SIMULATION OF LIQUID METALS VISCOUSITY BY MACHINE LEARNING INTERATOMIC POTENTIALS

P. V. Chirkov, G. S. Eltsov, V. V. Dremov, A. V. Karavaev

FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia

Due to advancements in modern computational power and artificial intelligence technologies in recent years, the approach of developing semi-empirical potentials for classical molecular dynamics (CMD) simulations using machine learning algorithms specifically machine-learned interatomic potentials (MLIPs) has gained widespread adoption. Within this framework, interatomic potentials are constructed not through physically justified functional forms and parameter fitting, but rather as a set (often very large) of computationally efficient descriptors. These MLIPs are parameterized using machine learning algorithms, primarily leveraging first-principles calculation results and existing experimental datasets. The use of multi-parametric MLIPs enables highly accurate approximations of CMD results to first-principles data, while allowing molecular dynamics simulations for significantly larger systems and longer timescales. Furthermore, MLIP-based CMD simulations retain access to the full computational tools developed for classical molecular dynamics.

In this work, the Moment Tensor Potential (MTP) [1] was employed as the MLIP model. This choice was motivated by prior studies [2] demonstrating that MTPs exhibit superior or comparable speed-accuracy trade-offs relative to other machine-learned models (e. g., GAP, SNAP, QSNAP). Additionally, MTP's adjustable "level" enables control over the balance between the accuracy of training/test data description and computational complexity (i. e. calculation time).

The optimization of the MTP coefficients for the studied materials (uranium, plutonium, platinum) was based on first-principles data. Since different temperatures within the investigated ranges (from melting points to 60 kK) correspond to distinct electronic subsystem contributions to free energy, independent classical MTP potentials were constructed for each temperature. MTP training, including on-the-fly active learning, was performed for specified temperatures across densities ranging from ~0.8 to ~2.2 times the density under normal conditions.

The dynamic viscosity of liquid metals under varying conditions determines the Reynolds number, a critical parameter in hydrodynamics that characterizes the ratio of inertial forces to viscous friction forces in fluids and gases. The relationship between the Reynolds numbers of contacting materials governs the development of instabilities and turbulence, such as during the propagation of shock waves across interfaces between substances of differing densities.

To determine dynamic viscosity across different densities and temperatures, the Kubo-Green formula was applied. This expresses the dynamic viscosity coefficient through the autocorrelation function of shear stress components:

$$\eta = \frac{1}{3TV}\int_0^\infty \mathrm{d}t \sum_{\alpha<\beta} \left\langle \sigma_{\alpha\beta}(t)\sigma_{\alpha\beta}(0)\right\rangle,$$

where α and β denote Cartesian coordinates. The values of $\sigma_{\alpha\beta}(t)$ were obtained from statistically independent classical molecular dynamics (CMD) trajectories in the *NVT* ensemble. Simulations were performed for systems of size $N = 4000$ atoms. Each *NVT* simulation ran for 2 million steps, with an averaging interval of 5000 steps for evaluating the autocorrelation function (yielding 400 statistically independent trajectories at each (ρ, T) point). Achieving such statistical reliability in first-principles MD calculations without employing the MLIP approach currently would be infeasible within a reasonable timeframe.

Using trained MTPs in CMD simulations, dynamic viscosity values were obtained for liquid uranium, plutonium, and platinum across a range of densities and temperatures. The calculated results were compared with available experimental data.

References

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2. **Zuo, Y.** Performance and cost assessment of machine learning interatomic potentials [Text] / Y. Zuo et al. // J. Phys. Chem. A. – 2020. – Vol. 124. – P. 731.