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ABSTRACT

Atomistic Monte Carlo Simulations of Diffusion and Ordering Kinetics in Fe-Ni and Ni-Cr Alloys

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We present atomistic Monte Carlo simulations of the ordering kinetics in Fe-Ni and Ni-Cr, two face-centered cubic (FCC) alloys that form the basis of many industrially relevant materials. These simulations are based on a vacancy migration mechanism that accounts for the dependence of vacancy jump frequencies on the local atomic environment, as well as the evolution of vacancy concentration during the ordering process.
To achieve this, we use a model of effective pair interactions on rigid-lattice that depend on both the local composition of the alloy and the temperature, allowing us to accurately reproduce the thermodynamic and transport properties of these systems. The parameters of the model are fitted using both ab initio calculations at 0 K (such as the formation enthalpies of ordered phases or disordered solid solutions, formation and migration enthalpies of vacancies) and experimental data at finite temperatures (such as the Gibbs free energy of mixing of Calphad databases, tracer diffusion coefficients, and interdiffusion coefficients).
Once this parameterization is completed, we simulate the ordering kinetics of FeNi3 (with a L12 structure) and Ni2Cr (with a Pt2Mo structure) and compare the evolution of long-range and short-range order parameters, as well as the size of ordered domains, with experimental data available in the literature. Particular attention is given to the magnetic properties of these alloys, which influence both phase stability and diffusion properties. We also discuss the effect of iron addition on the ordering kinetics of the Ni2Cr phase.