First-principles modeling and machine learning of the energy landscape of Fe-C in a magnetic field

Ming Li, Luke Wirth, Ajinkya Hire, Stephen R. Xie, Dallas R. Trinkle, Richard G. Hennig

Evaluation of the magnetic Gibbs free energy is required to model the thermodynamics and kinetics of steels in high magnetic fields. Density-functional theory (DFT) calculations can provide accurate energy calculations as the foundation of Monte Carlo and thermodynamic perturbation or integration methods. However, the high computational cost hinders its direct application to thermodynamic and kinetic modeling.

The ultra-fast force field (UF^3) [1] machine-learning potential provides effective two- and three-body potentials in a cubic B-spline basis with regularized linear regression. Our implementation of the UF^3 combines the speed to classical empirical potentials with the accuracy of modern machine-learning potentials. In this work, we adopt the UF^3 model to approximate the potential energy landscape based on a DFT database of Fe-C structural configurations in BCC and FCC phases with various magnetic states and C concentrations. We train and validate a UF^3 model for the Fe-C energy landscape on the energies and forces. We will discuss the machine learning approach and the resulting accuracy of the UF^3 model for making predictions.

[1] S. R. Xie, M. Rupp, R. G. Hennig, arXiv:2110.00624 (2021).