Direction de l'Energie Nucléaire – DEN
Département des Matériaux pour le Nucléaire – DMN
Service de Recherches de Métallurgie Physique – SRMP

ARTIFICIAL INTELLIGENCE FOR PHASE TRANSITION AND CRYSTALLIZATION (FINGERPRINT)

External forces such as severe mechanical solicitations, thermal stress solidification and quenching, particle irradiations and electro-chemical implantations of ions induce allotropic phase transitions, crystallization or amorphization of materials. The main goal of this project is to investigate and characterize the kinetics of these phase transitions, with ab-initio accuracy, in Fe and Si. In Fe, we will investigate the role of the excess of radiation-induced point defects on the phase transitions such as the body centered cubic - bcc - to hexagonal close packed - hcp. In Si, we will investigate the amorphization and crystallization processes, which are thermally, electro-chemically or mechanically induced. To this end, the community needs two groundbreaking ingredients: an accurate representation of the interatomic interactions and a reaction coordinate for the phase transformation. We believe that the last achievements in atomistic machine learning methods could provide the means to obtain both.

In FINGERPRINT project we propose to use an accurate machine learning potential (developed with the tools provided by our previous project) combined with *boosted* MD simulations in the framework of adapted biasing force or potential methods in order to characterize allotropic phase transitions, crystallization or amorphization. The goal is to obtain a free energy profile with DFT accuracy that sample the transition path during these processes.

We are looking for a well-motivated post-doctoral researcher, with strong skills in atomistic modelling of materials. A good knowledge on programming is also required. The experience in machine /deep learning offer an advantage but is not compulsory.   The position is available immediately in CEA Saclay (near Paris). The postdoc position is for 1 year with the possibility of a 1 year extension. The interested candidates will submit by email an application letter, a detailed CV including a list of publications and two reference names.

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