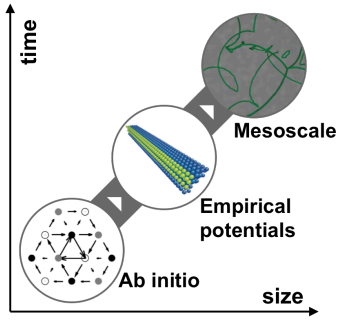
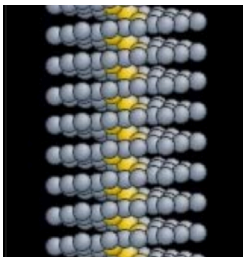
Ph.D. proposal Materials Science/Solid State Physics

Ab initio study of body-centered cubic metals plasticity

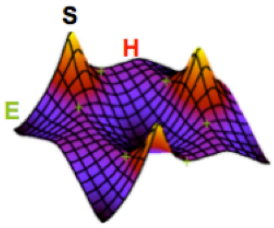
Summary – Body-centered cubic (BCC) metals are base components for many alloys and steels used for example in the nuclear and automotive industries. The optimization of these materials' mechanical properties is necessary to comply with increasingly demanding expectations such as structural lightening, resistance to radiation damage, energy savings, etc. The study of elementary mechanisms that control plasticity enables improving the performances of existing materials as well as guiding materials design. Here, we propose to investigate the plasticity of the following BCC transition metals: V, Nb, Ta, Mo, W and Fe. These metals display an atypical plasticity at low temperature that arises from screw dislocation core effects. The use of atomic-scale *ab initio* simulations that describe both the atomic and electronic structure of materials is necessary to investigate such effects. The approach consists in performing *ab initio* calculations of dislocation core properties in several BCC metals in order to (1) evidence differences and/or common behaviors between these metals at atomic scale and (2) improve existing models that describe BCC metals plasticity at higher scales. We will focus on the effects of stress on dislocation properties since the laws used to describe plastic deformation of materials do not apply to BCC metals. The results will be validated by comparison with experimental data and will be used to propose new laws to describe the plasticity of BCC metals. This work is part of the development of metals plasticity modeling in synergy with recent experimental progress, for example in the field of electron microscopy.



Multiscale modeling of dislocations and plasticity



Screw dislocation core in a BCC metal



Peierls potential in Fe calculated with dislocation

Context – The work will be performed at Jean Lamour Institute (Nancy, France), in the team *Physics, Mechanics and Plasticity* from the Department of Materials Science and Metallurgy, and in collaboration with CEA Saclay (France) and ILM in Lyon (France). The Ph.D. is co-funded by the LabEx DAMAS and the Grand Est region. The largest simulations will be performed on international supercomputers.

Profile – Masters of Physics and/or Engineering (quantum physics, solid state physics and/or materials science) interested in materials modeling. Programming skills will be appreciated.

Advisory team: The work will be co-advised by Lucile DEZERALD and Alain JACQUES. Frequent meetings will be scheduled with Lisa Ventelon and François Willaime (CEA) and David Rodney (ILM).

Information:
Funding: LabEx DAMAS and Grand Est region (fully funded)
Application deadline: August 15th 2017
Starting date: October 2017
Duration: 3 years

To apply, send a CV, statement of interest and transcripts to Lucile DEZERALD:
lucile.dezerald@univ-lorraine.fr