ABSTRACT ICTP-2014-SMR-2614

2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, 3–7 November 2014, International Centre for Theoretical Physics (ICTP), Trieste, Italy.

Energy landscape of point defects in body-centered-cubic metals.

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Progress in fusion and advanced fission power generation technology depends critically on the development of new high temperature materials. In metal alloys, including tungsten alloys, microstructural evolution occurring under irradiation is strongly dependent on the diffusion properties of point defects, such as interstitial atoms and vacancies, and also on the properties of extended defects, such as dislocations and surfaces. The mobilities of self-interstitial atoms and their clusters in metals, especially body-centered cubic (BCC) metals, are one of the main issues in multiscale models for the prediction of the microstructure evolution that these materials undergo under irradiation. Moreover, the morphology adopted by these defect clusters is a fundamental question with obvious practical consequences on the materials properties, since it controls also the dislocation obstacle strength and hence the strengthening of the materials and dimensional changes like swelling or growth for anisotropic materials. We investigate the energy landscape of defects in BCC metals by the means of the ab initio methods as well as the empirical potentials developed from electronic structure calculations.

For vacancy clusters there is a competition between planar loops and voids, and also stacking fault tetrahedra in face-centered cubic metals. On the other hand, the observation of clusters of self-interstitial atoms in metals by transmission electron microscopy (TEM) techniques reveals only nanometer size planar loops. In BCC metals these loops have a ½<111> Burgers vector, except in iron at high temperatures where it is <100>. Recently, we have proposed a three dimensional periodic structure for self-interstitial clusters in BCC metals, as opposed to the conventional two dimensional loop morphology [1]. The underlying crystal structure corresponds to the C15 Laves phase. The new three dimensional structures generalize previous observations [1, 2].Using Density Functional Theory (DFT) calculations on typical configurations, we demonstrate that in $\alpha $--iron these C15 aggregates are highly stable and immobile and that they exhibit large antiferromagnetic moments. These clusters form directly in displacement cascades and they can grow by capturing self-interstitials. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.

The mechanism of voids formation implies firstly the formation of smaller clusters as di-vacancy. Di-vacancy in tungsten, as in all BCC metals of the group VI B, has an unusual energy landscape. In tungsten, the first nearest neighbour is slightly repulsive or attractive depending of DFT calculations or exchange-correlation functional while the second nearest neighbour configuration is strongly repulsive [3]. The same tendency is observed for all elements of VI B group and is not the case for V B metals and iron for which the most stable configuration of di-vacancy is the second nearest neighbour configuration. However, in experiments, in the high temperature limit vacancy clusters are directly observed in tungsten [4]. Moreover, this work provides input data for kinetic models for microstructural evolution. The formation/migration free energies of mono- and di-vacancies / interstitials are computed using calculations. The vibrational part of the free energy is computed in the frame transition state theory (TST) using harmonic approximation. The anharmonic part is evaluated by the recently developed method based on adiabatic reweighting algorithm for computing the free energy along an external parameter from adaptive molecular dynamics simulations [5]. The electronic entropy contribution to the free energy is also taken into account. The defect binding free

energies and defect diffusion coefficients deduced from these calculations can be used to perform simulations of isochronal resistivity recovery experiments. We show that the temperature deeply impact the energy landscape of di-vacancy at higher temperature and can even change the relative stability of various configurations.

Using the ab-initio data we have developed empirical interatomic potentials to study ½<111> screw dislocations in bcc iron and tungsten. The potentials use the Embedded-Atom-Method formalism and are fitted to a mixed database, containing various experimentally measured properties and ab initio formation energies of defects, as well as ab initio inter-atomic forces computed for random liquid congurations. The availability of data on atomic force fields proves critical for the development of the new potentials. In agreement with predictions from ab initio calculations, the new potentials correctly reproduce the non-degenerate core structure of the screw dislocation, with a {110} glide plane and a single hump Peierls potential, without intermediate metastable configuration.

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