Ab-initio simulations of dislocations in bcc transition metals and alloys

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Understanding and predicting plastic deformation of bcc transition metals is a topic of intensive research. In comparison to fcc metals, bcc metals exhibit several unusual features of plastic deformation[1] including the presence several possible glide planes, i.e. the {110}, {112} and {123} plane, a pronounced temperature-dependence of the flow stress, solid solution softening, break-down of the Schmid law of the critical resolved shear stress, anomalous slip and a ductile-to-brittle transition. These features are all related to the properties and behavior of dislocations where a prominent role is assigned to the $1/2 < 111 >$ screw dislocation (in the following just referred to as screw dislocation). Due to its nonplanar core structure, this dislocation is relatively sessile and is regarded as a key limiting factor for plastic deformation. Recently, however, also the importance of other dislocations with a planar core structure, in particular the M111 dislocation, has been highlighted.[2]

In this talk we will present atomistic ab-initio simulations of screw dislocations and M111 dislocations in bcc transition metals. A special focus is laid on tungsten which is the metal with the highest melting point and a high ductile-to-brittle transition temperature. Furthermore, we also focus on Fe due to its obvious relevance as a structural material. The simulation techniques based on the periodic dipole approach and the Peierls-Nabarro model will be introduced. The fundamental properties of the screw dislocations and M111 dislocations in pure bcc metals will be discussed and their research history shortly outlined. On this basis, the impact of alloying on the core structure of screw dislocation at 0K within the framework of the virtual crystal approximation will be discussed.[1,2,3] It will be shown how the d-band filling induces a change in core structure in both W-Re and Fe-Co alloys (see Figure 1) but not, for instance, in W-Ta alloys.

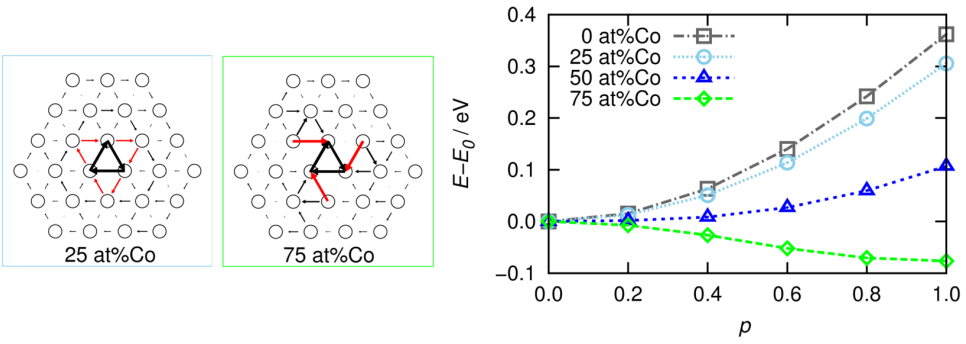

Figure 1: Differential displacement map of the screw dislocation in $Fe_{75}Co_{25}$ (left) and $Fe_{25}Co_{75}$ (middle) illustrating a change in core polarity p from 0 to 1. To the right, the energy per burgers vector of one dislocation as a function of core polarity is shown for several FeCo alloys.

Furthermore, the evolution of the Peierls stress with d-band filling of the screw dislocation for W-based alloys will be shown. A discussion on how these changes are related to other fundamental properties such as elastic constants, gamma surfaces or interstring potential and how they compare with available experiments from the literature will be presented.

As the next step we will discuss temperature-induced changes in the core structure of the screw dislocation. Such changes have been observed in some molecular dynamics simulations[6,7] but their occurrence is still unclear. For nonmagnetic materials the transition is rooted in the lattice vibrations and the arising lattice expansion. For Fe the situation is more complex as also a transition from the ferromagnetic to the paramagnetic state arises. We will present preliminary results where the spin-wave[8] method is used to model a screw dislocation in the paramagnetic state. After a short outline of the essential elements of the spin-wave method, we will show what the impact of the paramagnetic state on the core structure is.

After concluding the main topics and challenges for future ab-initio modeling of dislocations in bcc metals will be highlighted.

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