Institut Pprime

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Université de Poitiers

PhD proposal

Development of a supervised-learning method for grain boundary structure identification

The mechanical properties of polycrystalline materials are strongly dependent on the behavior of grain boundaries. These two-dimensional defects have long been studied, but their complexity and the vast parameter space make them a subject of study at the frontier of current knowledge. One of the main difficulties in studying these defects using atomistic simulations is identifying the fine structure (also known as complexion) of the grain boundaries present in the system. The aim of this thesis is to develop a machine-learning method, and more specifically supervised classification, for identifying the structures of grain boundaries in atomistic simulations.

We propose to adapt a machine-learning method called Steinhardt Gaussian Mixture Analysis (SGMA), recently developed for the identification of defects in complex crystals, to the identification of grain boundary complexions in a simple crystal. The first step is to establish a database of the structures to be identified. The second step is to calculate descriptors for each structure in the database, to represent the local atomic environments. These descriptors are then used to fit a Gaussian mixture model, enabling us to classify the unknown local atomic environments (see figure).

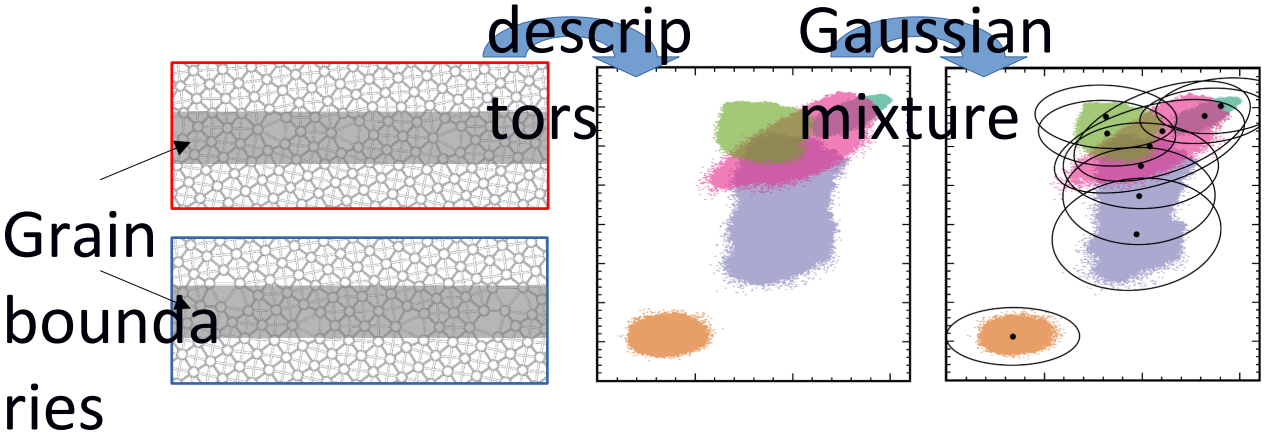

Figure : Illustrating the SGMA method, the atomic structures of grain boundaries are encoded by descriptors that are then fitted by a Gaussian mixing model.

This thesis will initially focus on the second stage of the method. Indeed, with the growing development of machine-learning techniques for materials physics, various descriptors have emerged, such as SOAP (Smooth Overlap of Atomic Positions) and ACE

(Atomic Cluster Expansion). These descriptors seem more promising for identifying grain boundary complexions than the descriptors initially used by the SGMA method. The thesis will first involve implementing the SOAP and ACE descriptors in AtomHIC (object-oriented C++) code, which already contains the other elements required to implement the SGMA method. We will then test the applicability of the method to the identification of grain boundary complexions, focusing on different complexions of the Σ3 grain boundary (twin boundary) in gold. One of the issues that this method will address, and which will be investigated during this thesis, is the establishment of relationships between grain boundary properties and their migration velocity.

Candidate profile

An interest in programming is required to successfully complete this thesis. Scientific curiosity, analysis, synthesis and communication skills are also desirable.

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