Neural Network Interatomic Potentials for Aluminum and Magnesium from Systematic First Principles Calculations

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Interatomic potentials are widely used for molecular dynamics (MD) simulation of a large system. Accuracy and transferability of potentials are important issues to be examined. Recently, a procedure for constructing interatomic potentials by a combination of the density functional theory (DFT) calculations and a neural network regression technique has been proposed, which has been called neural network potentials (NNP)[1]. In this study, we construct NNPs for aluminum and magnesium metals and evaluate the accuracy.

The total energy of a structure is generally obtained by the sum of the contributions from each atom. The neural network approximates the complex function of the atomic energy with respect to the atomic position. Figure 1 shows the structure of NNP applied to a system containing three atoms. In the NNP, a set of symmetry functions for each atom is introduced, which expresses the local geometric environment of the atom. It is used instead of the atomic position as inputs for the neural network. Using the symmetry functions, the regression coefficients of the neural network are estimated from a large set of DFT energies. We perform DFT calculations of 12000 FCC-, HCP- and BCC-based structures for both Al and Mg. Three quarter of them are used as training data. The rest of them are used as test data, estimating the predictive power for structures that are not included in the training data. Here we use eleven kinds of symmetry functions as inputs of the neural network of Al and Mg. We adopt Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm for optimizing the regression coefficients.

Figure 2 shows the energies of test data computed by the DFT calculations and NNP for (a) Al and (b) Mg, measured from the energy of the ground state structure. The root-mean square error (RMSE) between the DFT and NNP energies of test data for Al and Mg are 5 and 4 meV/atom, respectively. Prediction results by the embedded atom method (EAM) potential[2] are shown together in Fig. 2 (a). As can be seen, the energies of the test data with low energies can be accurately predicted both by the NNP and the EAM. On the other hand, the prediction for the test data with high energies by the NNP is much better than that by the EAM. The phonon dispersion curves obtained by the NNP are shown in Fig. 3, which is close to that obtained by the DFT calculation. These results imply that the NNP would be useful for the MD simulation when atomic arrangements are highly distorted and hence show high energies.

A support by a Grant-in-Aid for Scientific Research on Innovative Areas "Nano Informatics" (grant number 25106005) from JSPS is acknowledged.

References

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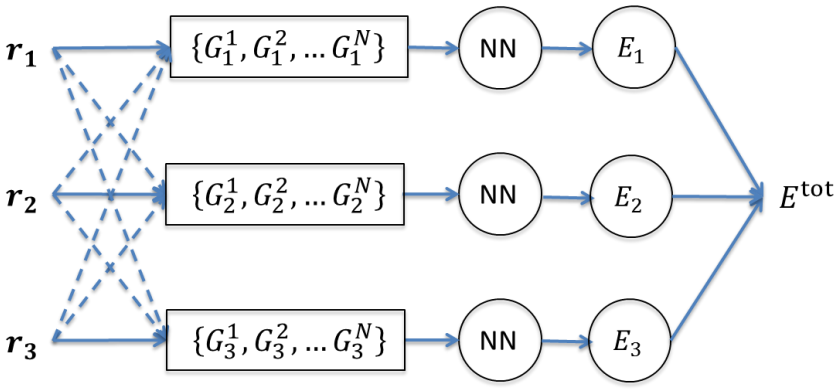

Fig. 1 Structure of NNP as applied to a system containing three atoms, where $\boldsymbol{r}_i$ and G_i^j denote the position and jth symmetry function of ith atom, respectively. The neural network approximates the complex function of the energy of ith atom, E_i, using the symmetry functions. The total energy E^{tot} is computed as the sum of atomic contributions E_i.

