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A comparative analysis of DeePMD and MTP models for short-range order prediction in Fe-V solid solutions

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Abstract: Body-centered cubic Fe-V alloys and their derived steels are extensively utilized in industry due to their outstanding mechanical properties, which include high strength, hardness, wear resistance, and improved impact toughness at elevated temperatures. Recent research has increasingly focused on the investigation of short-range order (SRO) in these alloys, particularly after the observation that the Cowley SRO parameter in a related Fe-Cr system changes with concentration. At low chromium concentrations, SRO is negative, indicating a propensity for short-range atomic ordering. Conversely, it becomes positive above 10 atomic percent, suggesting a tendency for segregation. Analyzing SRO in disordered alloys using molecular dynamics simulations requires the careful selection of highly accurate interatomic potentials to accurately represent the system's behavior. This study compares interatomic potentials derived from two prominent machine learning techniques: the Moment Tensor Potential (MTP) and the Deep Potential method (DeePMD). These potentials are applied to the Fe-V system across a vanadium concentration range of 0 – 25 atomic percent. Their performance is evaluated through error and efficiency analyses, concentrating on their ability to predict material properties such as the Cowley parameter, equilibrium volume, and lattice constants. This assessment aims to determine the effectiveness of these potentials in capturing the characteristics of Fe-V alloys, thereby providing a foundation for further investigations into their behavior.

Keywords: Fe-V alloys, short-range order, Cowley parameter, molecular dynamics, MTP, DeePMD

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1. Introduction

Short-range order (SRO) refers to the local atomic arrangement within an alloy and plays a critical role in determining its mechanical, thermal, and magnetic properties [1]. A comprehensive understanding of SRO is vital for elucidating the mechanisms underlying strengthening, diffusion, phase stability, and other properties that influence material performance [2]. The Fe-V system holds particular significance due to its applications in structural steels and high-entropy alloys, where the distribution of vanadium atoms within the iron matrix substantially affects strength and radiation resistance [3,4]. Experimental investigations of short-range order in the Fe-V system date back to 1982, employing neutron diffraction and nuclear magnetic resonance techniques [5]. However, these methods encountered challenges in clearly differentiating between the contributions of the first and second coordination shells, leading to the measurement of an averaged Cowley SRO parameter. It has been observed that the concentration dependence of this parameter is monotonous and relatively weak [5].

Recent interest in further examining SRO in Fe-V alloys has surged, influenced by findings in a comparable Fe-Cr system. In the Fe-Cr system, the short-range order parameter exhibits a sign change with increasing concentration: it is negative at low chromium levels, indicating short-range atomic ordering, but turns positive beyond 10 atomic percent, suggesting segregation [6,7]. This reversal of short-range order has been attributed to magnetic origins and is associated with the frustration effect [8,9]. The magnetic interactions in the Fe-Cr and Fe-V systems are entirely analogous [10], suggesting that similar features may manifest in the behavior of short-range order in iron-vanadium alloys.

When analyzing the short-range order in disordered solutions using the molecular dynamics method, a key consideration is the realism of the interatomic potentials employed. Existing parametric interatomic potentials of the MEAM type in the literature that describe well the elastic moduli and mixing energy of the Fe-V system are not able to replicate experimental data from work [5]. For this reason, we used an interatomic potential constructed using machine learning techniques from the DeePMD package in our study [11]. This potential allowed us to replicate the concentration dependence of the Cowley parameter α_{12} with good accuracy [5]. However, the process of developing machine learning potentials using DeePMD has proven to be time-consuming since it requires the creation of a large database of DFT calculations for a wide range of vanadium atom concentrations and configurations within the iron lattice. In this regard, it was found interesting to replicate

the concentration dependence of the Cowley parameters for the Fe-V solid solution using machine learning potentials based on the method of moments developed by A. Shapeev [14,15], and to compare the accuracy and performance of this approach with that of the DeePMD method.

