Neural-network descriptor and interatomic potential for accurately predicting atomic structure and properties of lattice defects

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Abstract
Atomic descriptors based on an artificial-neural networks (ANNs) were proposed to achieve high transferability to various lattice defects in silicon. Two- and three-body atomic environments, which are described by analytic functions for conventional ANN potentials, were expressed using separate ANNs. Four-body descriptors were also constructed in the same manner. Their output was then fed to another ANN, and all ANNs were trained with density-functional-theory calculation data at the same time. This approach enables constructing automatically optimal functions without manually selecting analytic functions. Our ANN potential is found to exhibit a lower error than a conventional ANN potential with respect to training datasets. The trained descriptors were found to form complicated functions that cannot be expressed using a single cosine function as used for symmetry functions.

1. Introduction
In crystalline materials, lattice defects are inevitably introduced due to thermodynamic conditions and material fabrication processes, having large impacts on material properties. To accurately predict their atomic structures and physical properties with practical computational cost, artificial-neural-network (ANN) interatomic potentials have been employed extensively. However, if an ANN potential learns various atomic environments of lattice defects at once, error with respect to training data becomes large. This leads to the limited ability to predict lattice defect properties. For this issue, this work proposed an alternative descriptor based on ANNs and compared its error with that of a conventional ANN potential. Here, Si was chosen as a model system.

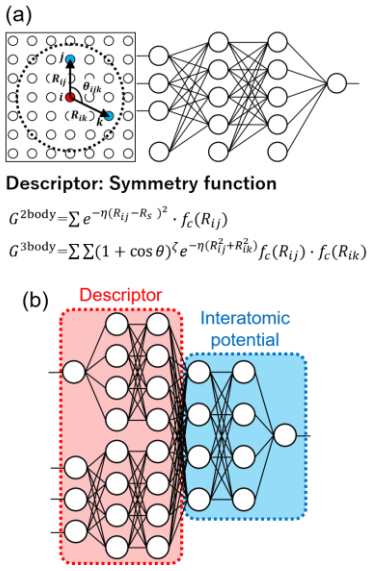

Fig. 1 (a) A conventional and (b) the present ANN potential. Conventionally, the ANNs surrounded by the red and blue rectangles are defined as the descriptor and interatomic potential, respectively.

2. Computational methodology
Figure 1 illustrates a conventional ANN potential and the present ANN potential. For the conventional ANN potential (Fig. 1(a)), a given atomic environment is converted to the input value by using the so-called symmetry function. This descriptor is commonly constructed from simple analytic functions, a Gaussian function and cosine function. However, it is unclear whether such analytic functions are optimal for describing atomic environments for lattice defects. For

this issue, this work expressed two- and three-body atomic environments by using two separate ANNs, as illustrated in Fig. 1(b). Their output was then fed to the input of another ANN. Finally, these ANNs were trained at the same time. Unlike conventional ANN potential, this approach enables us to construct the optimal functions for atomic descriptors without manually selecting analytic functions and their hyperparameters. Furthermore, four-body descriptors were also constructed in the same manner.

Training datasets were generated by performing density-functional-theory (DFT) calculations based on the projector augmented wave (PAW) method in VASP. Not only perfect crystals but also point defects, surfaces and grain boundaries were contained in the datasets.

3. Results and discussion

Figure 2 shows errors of the present ANN potential with respect to athe training datasets. All data points are distributed just near the diagonal line, indicating that it has successfully learned all training datasets. Using the same training datasets and the same architecture in the part of the interatomic potential, a conventional ANN potential with symmetry functions was also trained. The present ANN potential is found to exhibit a lower mean absolute error (MAE) of 0.71 meV/atom than that of the conventional one (2.20 meV/atom). Furthermore, an ANN potential with four-body atomic descriptors exhibits an MAE of 0.43 meV/atom, lower than that for only the two- and three-body potential. Our approach is thus expected to maintain higher accuracy with respect to lattice defects than conventional ANN potentials, although this work examined only training in terms of total energy.

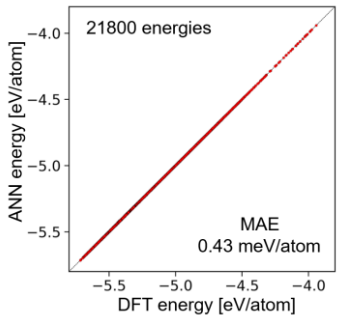

Fig. 2 Errors of the present ANN potential with respect to DFT data.

To understand the reason of the lower errors for our ANN potential, the functional forms of the trained descriptors were analyzed. The two-body descriptors have similar shapes to a single Gaussian function, although they can take both negative and positive values. In contrast, the three-body functions exhibit complicated shapes that cannot be reproduced a single cosine function as used for symmetry functions, as shown in Fig. 3. This difference may mainly contribute to the decreased errors mentioned above.

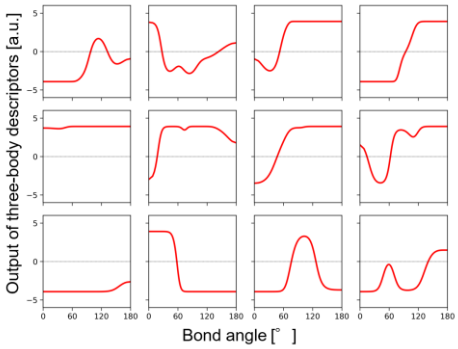

Fig. 3 Functional forms of the trained three-body descriptors as a function of bond angle.

4. Conclusions

This work proposed an atomic descriptor based ANNs. Unlike symmetry functions used in conventional ANN potentials, atomic environments were expressed using ANNs that separately account for two- and three-body atomic environments. The present ANN potential is found to exhibit a lower MAE with respect to the training datasets than a conventional ANN potential. In addition, an ANN potential with four-body descriptors shows a lower MAE than the ANN potential with only two- and three-body descriptors. The trained descriptors form complicated functions that cannot be reproduced using a single cosine function.

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