Efficient Interface Structure Searching using Geostatistics Approach

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Interfaces are two dimensional lattice defect inside materials, and they strongly influences to the properties of materials. For example, an interface in a polycrystalline material, namely, a grain boundary (GB), determines the electron and ion transportation properties and mechanical properties; an atomic abrupt heterointerface in a superlattice often gives peculiar properties such as two dimensional gas and superconductivity. The fact that the interfaces show different properties from the bulk is caused by the fact that the different atomic structures from bulk are present at the interfaces. Thus, determination of the atomic structure of the interface is essential to facilitate the understanding of the interface properties.

On the other hand, very exhaustive computations are necessary to determine even a single interface structure, because interface has many degrees of freedom. Even in the case of a simplified coincidence-site lattice (CSL) GB of a simple metal, the number of configurations to be considered still ranges from several hundred to several hundred thousand, depending on the complexity of the interface. Thus, developing efficient methods to determine the interface structure without searching all possible combinations is extremely important in material science.

Here, we demonstrate a powerful method to search the most stable interface structure with the aid of a geostatistics approach called “kriging”. Kriging is an effective interpolation method based on a Gaussian process governed by prior covariances, and has been used to predict the optimum access points for geological mining operations. We apply this kriging technique to find the stable structures of interfaces efficiently.

A GB of copper Σ5[001]/(210) was chosen as the model case and the stable structure was determined. Using the conventional approach, all configurations were calculated and the most stable structure was determined from the search space. To reach the most stable structure and energy, 17,983 complete calculations were necessary by the conventional method. The calculated most stable GB energy was 0.96 J/m². Similar to the previous studies, the GB is composed of an array with a six-membered structure unit (Fig.1 (top)). The trajectory of this method can be shows as Fig.1(Top). In the conventional method, all calculations of the possible configuration is necessary.

To accelerate the process for searching the stable structure, the kriging approach was used. From the results of 20 randomly selected configurations, the search space was interpolated based on the Gaussian process. By using this kriging method, the computation is dramatically decreased. In this case, the most stable point was found after only 69 trials (including initial 20 trials) as shown in Fig. 1(bottom). The most stable structure obtained is identical to the stable structure obtained by the comprehensive data searching method (Fig.1(top, bottom)). Furthermore, the calculated GB energy is 0.96 J/m², which is identical to that by the conventional method. This indicates that our method can accurately find the most stable structure [1].

In conclusion, our approach successfully determined the most stable interface structure with an efficiency almost 2 orders of magnitude better than the conventional
“brute force” approach [2].

References
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Figure 1: Trajectory of the calculated GB energy to the convergence using (top) the conventional method and (bottom) the kriging method. The obtained stable structures are shown in each figure.