18-month post-doctorate position at SRMP, CEA/Saclay, France, starting from April 2018

Title: Ab initio modelling of interactions between dislocations and solutes in body-centered cubic metals

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 of present and future nuclear power plants. It is essential to understand the sensitivity of their mechanical properties to both their microstructure and their chemistry. This involves the controlled addition of alloying elements, each offering specific attributes with respect to strength. The goal of this project is to study the origin at the atomic scale of solute effects on mechanical properties in metals and alloys and in particular to understand how dislocations interact with solute atoms. The study will focus on interstitial carbon solutes in bcc iron and bcc tungsten. Recent results based on ab initio electronic structure calculations – required to describe the core region of the dislocation adequately – suggest a strong attraction of carbon solutes with screw dislocation cores inducing a spontaneous reconstruction of the core structure. The present project involves ab initio calculations of interaction energies and Peierls barriers based on the VASP code in order to build an accurate picture of the segregation on dislocation cores and of the dislocation glide mechanisms in presence of carbon.

The post-doctorate fellow of 18 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. The most demanding calculations will be performed on national and European computing centers, and in particular on the MareNostrum supercomputer (BSC, Spain) through the PRACE AIMODIM project (Ab Initio Modelling Of Dislocations In Metals). This post-doctorate project will be in relation with the work performed within the framework of the EUROfusion Consortium.

Qualifications: Applicants must have an earned Ph.D. degree in Solid State Physics, Materials Science or in a closely related area. Good English language proficiency. Ideal candidates will have a few years of experience in atomic scale simulation and Density Functional Theory calculations.

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 30 full-time members with 25 graduate students.

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Time frame: The start date for the appointment is **April 2018** and the end date is **October 2019**.

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:

- L. Ventelon and F. Willaime, J. Computer-Aided Mater. Des. 14, 85 (2007).
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