



6-month research internship at SRMP, CEA/Saclay, France, starting from Feb. 2020

Title: Mobility of dislocations decorated by carbon atoms in iron

Research area: Solid State Physics, Materials Science

Summary of the project: Metals and alloys with body centered cubic (bcc) structure represent an important class of structural materials in industry, and in particular in the energy industry. The presence of interstitial impurities, such as carbon in iron, modifies the plastic behaviour of the material, notably by inducing the so-called dynamical strain ageing phenomenon, commonly observed in ferritic steels, which results from the interaction between dislocations and solute atoms. The goal of this project is to study the coupling between the dislocation mobility and the solute atom diffusion. To this end, numerical simulations will be used in order to improve our fundamental understanding of the effect of carbon on dislocation glide in iron. This requires a multi-scale coupling between ab initio electronic structure calculations and kinetic model of dislocation glide and solute diffusion, to describe the mechanisms underlying the dislocation glide kinetics in Fe(C) system. We will build on recent observations by in-situ straining experiments in a transmission electron microscope in Fe(C).

The research internship fellow of 6 months is funded by the ANR DeGAS project (Dislocation Glide in AlloyS: chemistry/microstructure coupling), based on a multiscale approach combining theoretical modelling, atomistic calculations and experiment. In this framework, this internship will be performed in close collaboration with two post-doctorate fellows working on both the modelling and the experimental part of DeGAS project. The most demanding calculations will be performed on national and European computing centers, and in particular on the Jewels supercomputer (Jülich, Deutschland) through the PRACE DIMAB project (Dislocations in bcc Metals: an AB initio study). This internship project will be performed within the framework of the EUROfusion European consortium on fusion materials modelling.

Qualifications: Applicants must have strong skills in Solid State Physics and Materials Science. Good English language proficiency.

Practical information: The Service de Recherches de Métallurgie Physique (SRMP) is part of the Department of Materials for Nuclear energy at CEA-Saclay. It is located 20 km south-west of Paris, in the area called Plateau de Saclay. The SRMP research laboratory has 28 full-time members with 29 graduate students. This internship can be followed by a PhD thesis funded by CEA.

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Time frame: The start date for the appointment is **Feb. 2020** and the end date is **July 2020**.

How to apply: Candidates must return a statement of research interests, CV, and names and contact information of two references to lisa.ventelon@cea.fr.

References:

- B. Lüthi, F. Berthier, L. Ventelon, B. Legrand, D. Rodney and F. Willaime, Modelling Simul. Mater. Sci. Eng. 27, 074002 (2019).
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- D. Rodney, L. Ventelon, E. Clouet, L. Pizzagalli and F. Willaime, Acta Mater. 124, 633 (2017).
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- D. Caillard, Acta Mater. 112, 273 (2016).
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