



Five-month interim replacement at SRMP, CEA/Saclay, France, starting from March 2015

Title: Ab initio modeling of dislocations in body-centered cubic metals

Research area: Solid State Physics, Material 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. The specific plastic deformation behaviour of bcc metals is related to the fact that dislocations have deep Peierls valleys, i.e. they must overcome high energy barriers to glide in the crystal. An atomistic description of the core of these linear defects is required to account for this behaviour. The electronic structure of the material is itself at the origin of the geometry of the dislocation core. Our recent electronic structure calculations have for instance shown that the relative stability of dislocation core configurations in bcc Fe(C) is profoundly modified compared to pure iron by the presence of carbon solutes.

The goal of this project is to explore the relation between atomic-scale dislocation core properties and macroscopic mechanical behavior in bcc transition metals. This work will be based on electronic structure calculations, using ab initio techniques in the framework of the Density Functional Theory based on the VASP code. The project will focus on the ab initio modelling of the Peierls potential, i.e. the energy landscape seen by dislocations, under applied stress in bcc transition metals (V, Nb, Ta, Mo, W and Fe). This will allow us to study the dependence of the Peierls stress, i.e. the applied shear stress needed for dislocation motion at 0 K, on crystal orientation.

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.

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 29 full-time members with 13 graduate students.

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Time frame: The start date for the appointment is **March 2, 2015** and the end date is **July 17, 2015**. Applications received before **January 30, 2015** will be given full consideration but the review of applications will continue until the position is filled.

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 et F. Willaime, J. Computer-Aided Mater. Des. 14, 85 (2007).
- L. Ventelon, Ph. D. Thesis, Université Claude Bernard Lyon 1, France (2008).
- E. Clouet, L. Ventelon et F. Willaime, Phys. Rev. Lett. 102, 055502 (2009).
- L. Ventelon, F. Willaime, E. Clouet et D. Rodney, Acta Mater. 61, 3973 (2013).
- L. Dezerald, L. Ventelon, E. Clouet, C. Denoual, D. Rodney et F. Willaime, Phys. Rev. B 89, 024104 (2014).
- L. Dezerald, Ph.D. thesis, Institut National Polytechnique de Grenoble, France (2014).

For additional information about the related research area, please visit:
<http://lisa.ventelon.pagesperso-orange.fr>