Artificial Neural Network Modeling of Phase Transition of ZrO2 Ceramics

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Purpose To construct an artificial neural network potential for the atomic-scale simulation of the inner mechanics of phase transition in ZrO2 ceramics.

Outline 1. The train data including energy under different distortion pattern, energy under loading, surface energy, stacking fault energy and so on were calculated via DFT.
2. Additional reference structures by short molecular dynamics (MD) simulations for each polymorph at various temperatures over 1000 fs with a time step of 1 fs; after every 20th MD step, the structures were extracted and their total energies were computed using DFT.
3. This process, i.e., fitting a potential and using it for the generation of additional reference structures, was repeated until the newly generated structures were already found to be accurately represented by the potential.

Result The most accurate artificial neural potential we obtained used the hyperbolic tangent activation functions and contained two hidden layers with 17 nodes per layer. The mean-absolute-error (MAE) of training set and testing set were 1.9 meV/atom and 2.1 meV/atom, and the root-mean-square error (RMSE) are 3.1 meV/atom and 3.6 meV/atom, respectively. They are similar to each other which is an indication that our artificial neural network potential has not been over-fitted.

Computing system: SQUID

node-hour 1200 node-hour
parallelize 2-4 node