PhD offer: *Atomistic modelling of the interaction between hydrogen atoms and structural defects in ferritic steels*

Key words: Hydrogen, Phase field crystal, ferritic steels, Hydrogen induced embrittlement, Machine-learning, Ecological transition.

PhD topic: Over the last years, the behaviour of hydrogen in metals has raised particular attention from the scientific community, in the background context of ecological transition and clean means of transport. Due its very small atomic radius, a tiny amount of hydrogen can indeed diffuse within the steels that come into contact with the liquid/gaseous dihydrogen during transportation and storage. With this, hydrogen atoms interact with the structural defects of the material, with respect to dynamical processes yet poorly understood. This phenomenon can lead to the embrittlement of the material, and eventually component failure. The understanding of the interaction of hydrogen atoms with structural defects in steels is therefore of paramount importance, both at the fundamental and technological levels.

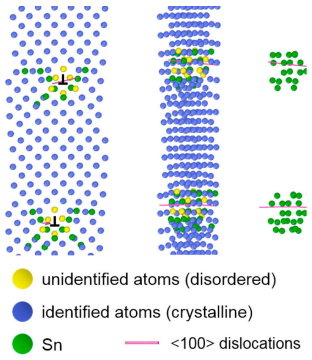

Figure 1: *QA simulation of the adsorption of Sn atoms in Iron.*

In this context, this project aims at developing a theoretical and numerical approach based on atomic scale modelling, in order to understand the underlying mechanisms of the interaction between hydrogen atoms and crystalline defects in ferritic steels. The ultimate purpose will be to decipher the entangled mechanisms that root hydrogen induced embrittlement in steels. In this perspective, an alternative approach to the traditional atomistic models (*ab initio* calculations, molecular dynamics, kinetic Monte-Carlo, etc.) named Quasi-particles approach (QA) [1, 2] will be used. This recent numerical method allows to simulate the evolution of the system on a time scale of diffusion and in continuous space, while preserving the description of the system at atomic scale. This approach is thus particularly suitable to address phenomena related to structural defects (dislocations, JG, incoherent interfaces, etc.), where the lattice periodicity is lost (figure 1). This numerical approach will be aided by an original machine-learning procedure based on Recurrent Neural Networks, which will allow to upscale QA simulations, for purposes of unravelling the coupled mechanisms at the origin of hydrogen induced embrittlement in steels for the first time, on space and time scales comparable to experiments.

The PhD student will carry out his or her PhD within the ERAFFEN team of the GPM laboratory, which has a strong expertise in the field of modelling and simulation for materials. He or she will have access to the supercomputer of Normandy (CRIANN). The geographical environment of the thesis will be the city of Rouen, very close to Paris.

[1] M. Lavrskyi *et al.*, Npj Computational Materials **2**, 1 (2016).

[2] G. Demange *et al.*, Acta Materialia **226**, 117599 (2022).

Expected skills:

1. The candidate will have twofold skills in numerical modelling and condensed matter physics.
2. The candidate will have solid knowledge in one topic at least among the following: condensed matter physics, (statistical) thermodynamics, cristallography, materials science.
3. The candidate will show solid basis in numerical physics.
4. Programming skills in one of the following languages are required: Fortran, Python. Skills in C/C++ may be acceptable.

Practical information: the PhD thesis will be carried out at the Groupe de Physique des Matériaux (GPM, UMR 6634, Université de Rouen-Normandie), under the direction of Helena Zapolsky (Professor) and the supervision of Gilles Demange (Maître de Conférences), starting 01/09/2023.

Contacts: gilles.demange@univ-rouen.fr, helena.zapolsky@univ-rouen.fr

---