Polycrystalline materials comprised numerous crystal grains, and grain boundaries are formed by the attachment of different crystals. Since two differently oriented crystals form a grain boundary, the atomic arrangement at the grain boundary differs significantly from that in the bulk. This different atomic arrangement endows the grain boundary with peculiar properties, such as fast ion transportation and preferential deformation. The atomic arrangement at the grain boundary is thus of significant interest to the research of materials science and engineering.

Computations of grain boundary structures using first-principles calculations and static lattice models have been extensively performed. However, exhausting calculations are necessary to determine the complete grain boundary structure. This mainly results from the geometrical freedom of the grain boundary. Generally speaking, nine degrees of freedom, including five macroscopic and four microscopic, are present in a grain boundary. Even in the coincidence site lattice (CSL) grain boundary, called the four-dimensional rigid body translations and one grain-boundary plane must be considered. With simplified CSL grain boundaries, the number of configurations to be considered still remains anywhere from 1,000 to 10,000, depending on the complexity of the grain boundary structure. The theoretical calculations (static-lattice calculation or first-principles calculation) must be run by the number of these configurations to optimize the atomic structure and calculate the interface energy.

Figure 1 shows the four dimensional plot of the three dimensional rigid body translation and the grain boundary energy. One has to determine the most stable point in this data set. Only after this computation can the most stable atomic configuration and its grain boundary energy for one grain boundary type be determined. This computation for determining grain boundary structures is truly exhaustive, limiting systematic studies of grain boundary interfaces to simple metal systems. Despite the importance of these interfaces, accelerating the computation is not easy.

For instance, Chua et al. reported predictions of the stable structure of complex-oxide grain boundaries using a generic algorithms[1]. Similar methods for predicting unknown grain boundaries were performed by ab initio random structure searching algorithms by Schusteritsch et al.[2]. These methods have successfully predicted unknown grain boundary structures. However, even with these methods, many trial calculations are necessary to determine a single grain boundary structure. If the prediction of an unknown grain boundary can be achieved with less calculation, systematic investigations of more grain boundary types can be achieved within practical time frames. This systematic study of the grain boundary can provide deeper understanding of the structure-property relationships at this region.

Here, we demonstrate the two efficient informatics approaches for unveiling the structure and energy of grain boundary. The first one is the prediction of the structure and energy with the aid of a virtual screening based on machine learning technique.
After training the relationships between the grain boundary energy and the interface structure, this method can predict the structure and energy very efficiently [3]. The second method is the acceleration of the structure searching using Bayesian inference, namely kriging. We found that this kriging method is at least two order of magnitude better than the conventional approach [4] [5].

References
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Figure 1: the four dimensional plot of the three dimensional rigid body translation and the grain boundary energy.