INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

The ICAMS Seminar presents

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Coupling elasticity theory and atomic simulations to model dislocations in iron

Plastic deformation in crystals is heavily related to the dislocation core properties. As experimental investigation of the dislocation core is difficult, atomic simulations have become a common tool in dislocation theory. But dislocations induce a long-range elastic field, and one has to take full account of it in the atomic modelling. We illustrate how this coupling between elasticity theory and atomic simulations operates for the case of dislocations in bcc iron. A proper definition of the elastic energy allows extracting from atomic simulations a dislocation core energy which is a real intrinsic dislocation property [1]. Calculations for edge dislocation shows that dislocations gliding in {110} planes are more stable than those gliding in the {112} planes. For the screw dislocation, ab initio calculations indicate that the elastic displacement cannot be described only by the Volterra solution. A supplementary elastic field is also created by a dilatation of the dislocation core. The modelling of this core field in anisotropic elasticity theory leads to atom displacements in perfect agreement with the ones observed in ab initio calculations. The inclusion of this core field in the computation of the elastic energy allows deriving a core energy which does not depend on the simulation conditions [2]. Finally, we model the interaction of C atoms with dislocations using both atomic simulations and elasticity theory. A quantitative agreement is obtained between both modelling techniques. The comparison shows that elastic calculations remain valid even when the C atom gets really close to the dislocation core [3].

[1] E. Clouet, Philos. Mag. **89**, 1565 (2009).
[2] E. Clouet, L. Ventelon, and F. Willaime, Phys. Rev. Lett. **102**, 055502 (2009).
[3] E. Clouet, S. Garruchet, H. Nguyen, M. Perez, and C. S. Becquart, Acta Mater. **56**, 3450 (2008).