Machine learning and Monte Carlo simulations of the Gibbs free energy of the Fe-C system in a magnetic field

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Modeling the thermodynamics and kinetics of steels in high magnetic fields requires knowledge of the magnetic Gibbs free energy. Although accurate, density-functional theory (DFT) calculations introduce heavy computational burden. To solve this problem, we assembled a DFT database which includes the energies and forces as a function of magnetic field for different structural and magnetic configurations of bcc and fcc Fe(C) systems. Ultra-fast force field (UF^3) machine learning models [1] are trained and validated on this database and are proved to be efficient to approximate the DFT energy landscape.
These UF^3 models are then implemented in the subsequent Monte Carlo simulations to quickly evaluate the energies of ensembles. Thermodynamic integration is utilized to achieve the magnetic Gibbs free energy models at different temperatures for the two Fe(C) phases as a function of atomic fraction of carbon and magnetic field.

References

[1] S. R. Xie et al, arXiv:2110.00624 (2021).