

Rapid Algorithm for Creation of Machine Learning Potential for Viscosity Calculation of Liquid Ni₃₀Fe₇₀

A. A. Tsygankov^{a, b, *}

^a Kazan (Volga region) Federal University, Kazan, 420008 Russia

^b Udmurt Federal Research Center, Ural Branch, Russian Academy of Sciences, Izhevsk, 426067 Russia

*e-mail: tsigankov.artiom@yandex.ru

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Abstract—The use of machine learning methods in materials modeling is a powerful tool for reproducing the properties of a medium with an accuracy close to ab initio calculations. Describing the properties of even binary disordered systems is a nontrivial task due to the complexity of finding the global minimum of potential energy to describe the medium. This problem can be solved using machine learning methods. Using the deep learning method implemented in the DeePMD package, we demonstrate that a machine-learned potential can be obtained for calculating the viscosity of Ni₃₀Fe₇₀ melt using classical molecular dynamics. Moreover, the accuracy of viscosity calculation will be close to the experimental one. This result opens up prospects for developing procedures to rapidly obtain potentials for modeling the dynamic properties of binary alloys.

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Machine learning (ML) in computational materials science is a well-developed and rapidly growing field [1–5]. The basic principle of obtaining a machine-learned force field relies on ab initio simulation data and the use of reference energy, force, and stress tensors to describe the dynamics of the material under study [6]. This approach overcomes the key challenges of the system size and computational complexity of ab initio simulation without significant loss of computational accuracy.

One under-explored problem is constructing a force field for disordered systems, such as liquids. The lack of short-range order necessitates the availability of supercell modeling data on the order of hundreds of atoms and a large dataset of tens of thousands of time steps. However, this requires access to a powerful supercomputer capable of performing ab-initio simulation with Projected Augmented Wave (PAW) method. This paper demonstrates the feasibility of rapidly creating a machine-learning capability for predicting observable quantities, such as viscosity. The Ni₃₀Fe₇₀ melt will be considered above melting temperatures of $T = 1773, 1823, 1873, \text{ and } 1923$ K at a normal pressure of $P = 1$ atm, since the system as a whole has been poorly studied.

Ab initio simulation data were generated using the Vienna ab initio simulation package (VASP) in the Born–Oppenheimer approximation at a temperature of 1773 K in the NVT ensemble [7–9]. An ultrasoft exchange–correlation functional with a kinetic energy

cutoff of 500 eV was used [10]. The density was chosen to be identical to the experimental data and equal to 7105 g/m³ [11]. First-principles simulations were performed in a cell of 128 atoms in length with 5000 time steps, of which 1000 were used to validate the resulting machine-learned potential. The integration timestep was 3 fs.

Following the ab initio simulations, machine learning was performed with the DeePMD package using a deep neural network [12]. The `se_e2_a` descriptor was used, which takes into account non-spherical interactions between atoms and is the most popular. The embedding network consists of two layers and contains 60 and 120 neurons, respectively. The training network consists of three layers, each containing 240 neurons. The initial learning weights are 1000 for energy, 10 for forces, and 0 for the virial. The final learning weights are 0 for energy, 1 for forces, and 0 for the virial. Training was performed over 1000000 steps with the learning rate changed every 500 steps. The root-mean-square error of force calculations is 0.4 eV/Å. The root-mean-square error of energy calculations is 0.5 eV.

After obtaining the potential, simulations were performed using the LAMMPS package [13]. An NVT ensemble with 3456 atoms was used, and the Ni₃₀Fe₇₀ melt density was selected to match the experimental data. The simulation step was 1 fs. Viscosity was calculated using the Kubo–Green formula [14]:

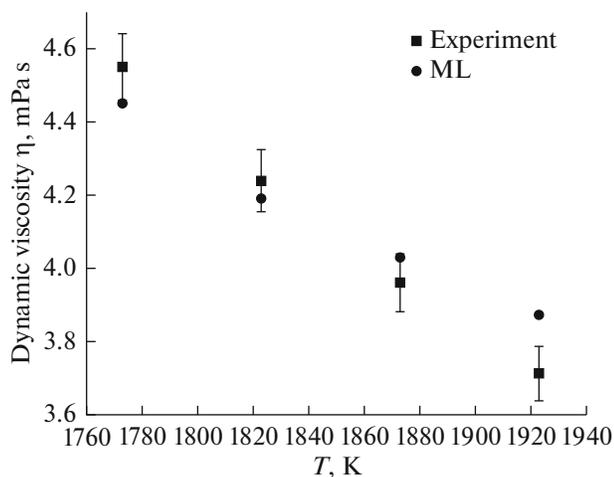


Fig. 1. Viscosity of Ni₃₀Fe₇₀ [11]. The error in viscosity measurement is 2%.

$$\eta = \frac{V}{3k_B T} \int_0^{\infty} \langle \mathbf{J}(0) \cdot \mathbf{J}(t) \rangle dt, \quad (1)$$

where V is the system volume, k_B is the Boltzmann constant, T is the system temperature, and \mathbf{J} is the material flux. The viscosity calculation results are shown in the figure below.

The data in Fig. 1 demonstrate that it is possible to develop a machine learning capability for viscosity prediction with sufficient accuracy within the experimental measurement uncertainty. However, at $T = 1923$ K, the viscosity obtained from molecular dynamics simulations falls outside the experimental uncertainty range. This result indicates that extrapolating viscosity from the initial state where machine learning was performed is of limited use. This problem can be addressed by conducting machine learning from ab initio simulation data at multiple states. For example, conducting first-principles simulations and machine learning at multiple states: the initial state ($T = 1773$ K) and the final one ($T = 1923$ K).

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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