Machine-learning potential for multi-phase titanium molecular dynamics modeling

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Molecular dynamics gives us an opportunity to investigate the behavior of different materials on the micro-level. In recent years, the so-called machine-learning potentials become more and more popular. They can describe high entropy alloys, several phases of pure material.

In this work, the approach of constructing multi-phase titanium machine-learning potential will be presented. The paper gives an overview of codes for constructing and using machine-learning potential. Basic types of such potentials are considered. Methods for training set preparation are described and compared with one another.

Titanium is taken to demonstrate feasibility of machine-learning potentials construction. The classical EAM potential is used to get energies, forces, and stress. The resulted machine-learning potential reproduced the initial EAM potential well.