Elastic effects in Materials Modelling

A talk by Céline Varvenne

Laboratory for Multiscale Materials Modelling, EPFL, Switzerland

DATE / TIME: Monday, March 17th 2014, 04:00 p.m.
LOCATION: Ludwig Boltzmann Lecture Hall, ground floor, Strudlhofgasse 4, 1090 Vienna

Céline Varvenne | celine.varvenne@epfl.ch

Including elastic effects is necessary when studying materials properties. In metallic alloys, they arise from alloying elements, from point defects, or from dislocations. These spatial inhomogeneities induce atomic relaxations that have consequences both on the thermodynamics and the kinetics of the material. Such relaxations can also lead to numerical issues due to finite size effects in simulations, when trying to obtain reliable defect properties.
We first examine, at the atomic scale, the effects of atomic relaxations that are present in any alloy involving elements with different atomic radii. Relaxations are incorporated in this work within the Lattice Green's functions formalism, where elasticity is embedded into a long-range Hamiltonian (effective pair interactions). The characteristic time scale in this framework is the diffusion one, which allows us to study microstructural evolutions at the atomic scale, using a lattice Monte Carlo code. A quantitative analysis of the precipitation processes is provided for binary alloys with varying atomic size mismatch. In addition, we establish in a clear way the link between discrete and continuous homogeneous linear elasticity. This shows how to easily parametrize elastic interactions at the atomic scale from macroscopic quantities, for any alloy.

In a second time, we adress the question of point defect modelling, such as vacancies, interstials and their clusters. Indeed, ab initio approaches are the most accurate way to model these defects, but they suffer from strong size limitations (a few hundred atoms). Consequently, when using periodic boundary conditions to calculate their properties, each defect interacts with its periodic images. This is due to the atomic relaxations around the defect and make the converged values of the defect properties out of reach in many situations. We propose an elastic corrective scheme able to get rid of this limitation and to obtain the properties of isolated defects. The reliability of the method is demonstrated on three different problematic cases: the self-interstitial atom in hcp zirconium, the vacancy in diamond silicon and self-interstitial clusters in bcc iron.