2. Methods

2.1. Machine Learning of Interatomic Potentials

The foundational concept of Machine Learning for Interatomic Potentials (MLIP-potentials) utilizing neural networks was initially introduced by J. Behler and M. Parrinello [16] and is predicated on the following principles:

1. Locality of Atomic Interactions: It is assumed that atomic interactions are local, leading to the total energy of the system being represented as the sum of the energies of individual atoms E_i, which are determined by their local environment (N_i). This local environment is defined as a set of positions ($\mathbf{r}_{i1}$; $\mathbf{r}_{i2}$;…; $\mathbf{r}_{in}$) of the n nearest neighbors within a spherical region of radius ($\mathbf{r}_c$).

$$E = \sum_{i=1}^{n} E_i \qquad (1)$$

2. Input Representation for Machine Learning: The local environment N_i is not an optimal input representation for atomistic systems in the context of machine learning. The number of particles in an atom's local environment can vary, complicating the development of a direct machine learning algorithm. Additionally, it lacks invariance to rotation or translation. Consequently, the local environment N_i is represented by a fixed-dimensional vector composed of local structural parameters $\mathbf{G}_i = (\mathbf{G}_{i1};\mathbf{G}_{i2};\ldots;\mathbf{G}_{ik})$. These parameters are smooth functions of ($\mathbf{r}_i$) that maintain invariance under translations and rotations of the coordinate axes, as well as permutations (relabeling) of atoms, and are referred to as descriptors. Effective descriptors for atomistic machine learning must meet several criteria, including: 1) invariance to spatial displacement of the coordinate system, ensuring homogeneity of space; 2) invariance to rotation of the coordinate system, ensuring isotropy of space; 3) invariance to permutation of atomic indices, such that changes in atom numbering do not affect the physical properties of the system; 4) continuity, where small alterations in atomic structure yield minor changes in the descriptor; and 5) low computational costs.

3. Mapping and Regression Model: The vector ($\mathbf{G}_i$) is mapped to the energy E_i through a regression model that is pre-trained on the results of density functional theory (DFT) modeling of the system in question. The constructed regression (R) maps the K-dimensional space of descriptors onto the one-dimensional space of atomic energies. The potential is trained to approximate the total potential energy surface (PES) of the system, rather than specific physical properties. However, the PES uniquely determines all system properties, with its local minima corresponding to stable or metastable structures and saddle points representing the energy barriers of thermally activated kinetic processes.

A significant number of methods for constructing Machine Learning Interatomic Potentials (MLIPs) have been developed. The two primary components of machine learning for potentials are the numerical representation of input data through descriptors and the regression learning algorithm. Numerous methods for the machine learning of potentials in atomistic modeling have already been established. The rationale behind this proliferation is that if the quality of the training model is the main focus, it typically necessitates a comprehensive expansion of the descriptor space. This approach can be conventionally termed "mathematical". It is characteristic of neural network potentials (NNP), where artificial neural networks and atom-centered symmetric functions (ACSF) serve as the regression model. These descriptors are radially symmetrized two- and three-particle functions that can be finely tuned to identify specific structural features. This methodology is implemented in the DeePMD package. Conversely, the "physical" approach aims to select a descriptor space that closely aligns with the physics of interparticle interaction processes. In this scenario, the descriptor space is more constrained, yet performance is enhanced. Identifying the optimal balance between "mathematical" and "physical" approaches for each material type and modeled property is crucial, as this will ensure the desired accuracy alongside high performance. We contend that, in the context of short-range order in binary alloys, the Moment Tensor Potential (MTP) method proposed by A. Shapeev exemplifies this property. Recent evaluations of various MLIP types have revealed that MTP potentials exhibit an optimal combination of accuracy and computational efficiency.

