Machine Learning based Efficient Exploration of Crystal Interface Structures

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(FY2017-2020)

Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences (PO:Shinji Tsuneyuki)

Brief overview

Interfaces created by crystals have significant effect on important properties of materials. Because of recent development of computational resources, theoretical calculations become a quite useful tool for materials analysis. However, for interface structures, exhaustive investigation by theoretical calculations is not feasible because there exist infinite number of possible interface structures. To overcome this difficulty, we utilize machine learning models estimated from limited amount of simulation results, and show that it provides fast and accurate prediction of interface properties for efficient screening of materials.

Achievement

In this study, we built machine-learning based methods which drastically accelerate grain boundary (GB) analysis. Our main results are 1) GB atomic energy prediction, and 2) simultaneous structure search for multiple energy surfaces. Local energy distribution around the boundary is an essential information about GB. We showed that machine-learning based local energy prediction model accurately recovers the DFT atomic energy (Fig. 1). For the structure search study, we constructed an efficient machine-learning method for solving a set of structure searches of different rotation angle (Fig. 2). Based on transfer learning framework, faster exploration was realized, and further we introduced cost-effective strategy by which time-consuming larger cell calculations can be reduced.

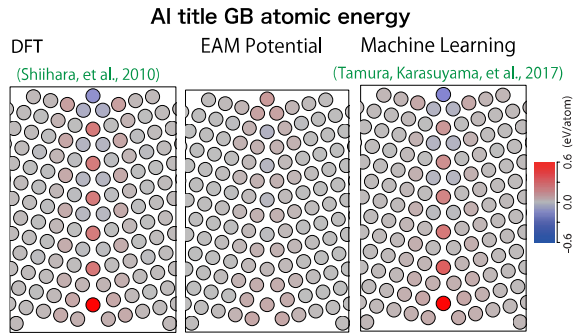

Fig.1: atomic energy prediction

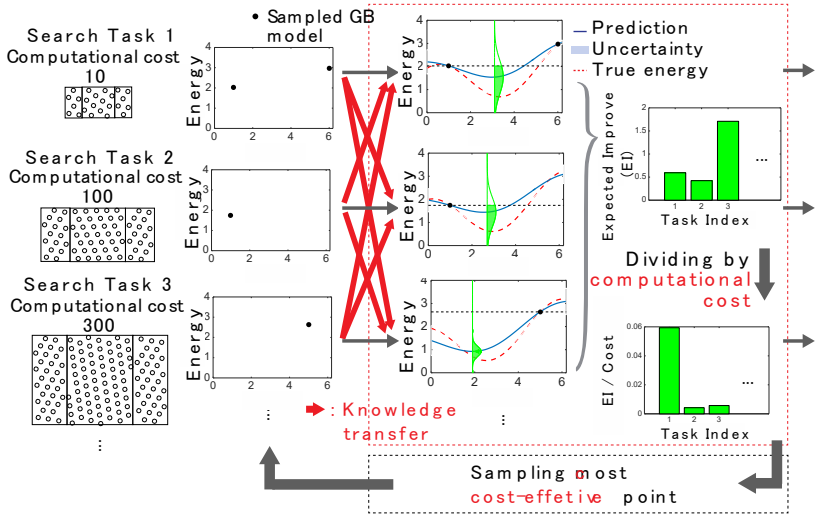

Fig. 2: GB structure search

Reference/Link

T. Yonezu, T. Tamura, I. Takeuchi, **M. Karasuyama**, *Physical Review Materials*, 2, 113802, 2018.

T. Tamura, **M. Karasuyama**, R. Kobayashi, R. Arakawa, Y. Shiihara, and I. Takeuchi, *Modelling and Simulation in Materials Science and Engineering*, vol.25, no.7, 075003, 2017.

As for related strategic objectives related to this research area, see http://www.senryaku.jst.go.jp/teian/en/koubo/h29youkou_7_en.pdf