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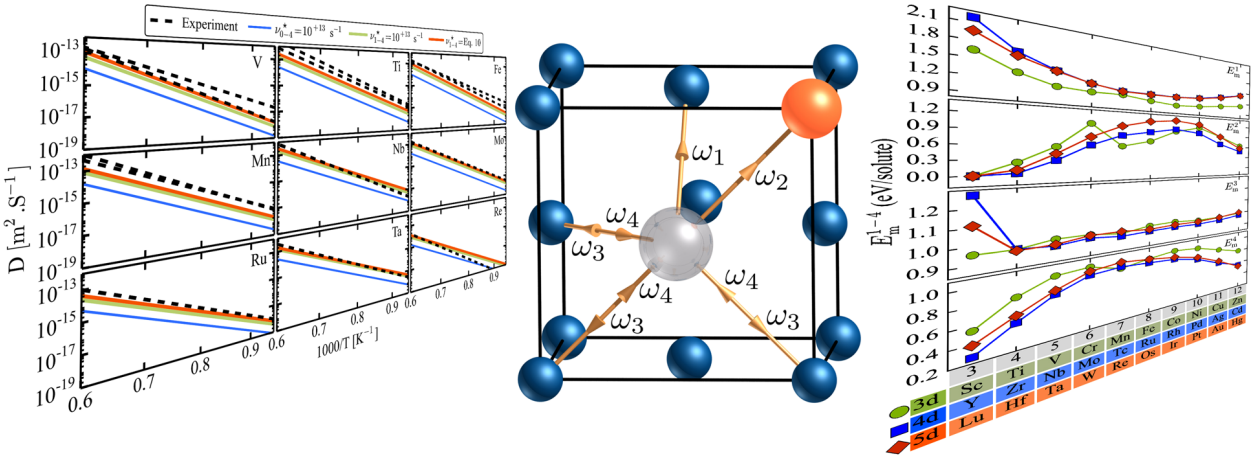
Diffusion coefficients of transition metals in fcc cobalt.

Shahab Naghavi, V. I. Hegde and C. Wolverton.



Scientific Achievement

We have assembled a large database of energetic and kinetic properties for Co-based alloy systems. This database should significantly accelerate Co alloy design activities. Specifically, we have constructed:

1. A large first-principles database for solute diffusion in fcc cobalt, including diffusion coefficients, diffusion prefactors, activation energies, and individual jump frequencies.
2. A thermodynamic database for many solutes that includes solute-vacancy binding energies, solid solution mixing energies, compound formation energies, and solubility energies.
3. We have provided our diffusivity database to NIST scientists working on developing a mobility database for cobalt-based superalloys.

Significance

The development of these Co thermodynamic and kinetic databases of "pre-CALPHAD data" will enable researchers who are developing CALPHAD and DICTRA databases of thermodynamics and kinetics. The DFT-derived data will be invaluable in cases where experimental data is limited or missing. In turn, these CALPHAD databases will provide an essential tool in alloy design activities and the acceleration of Co alloy development.

Citation

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