Magnetic moment tensor potentials for investigating magnetic materials

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1. Introduction

Machine-learning interatomic potentials (MLIPs) have become a reliable tool in computational materials science. Since 2020, many MLIPs that explicitly include magnetic moments have been developed and used for investigating magnetic materials (see, e.g. the papers [1, 2, 3], where the Curie and the Neel temperatures were predicted with magnetic MLIPs for different magnetic materials).

In this work, we use one class of magnetic MLIPs, namely, collinear magnetic moment tensor potentials (mMTPs), to investigate the Fe-Al and CrN systems. Magnetic MTPs were proposed in [4] for single-component magnetic systems and then generalized to the case of multi-component magnetic materials [5]. To create training sets needed to fit mMTPs, we use spin-polarized density functional theory (DFT) with hard constraints on magnetic moments [6].

2. Fe-Al

We applied mMTP to investigate the bcc Fe-Al system with different concentrations of Al and Fe and different ways in which Al and Fe atoms occupy the supercell sites. We demonstrated that the equilibrium magnetic moments of the unit cell and the equilibrium lattice parameters (see Fig. 1) for different Fe-Al structures calculated with mMTPs are in good correspondence with the ones obtained with DFT. We also showed that the theoretical calculations conducted in this study qualitatively reproduce the experimentally observed anomalous volume-composition dependence in the Fe-Al system at $T = 300$ K (see Fig. 1). A detailed description of our study on the Fe-Al system is provided in [7].

3. CrN

Another material investigated in this study with mMTP is chromium nitride (CrN) in the B1 phase (rock-salt structure) in the paramagnetic state (B1-CrN). To automate the creation of a training set needed for fitting mMTP, we generalized the active learning (AL) algorithm originally proposed in [9] for non-magnetic MTP to accommodate mMTP. The scheme of the AL process is illustrated in Fig. 2.

To describe the paramagnetic state, we averaged over different randomly disordered collinear magnetic states. Using the actively trained mMTP in the paramagnetic state, we calculated the elastic constants and phonon spectrum (see Fig. 3) and demonstrated that these properties predicted with our mMTP align closely with those obtained with DFT. In addition, we used the quasi-harmonic approximation to predict thermal properties, namely, the lattice thermal expansion coefficient (see Fig. 4) and the specific heat capacity of paramagnetic B1-CrN. Both thermal properties predicted with the mMTP are in good agreement with experimental results. A detailed description of our study on the CrN system can be found in [10].

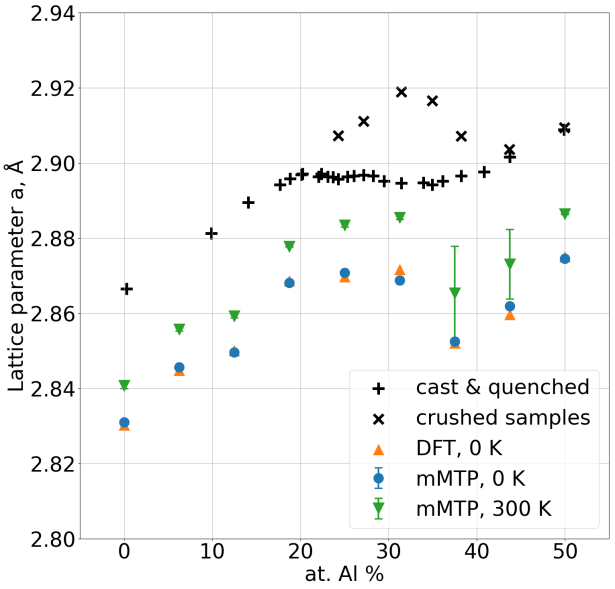

Fig. 1: Lattice parameters calculated at $T = 0$ K and $T = 300$ K using mMTP. Experimental points at $T = 300$ K are taken from [8] and DFT calculations were obtained at $T = 0$ K. This figure is taken from the paper [7].

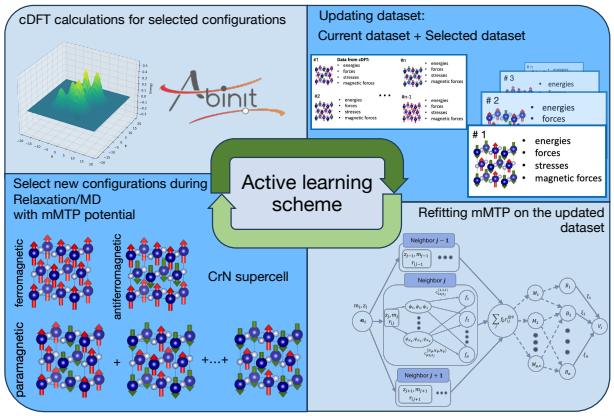

Fig. 2: Protocol of magnetic MTP active training.

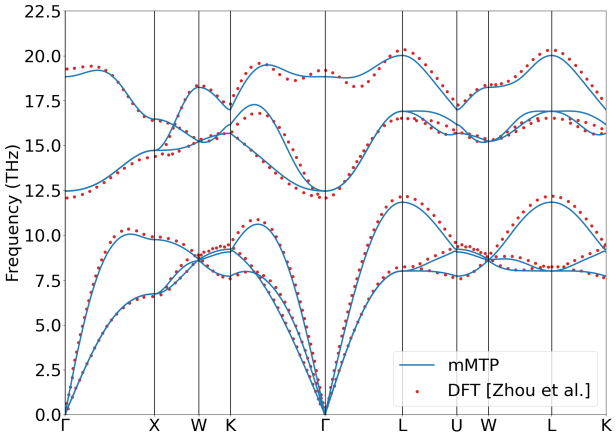

Fig. 3: Phonon spectrum for B1-CrN in the paramagnetic state obtained with the fitted mMTP (solid lines) and DFT [11].

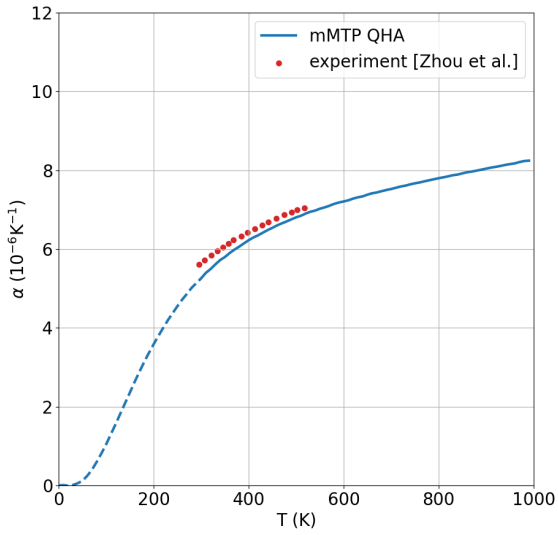

Fig. 4: Linear thermal expansion coefficient for B1-CrN in the paramagnetic state obtained with the fitted mMTP (dashed and solid line) and experimentally [11].

Acknowledgments

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