# Interface structure determination using machine learning and atomic resolution analysis

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Interfaces are a kind of lattice defect inside crystalline materials, and can have significant effects on the mechanical and functional properties of materials. For instance, interfaces in polycrystalline materials, i.e., grain boundaries (GB), determine the ion transportation properties and high temperature mechanical properties; an atomically controlled interface in a thin film often provides unique properties such as the formation of two-dimensional gases. The fact that interfaces have different properties from the bulk is a consequence of the fact that they have different atomic structures from the bulk. Thus, for a comprehensive understanding of interface properties, determination of the atomic structure of the interface is one of the most important tasks for the materials research.

Since the atomic structure of the interface is strongly dependent on the crystal orientation, lattice planes, and terminations, a systematic study of the interface structure is indispensable for achieving a comprehensive understanding. Thus, the atomic structures of interfaces have already been extensively investigated. Because these characteristic atomic configurations at the interface appear within a very limited area (below 10nm), atomic resolution observations using transmission electron microscopy and theoretical calculations using atomistic simulations have been effectively applied to investigate interfaces.

To determine the interface structure via calculation, extensive calculations are usually necessary to determine even one interface structure because of the geometrical freedom of the interface. Nine degrees of freedom (five macroscopic and four microscopic) are present in an interface. The number of atomic configurations to be considered often reaches 10,000 in even the simplified coincidence site lattice (CSL) grain boundary, namely S grain boundaries.

If the structure and energy of unknown interfaces could be determined more efficiently and accurately, the investigation of interfaces would be dramatically accelerated, which could lead to a deeper understanding of the mechanisms that give rise to interface properties. To more efficiently determine interface structures, a genetic algorithm method and a random structure searching algorithm method have been proposed. However, many trial calculations are still necessary to determine a single grain boundary structure. More recently, much more efficient methods based on machine learning techniques, including virtual screening and Bayesian optimization have been proposed by the present authors.

Here, we demonstrate powerful approaches for unveiling the structure of the interface with an aid of machine learning. In my presentation, I am going to introduce two machine learning methods based on virtual screening [1] and Bayesian optimization (Kriging) [2,3]. We also combined transfer learning to the Kriging to accelerate the interface structure searching [4].

In addition, atomic resolution analysis is also using to investigate liquid, gas, glass, and interfaces [5-10]. I am going to presents those researchs in my presentation.

 

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Keywords: Crystal interface, Grain boundary, Machine learning, Atomic structure, Theoretical calculation, Kriging

 