2.2. Methodology for constructing MLIP potentials using the moment tensor method

The Moment Tensor Potential (MTP) method, proposed by Shapeev, is designed for constructing MLIPs for alloys of a specified structure. The total interaction energy (E) of the atoms in the modeled system is determined by a quantum-mechanical Density Functional Theory (DFT) model that must be approximated. According to Eq. (1), the total energy E is approximated as the sum of the interaction energies ($V(N_i)$) of individual atoms i with their local environment N_i. The potential $V(N_i)$ is linearly decomposed in terms of a set of basis functions B_α:

$$V(N_i) = \sum_{\alpha} \xi_\alpha B_\alpha(N_i), \qquad (2)$$

In this equation, B_α represents a set of predefined basis functions constructed from moment tensor descriptors [14], and ξ_α are coefficients that need to be trained and optimized by minimizing the mean square error of predicting the total energy, forces, and stresses from the DFT dataset [14].

The basis functions depend on the moment tensor descriptors defined as

$$M_{\mu,\nu}(N_i) = \sum_j f_\mu\left(\left|\vec{r}_{ij}\right|, z_i z_j\right) \underbrace{\vec{r}_{ij} \otimes \ldots \otimes \vec{r}_{ij}}_{\nu \text{ times}}, \qquad (3)$$

where the index (j) enumerates all the atoms in the local environment N_i surrounding the (i)-th atom. The symbol "⊗" denotes the outer product of vectors; thus, in Eq. (3), ($\mathbf{r}_{ij}\otimes\ldots\otimes\mathbf{r}_{ij}$) represents a tensor of rank ν. Each descriptor in Eq. (3) consists of a radial component $f_\mu(|\mathbf{r}_{ij}|, z_i, z_j)$, which depends solely on the relative distances between atoms and their types (z_i) and (z_j), and an angular component ($\mathbf{r}_{ij}\otimes\ldots\otimes\mathbf{r}_{ij}$),

reminiscent of moments of inertia. The functions $B_\alpha(N_i)$ enumerate all possible scalar convolutions of any number $M_{\mu,\nu}(N_i)$ [14]. By design, $M_{\mu,\nu}(N_i)$ is invariant under translations of the system and permutations of equivalent atoms. Their scalar convolutions are also invariant under rotations of the neighborhood. Consequently, the resulting function ($V(N_i)$) retains all the specified symmetries.

3. Results and discussion

3.1. Machine learning interatomic potentials: DeePMD

As one of the methods in this comparative study, we used a machine learning potential that was constructed and thoroughly investigated in our previous work [11]. For completeness, we provide the key parameters of its training below. The interatomic potential was constructed using the DeePMD-kit v2 package [12]. The training employed an active learning approach implemented in the DPGEN package to automatically generate and curate the training database. The DeePMD model was built using descriptors of the "se_e2_a" type with a cutoff radius of 7.0 Å. The neural network architecture consisted of an embedding network with three hidden layers (25, 50, and 100 neurons) and a fitting network with three hidden layers (255 neurons each). The training utilized an active learning approach where four replica models were used to run classical molecular dynamics ensembles. Configurations with high uncertainty, identified by a large standard deviation of interatomic forces between the replicas, were selected for *ab initio* calculation and added to the training set. This iterative process continued until convergence was achieved. The active learning simulations used supercells of 100–150 atoms with a time step of 0.1 fs, covering temperatures from 100 to 1500 K and pressures from 0 to 50 GPa to ensure broad coverage of the configurational space. The final model demonstrated an accuracy of 2.6 meV/atom for energy and 0.17 eV/Å for forces (RMSE) relative to the reference DFT calculations.

