MS006.O05

Uranium phase diagram built using machine learning interatomic potential

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The classic interaction potentials are often used in modern computational methods. Usually the accuracy of these potentials is not enough for different applications. DFT methods can replace classic potentials but they are much more computationally expensive. Machine learning algorithms are known to possess both high accuracy and high operating speed. The aim of our study was to build machine learning potential that can with high accuracy predict energies and forces acting on each of the atoms in the compound (e.g. during molecular dynamics run).

As a descriptor of the crystal structure that does not depend on translations and rotations we used a vector of exponents with different parameters (similar to [1]). Linear regression was chosen as a learning algorithm. Therefore, energies and forces were sought as a multiplication of linear regression coefficients by a feature vector (descriptor). In this work we showed how properly choose optimal training set, number of parameters in exponential decomposition and how to prevent overfitting. The developed potential was implemented in LAMMPS code.

We compared forces and energies predicted by our interatomic potential (Fig. 1, "1000K" and "5000K") with different trained on the same database (Fig.1, "EAM") and published EAM potentials for uranium (Fig. 1, "1,2,3,4"). For the solid (alpha uranium) and liquid phases the accuracy was 15% and 50%, respectively, higher than that of EAM potentials. Using evolutionary algorithm USPEX we investigated uranium phase diagram at 0K and pressures up to 1TPa. We found stable alpha- and gamma- phases with phase transition at about 255GPa (comparable with [2]), and also more than 5 new phases, which could be stable at higher temperatures. After, using developed potentials, phase diagram of uranium was built at pressures and temperatures up to 1TPa and 15000K .

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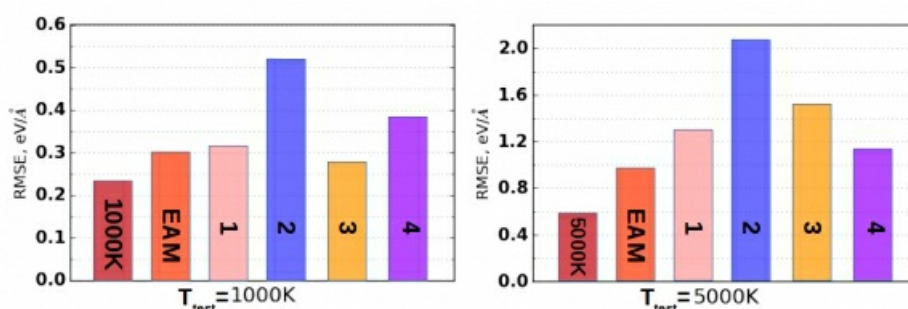
Keywords: machine learning, molecular dynamics, phase diagram