Unité Matériaux et Transformations

Université Lille - UMR CNRS 8207
Bâtiment C6
59655 Villeneuve d'Ascq – France

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Atomistic Modelling of Dislocation climb in Oxide

Convection and flow in the Earth's mantle involves the deformation of crystalline rocks in creep conditions, characterized by high temperatures and extremely low stresses. Creep usually occurs by the operation of various deformation processes, at different scales of length and time. In particular, the glide and climb of dislocations (crystalline defect responsible for plastic deformation) are expected to play a major role. Whereas glide has attracted a lot of attention, climb remains poorly constrained and controversial. Since the latter is enhanced under extremely low stress conditions typical of the mantle, it is extremely challenging to study dislocation creep using laboratory experiments. In this context, numerical modelling represents the most promising approach to study creep behaviour of Earth's minerals under relevant natural conditions.

Understanding creep requires a proper description of dislocation climb processes (i.e. the emission or the absorption of point defects that allows a row of the dislocation line to move out of its glide plane). At the scientific interface between geosciences and materials science, the goal of this PhD project is to provide a new understanding of climb processes in ionic materials. The PhD project will be first dedicated to the climb of dislocation in magnesium oxide MgO, which with a typical rock salt structure, can be viewed as an archetype of ionic system. The major part of the project will be to undertake atomistic simulation of jogged dislocation line configurations, in the scope of computing jog nucleation and migration enthalpies. Molecular static calculations will be performed using classical packages such as LAMMPS or GULP.

The successful candidate should hold a Master degree in Condensed Matter, solid state physics/chemistry, or materials science. He/she should have a pronounced taste for theoretical modelling and knowledge of basic programming. Applications must be sent to philippe.carrez@univ-lille1.fr