Neural Network Potential for La polytypes

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A three-dimensional crystal forming a dense structure can have various structures consisting of a combination of three types of stacking called polytypes. For the same number of layers, different polytype structures have different physical properties such as bandgap and volume [1][2]. Therefore, it is useful from an engineering point of view to create a polytype with the appropriate physical properties for the application by crystal growth.

In order to search for new functional materials and to investigate the process of crystal growth, it is necessary to perform dynamic simulations that accurately reproduce the microscopic mechanism of polymorphs. A method called ab initio molecular dynamics (AIMD) has been considered as

the main method to perform such simulations[3]. However, since crystal growth requires a long simulation time, it is difficult to use AIMD because of its high computational cost. In order to solve these problems, we created a molecular dynamics potential for La polytypes by creating a neural network using a symmetry function, which reproduces the results of first-principles calculations based on density functional theory (DFT). By mapping the stacking order of the polytypes, a quantity called hexagonality can be created, and it is believed that there is a correlation between the physical properties and the hexagonality. In this study, we aimed to construct a neural network potential (NNP) that reproduces the correlation between energy and hexagonality by DFT.

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