Ultra-fast machine learning potential for Fe-C in high magnetic fields

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Induction-coupled thermomagnetic processing combines the efficiency of induction heating with high static magnetic fields to treat steels, enabling rapid processing and reducing energy consumption. Understanding the fundamental impact of the magnetic field on phase stability and kinetics is critical to realizing the benefits of this novel processing approach. Modeling the thermodynamics and kinetics of steels in high magnetic fields requires magnetic Gibbs free energy, which involves millions of energy evaluations to sample the energy landscape, which is computationally too demanding for density-functional theory (DFT) calculations.

To address the challenge, we turn to an ultra-fast force field (UF^3) machine-learning method [1] that combines effective two- and three-body potentials in a cubic B-spline basis with regularized linear regression. We prepare a DFT database to train and validate the UF^3 potentials. The database includes different structural and magnetic configurations of bcc and fcc Fe(C) systems and is assembled using modified VASP with the fixed-field method, which can provide information on energies and forces under various magnetic fields. Our analysis based on the following phonon frequency calculations can approximate the experimentally observed transition temperature shift under applied fields [2], verifying the efficiency of the finite-field calculations.

We demonstrate that treating Fe atoms using an Ising model for the spin states improves the accuracy of energies and forces for the UF^3 potentials, indicating the importance of the spin degree of freedom for the machine-learning of the energy landscape. Motivated by this observation, we implement a magnetic UF^3 approach that incorporates the effect of the local magnetic moments and external magnetic fields using a Landau-Heisenberg Hamiltonian. Training and validations of both the non-magnetic and magnetic UF^3 models are performed on our database. Comparisons between the models reveal the improved accuracy of the magnetic UF^3 model while retaining its ultrafast speed.

[1] Xie, S.R., Rupp, M., and Hennig, R.G., npj Comput Mater 9, 162 (2023)

[2] G. M. Ludtka, DOE technical report ORNL/TM-2005/79 (2005)