_4: association rate of impurity-vacancy pair.*

Scientific Achievement

We showed diffusion coefficients in fcc Co follow a parabolic trend for solutes across the transition metal series. Here the change in the diffusion coefficient correlates with d-band filling, peaking near half d-filling, and then finally decreasing back down as the d-shell completely fills. We find that large solutes diffuse much faster than small ones due to what we named the **strain-mediated mechanism**. We found for the extremely large solutes (group III), the monovacancy mediated mechanism of diffusion is not valid.

Significance

Beside the scientific understating of diffusion in fcc metals, this research provides valuable information for larger-scale ICME tools: 1) developing CALPHAD type diffusion mobility databases, similar to the ones that exist for Mg alloys and Ni-based superalloys, and 2) constructing predictive, quantitative phase-field models of microstructural evolution.

Citation

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