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ABSTRACT:

Atomic Diffusion in Magnetic Metallic Alloys via ab-initio Based Spin-Atomic Monte Carlo Simulations

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Steels are used for numerous technological applications. Several properties of the underlying Fe alloys are strongly affected by magnetism. With increasing temperature, magnetic excitations and lattice vibrations emerge and interact with chemical variables.. So far, a quantitative modelling of these coupled effects is still challenging and attracting extensive efforts worldwide.

We propose an efficient modelling approach to predict atomic-diffusion properties versus temperature and composition. It consists in coupled spin-atomic Monte Carlo simulations using magnetic effective interaction models parameterized from density functional theory (DFT) predictions. We apply the method to predict vacancy-mediated diffusion properties including tracer diffusion coefficients and kinetic correlation factors, in dilute and concentrated Fe alloys [1 – 4]. We focus particularly on the effects of magnetic excitation and transition. Our modelling results are fully consistent with experimental data, usually available only at high temperatures, and provide reliable predictions at low and intermediate temperatures. This approach is fully transferable to other magnetic alloys. It is also promising for the study of more complex kinetic processes such as phase ordering and precipitation.

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[3] V. Kulitckii, A. Schneider, O. Lukianova et al., Acta Mater. 251, 118883 (2023).

[4] K. Li and C.-C. Fu, Phy. Rev. Materials 9, 083401 (2025).