2024-2025

Master thesis proposal

SIMAP
Grenoble-INP-UGA, Saint-Martin d'Hères
Director: Didier Chaussende

Title: Machine learning potentials for atomistic simulations of Al-Al_2Cu interphase boundaries

Keywords: interfaces, atomistic simulations, machine learning, atomistic potentials

Scientific description: The identification of the atomic-scale structure of heterophase interfaces at equilibrium in a two-phased solid (interphase boundaries) is the key to a good understanding of both the elaboration process and the resulting physical properties of as-grown composite materials. It also represents a challenging research task, considering the complexity of the interactions between atoms of different chemical nature and the great variety of possible arrangements at the interfaces between crystal lattices of different symmetries. Indeed, numerical-simulation approaches using classical molecular dynamics methods are based, as a key input, on empirical interatomic potentials that actually remain only partly reliable as regards an accurate prediction of the relevant thermodynamic characteristics.
Objective: Bringing significant improvements in atomistic simulations of interphase boundaries by the use of machine learning (ML) algorithms for the construction of empirical potentials. During the internship, *ab initio* calculations of a sufficiently large number of representative configurations will be carried out. The resulting structures will be used for the numerical training of a high-dimensional neural-network dedicated to the construction of a well-calibrated potential. As a model system, we propose to consider the Al-Al_2Cu eutectic, with a motivation for the formation of solidification microstructures in lamellar-eutectic grains presenting remarkable orientation relationships between the two crystal phases. The aim is to get quantitative information on the anisotropy of the surface free energy of the interphase boundaries between the fcc Al-rich solid solution and the tetragonal Al_2Cu intermetallic at a finite temperature close to the eutectic. A particular orientation relationship, which has been recently identified experimentally in this system, will be considered in priority. Focus will be put on the simulation of interphase boundaries with various inclinations in the vicinity of the characteristic coincidence plane.

Techniques/methods in use: ab initio simulations (VASP), molecular dynamics (LAMMPS), machine learning tools (Scikit-Learn, N2P2 package).
Applicant skills: Applicants should have some knowledges in chemistry, physics and materials including phase transformations, as well as in modelling approaches (quantum mechanics, *ab initio, molecular dynamics*). Strong interest in computer science oriented towards machine learning approaches is a plus.
Industrial partnership: N

Internship supervisor(s) (name, email, phone, webmail):
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http://www.insp.jussieu.fr/-Dynamique-des-interfaces,583-.html
Internship location: The master thesis will be located in SIMAP, one of the leading Materials academic Lab in Grenoble under the auspices of a collaborative project between SIMAP at Grenoble-INP-UGA and INSP at Sorbonne University, Paris. The Lab is located on the campus of Saint Martin d'Hères, next to Grenoble, the capital of the Alps, and offers an international and simulating environment for both leisure (mountain sport) and science.
Possibility for a Doctoral thesis: Probable