Application of machine-learning potentials to high-entropy alloys investigation

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High-entropy alloys represent a class of refractory materials, which have a rare combination of ductility and strength. Their ability to form a stable single-phase solid solution gives them extraordinary physical properties, gives them the ability to compete with nickel superalloys.

In order to design a new HEA, it is necessary to know phase transitions temperatures. Experimental investigations of HEA are very time-consuming: it may take a few weeks even to prepare a sample. Hence, computational investigation of HEA is of a great interest.

In this work, a new computational method of order-disorder phase transition investigation is presented. The new approach is based on the application of the machine-learning potentials as the interatomic interaction model in canonical Monte Carlo algorithm. This new method turned out being competitive with other data-driven methods.

The interatomic potentials training for the NbMoTaW system is described in this work. The results of the phase transition investigation for NbMoTaW alloy turned out being close to previous theoretical works. A new ground-state structure of the equiatomic NbMoTaW alloy system was found and described. The new method is better than the ones that were used before in accuracy and efficiency.