3.2. Machine learning interatomic potentials: MTP

The initial training dataset for the first version of the Moment Tensor Potential (MTP) was developed using body-centered cubic (BCC) supercells containing 128 atoms. These supercells featured varying volumes and a random distribution of iron (Fe) and vanadium (V) atoms across lattice sites. The vanadium concentration ranged from 0 to 25 at.%, divided into 17 discrete compositions with increments of 2 V atoms per supercell. For each composition, 12 supercells were generated, corresponding to volumes ranging from 94% to 105% of the experimentally determined equilibrium volume, yielding 204 unique configurations. First-principles calculations of energies and atomic forces within the framework of density functional theory (DFT) were performed for these configurations, employing the projector-augmented wave (PAW) method and GGA-PBE exchange-correlation functional [17], as implemented in VASP software package [18]. All density functional theory (DFT) calculations included spin polarization, using a plane wave energy cutoff of at least 400 eV, and a 4×4×4 Monkhorst-Pack k-point grid in the Brillouin zone. Initially, training utilized 204 configurations for which DFT-calculated energies, atomic forces, and stress tensors were available. Subsequently, active learning [19] was conducted using hybrid Monte Carlo and molecular dynamics simulations in the LAMMPS software package [20]. Simulations were performed on 4×4×4 BCC supercells of the Fe-V system at various temperatures and constant pressure (NPT ensemble), employing a Nosé-Hoover thermostat. To enhance sampling, periodic random swaps of Fe and V atoms were implemented. This process was repeated for compositions containing 0, 2, 4,…, 32 V atoms per supercell. During active learning, configurations were selected based on the $\gamma(X_i)$ information metric [21], which quantifies the novelty of a given configuration X_i if added to the training set. In total, 1160 configurations were selected throughout the active learning process. Initially, the MTP model of level 20 was trained using the recommended set of weighting coefficients: $w(E)=1$, $w(f)=0.01$, and $w(S)=0.001$. However, this setup led to a slight underestimation of the lattice parameter. Improved agreement with DFT values was achieved by setting the stress weight to zero ($w(S)=0$). The comparison of lattice parameters for Fe-V solid solutions calculated using DFT and MTP is shown in Table 1, while the accuracy of energy and force predictions is illustrated in Fig. 1. The root mean square errors (RMSE) for the MTP model relative to the reference DFT data are 1.6 meV/atom for energy and 0.097 eV/Å for forces.

Both the data in Table 1 and Fig. 1 indicate a high accuracy of the regression of the results of calculating the energy and lattice parameters of alloys using the MLIP-potentials constructed by the MTP method.

Table 1. Calculated values of lattice parameter *a* for different vanadium concentrations in the Fe-V system.

Vanadium concentration at.%	0	5	10	15
Calculation by DFT method, Å	2.837	2.847	2.854	2.855
Calculation by the MTP method, Å	2.838	2.841	2.846	2.853

3.3. Calculation of short-range order parameters in Fe-V alloys and comparison of machine learning methods

In our investigation of short-range order, we employed a combined approach utilizing classical molecular dynamics alongside the Monte Carlo method. We began by generating structures that represented binary random substitutional BCC Fe-V alloys, which were then equilibrated at a fixed temperature of 1000 K and a pressure of 1 atm for 1 ns. The simulations used a time step of 1 fs and were conducted under periodic boundary conditions. During the simulation, every 1 ps, 5% of the vanadium atoms were replaced with iron atoms using the lattice Monte Carlo method and the Metropolis algorithm. This replacement process required adjusting the velocities of the atoms according to their mass to ensure that the total kinetic energy of the system remained constant throughout the rearrangement. For these calculations, we utilized a supercell composed of 15×15×15 elementary BCC cells of the Fe-V alloy, containing a total of 6750 atoms.

The short-range order parameter, also referred to as the Warren-Cowley parameter, for the *i*-th coordination sphere

in a disordered solution was calculated using the following formula [22]:

$$\alpha_i = 1 - \frac{Z_{AB}}{Z_A x_B},$$

where Z_{AB} is the number of B atoms in the coordination shell centered on an A atom, Z_A is the total coordination number of the A atom, and x_B is the concentration of B atoms in the alloy (in at.%).

The coordination numbers were calculated using the LAMMPS software package by analyzing radial distribution functions.

To enable a direct comparison of the simulation results with experimental data [5], a weighted average SRO parameter for the first and second coordination shells was also calculated:

$$\alpha_{12} = \frac{8\alpha_1 + 6\alpha_2}{14}.$$

The simulated Cowley parameters, α_1 and α_2, as well as a comparison between the calculated α_{12} values and experimental data, are presented in Fig. 2 a, b.