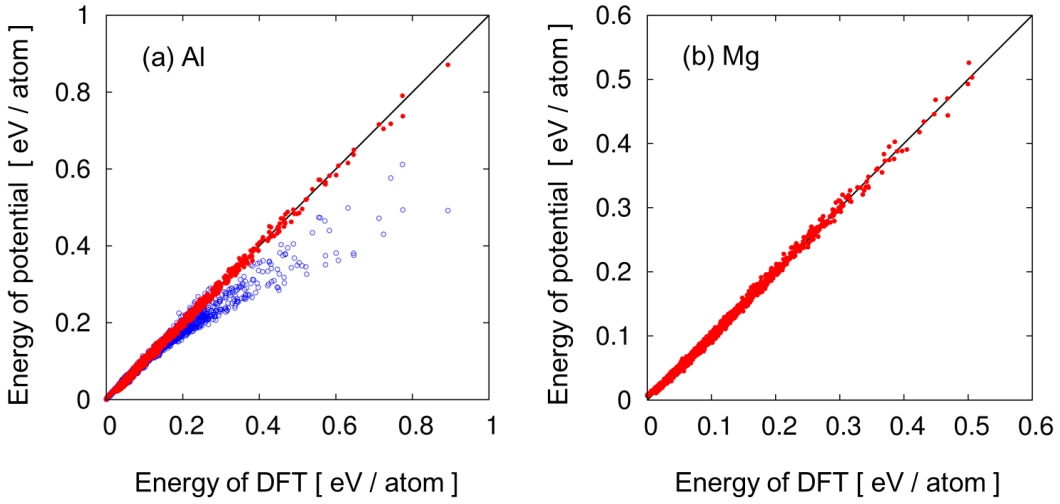

Fig. 2 Energies of test data predicted by DFT calculations and NNP for (a) Al and (b) Mg, shown by red closed circles. On the solid line, DFT and NNP energies are exactly the same. Blue open squares show EAM energies of the corresponding structures.

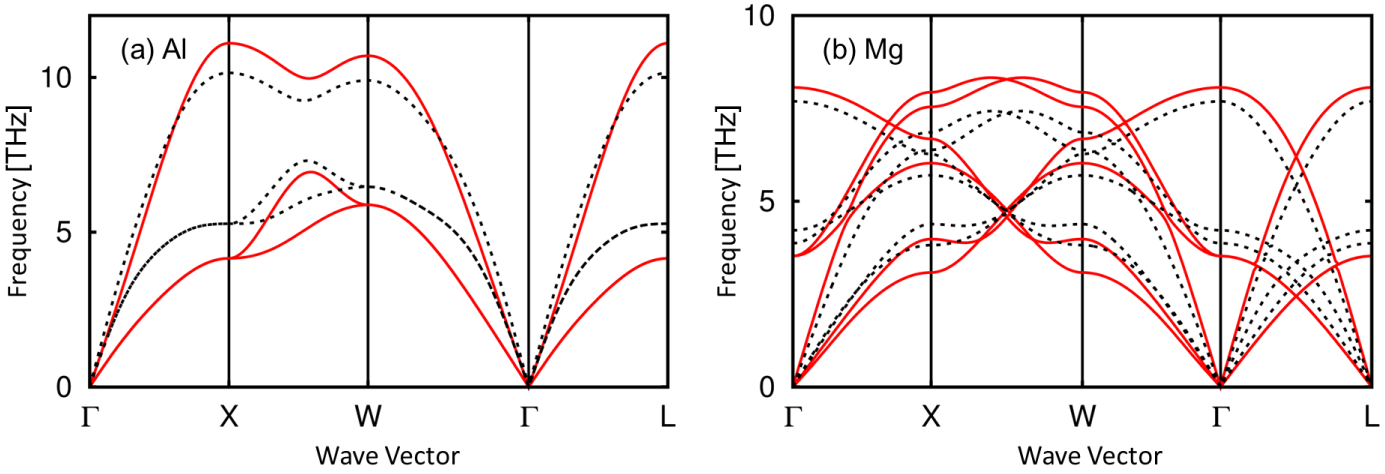

Fig. 3 Phonon dispersion curves obtained by NNP (red solid lines) and DFT (black broken lines) for (a) Al and (b) Mg.