Constructing Machine-learned Interatomic Potentials for Covalent Bonding Materials and MD Analyses of Dislocation and Surface

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In recent years, machine learning (ML) methodology has come to be utilized in various fields. In computational engineering, ML is effectively used for the development of interatomic potential. Such ML potentials are usually constructed on a general functional form and a large number of parameters, and many results of DFT calculations are needed for the learning.

The SNAP, or as its advanced type qSNAP, is one of the ML potentials. In this research, we actually construct SNAP and qSNAP for silicon (Si) and 3C-silicon carbide (SiC) crystal systems and confirm their reproducibility in MD simulations by comparing with an empirical potential such as Tersoff potential. Using a genetic algorithm, optimization calculations are performed so that the errors of the lattice constants and elastic moduli are sufficiently minimized.

We found that the SNAP is capable of reproducing lattice constant and elastic moduli for 3C-SiC, and the lattice constant, elastic moduli, and melting point for Si. Besides, the experimentally observed dimer structure in the free surface of Si {100}, which has not been predicted by empirical potentials, is successfully obtained by qSNAP.

Unfortunately, at this stage, the dislocation behaviour has not yet sufficiently been reproduced in either Si or 3C-SiC crystal. For Si crystal, dislocation cores are generated successfully. But, while pure shear strain is being applied to the crystal, some wrong partial dislocations occur, and the dislocation cores lose their stable shape in sliding. In cases above, we recognize that the reproducibility in the elastic region are sufficiently good, but the behaviour in the plastic region is by no means satisfactory for further MD analyses. So that, some improvement of the SNAP and qSNAP potential is expected by adding extra data on stacking defects to the learning process.

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