As shown in Fig. 2 b, the Cowley parameter α_{12}, averaged over two immediate environments, aligns excellently with the experimental data from classical work [5]. Additionally, there is a strong correspondence between the α_{12} values and the results obtained using another machine learning method, DeePMD [11]. The constructed MLIP potentials enabled the determination of all Cowley parameters up to the fourth order. The most informative short-range order parameters are those in the first (α_1) and second (α_2) environments, as illustrated in Fig. 2 a. Notably, the nearly linear increase in the negative values of the α_1 parameter with vanadium concentration suggests that V atoms are surrounded solely by Fe atoms, indicating that nearby vanadium atoms repel each other. This conclusion is entirely consistent with the findings of [4].

The cutoff radius is a critical parameter in machine learning potentials, as it determines the maximum range of interactions between atoms, which is essential for achieving accurate predictions. Consequently, we have selected a consistent cutoff radius of 6.0 Å for all simulations. The root mean square error (RMSE) for the energies predicted by the MTP potential, relative to the reference density functional theory (DFT) data, was 1.6 meV/atom, while the RMSE for the interatomic forces was 0.097 eV/Å. In comparison, the corresponding values

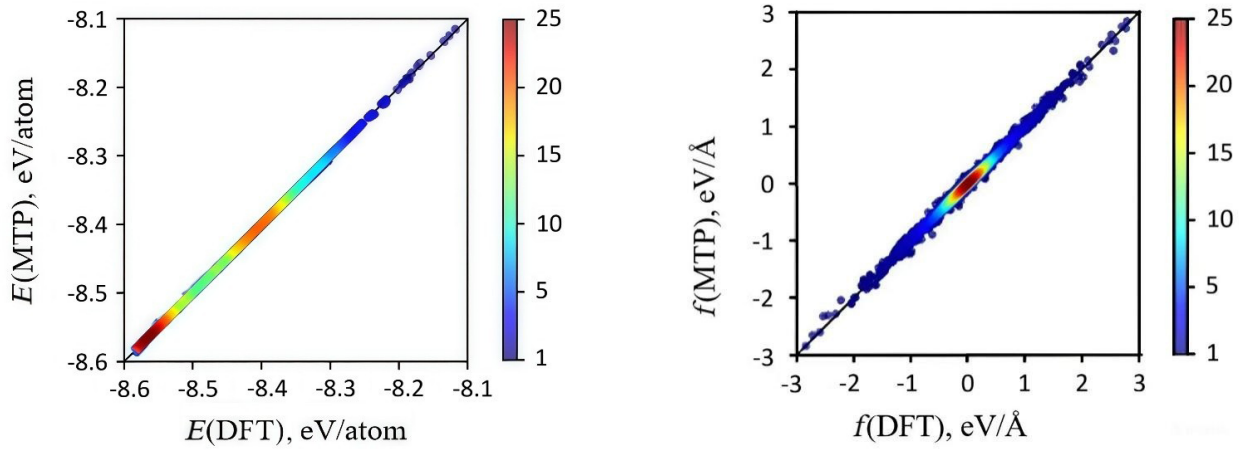

Fig. 1. (Color online) Comparison of energies (a) and interatomic forces (b) obtained using the DFT method and MTP potential. The color bar represents the density of data points, with warmer colors indicating higher density regions. The RMSE for the MTP model are 1.6 meV/atom for energy and 0.097 eV/Å for forces, calculated relative to the reference DFT data.

