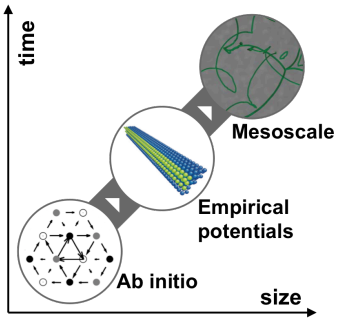
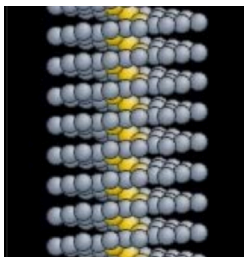
Ph. D. proposal in Materials Science/Solid State Physics

Ab initio study of plasticity in body-centered cubic metals

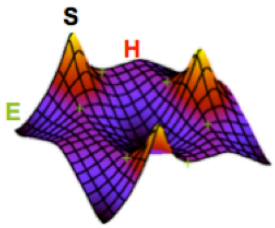
Summary – Body-centered cubic (BCC) metals are base components for many alloys and steels used for example in the nuclear and automotive industries. The optimization of these materials' mechanical properties is necessary to comply with increasingly demanding expectations such as structural lightening, 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 the design for new materials. The proposed work aims at investigating 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 envisionned 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*. The research topics will include the impact of stress and chemical composition on screw dislocations core properties and BCC metals plasticity. This work is part of the development of metals plasticity modelling in sinergy with recent experimental progress, for example in the field of electron microscopy.



Multiscale modeling of dislocations and plasticity



Screw dislocation core in a body-centered cubic metal



Peierls potential in Fe calculated with ab initio

Context – The research will be performed at IJL (Nancy, France). The largest calculations in terms of cpu time (~ million hours cpu) will be performed on supercomputers (French and European), in collaboration with CEA (Saclay, France) and ILM (Lyon, France). An additional collaboration with UCLA (CA, USA) is envisionned. This research is part of the topics covered by the labex DAMAS.

About the candidate – The position requires holding a MS or ME with knowledge in quantum physics, solid state physics and/or materials science. Programming skills will be appreciated.

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Coadvisor – Alain JACQUES (IJL)

Information :
Envisionned grant : MSER Ph.D fellowship
Starting date : September/October 2016
Duration : 3 years
Location : Institut Jean Lamour, 54000 NANCY
Département de Science et Ingénierie des Matériaux et Métallurgie
Equipe de Physique, Mécanique et Plasticité

The proposed work is in continuity with the following: Dezerald et al., Phys. Rev. B **89, 024104 (2014) et Dezerald et al., Phys. Rev. B **91**, 094105 (2015)*