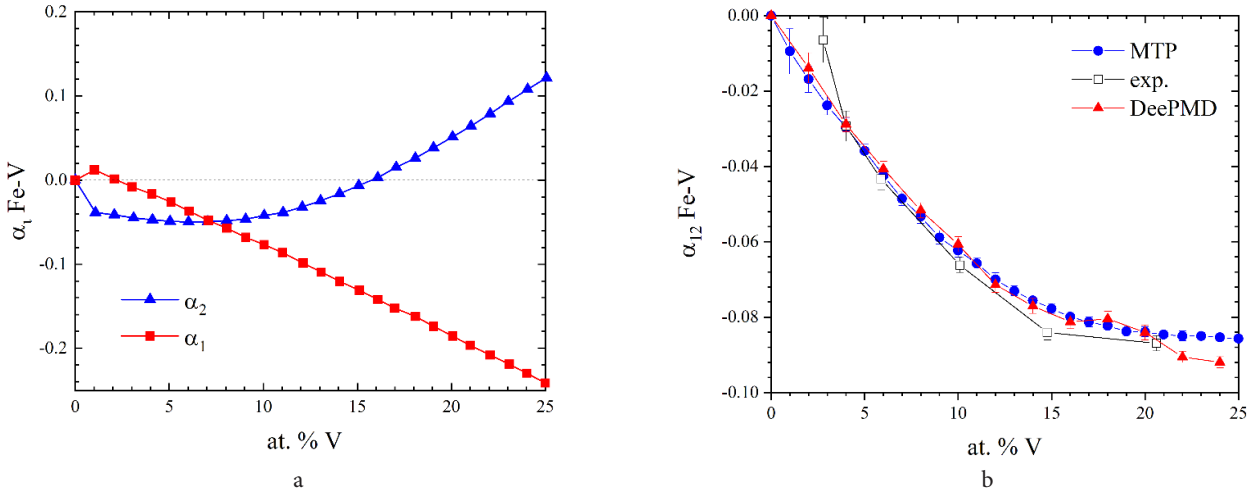

Fig. 2. (Color online) Warren-Cowley parameters for Fe-V structures from MTP simulations: α_1 and α_2 (red squares and blue triangles) (a), comparison of the calculated α_{12} parameter obtained using the MTP and DeePMD [11] potentials with experimental data [5] (b). Data are shown for a temperature of 1000 K.

for the DeePMD model were 2.6 meV/atom and 0.17 eV/Å, respectively. It is noteworthy that achieving comparable accuracy with the DeePMD model necessitated three times more training configurations than the MTP model. Despite this, the simulated short-range order (Warren-Cowley) parameters obtained from both potentials demonstrate good agreement (Fig. 2 b). Thus, the MTP potential exhibits a robust capacity to accurately reproduce the short-range order in binary Fe-V solid solutions using a relatively small training dataset of approximately 2000 configurations. In contrast, comparable accuracy with the DeePMD method requires a substantially larger volume of training data.

4. Conclusions

In this study, we demonstrated the effectiveness of machine-learned interatomic potentials (MLIPs), specifically the Moment Tensor Potential (MTP) method, for investigating the features of short-range order in Fe-V solid solutions. Our calculations revealed a complex, sign-alternating character of the Cowley parameters: negative values of α_1 and α_4 indicate a tendency toward ordering in the first and fourth coordination shells, while positive values of α_2 and α_3 suggest a tendency toward clustering in the second and third shells. This sign-alternating pattern is what characterizes the SRO in this system as "complex". The novelty of this work lies in the comparative analysis of two state-of-the-art MLIP methods (MTP and DeePMD) for accurately predicting this intricate behavior, with the MTP method achieving comparable accuracy at a substantially higher computational efficiency. The main conclusions drawn from this work are:

1. The results obtained from short-range order parameter modeling using machine learning potentials through the MTP method align closely with experimental data, performing comparably to DeepPMD training.

2. Both methods successfully reproduced the intricate nonmonotonic concentration dependence of the Cowley parameters in the Fe-V solid solution, with the underlying features elucidated in terms of magnetic interactions between iron and vanadium atoms as detailed in [6].

3. However, the development of interparticle potentials using the MTP method exhibits a notably superior balance of accuracy and computational efficiency compared to the DeepPMD models.

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