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Atomistic simulations of screw dislocations in bcc tungsten: From core structures and static properties to interaction with vacancies

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ABSTRACT

Atomistic simulations have been used to investigate the core structures, static properties of isolated 1/2 <1 1 1> screw dislocations, and their interaction with vacancies in bcc tungsten (W) based on three empirical interatomic potentials. Differential displacement maps show that only one embedded atom method potential is able to reproduce the compact non-degenerate core as evidenced by *ab initio* calculations. The obtained strain energy and stress distribution from atomistic simulations are, in general, consistent with elasticity theory predictions. In particular, one component of the calculated shear stress, which is not present according to elasticity theory, is non-negligible in the core region of our dislocation model. The differences between the results calculated from three interatomic potentials are in details, such as the specific value and the symmetry, but the trend of spatial distributions of static properties in the long range are close to each other. By calculating the binding energies between the dislocations and vacancies, we demonstrate that the dislocations act as vacancy sinks, which may be important for the nucleation and growth of hydrogen bubbles in W under irradiation.

1. Introduction

Dislocations are the main features to accommodate plastic deformation in crystalline materials [1]. It is generally recognized from both experimental and theoretical studies that the plasticity of bcc transition metals is controlled by the motion of ½<1 1 1> screw dislocations, whose non-planar core structures lead to a high lattice friction stress [2–5]. To date, extensive a*b initio* calculations [4–7] demonstrated that the non-degenerate (symmetric) core structures are energetically more stable than their degenerate (asymmetric) counterparts in pure bcc transition metals. Notably, the preferred core structure may change from non-degenerate to degenerate upon substitutional solute alloying or interstitial solute segregation [8–12].

Tungsten (W) is considered to be the leading candidate for plasma facing materials (PFMs) in future fusion devices. However, the mechanical properties of W-PFM will be severely degraded by hydrogen (H) or helium (He) irradiation, retention and bubble formation. Most recently, comprehensive computational and experimental efforts [13–15] showed that dislocations can increase H retention in W by trapping H at the dislocation core. These interstitial H atoms can subsequently undergo fast one-dimensional migration along the dislocation line, resulting in H aggregation, jog-punching, and eventually the nucleation and growth of H bubbles. However, the high computational cost of *ab initio* calculations and difficulty of observing atomistic processes by experimental means point out the necessity of investigating the basic static properties [16–19] and dynamic behaviors of dislocations from classical atomistic simulations based on empirical interatomic potentials. An essential step towards the above-mentioned dynamic simulations is whether the core structures, static properties of dislocations and their interaction with defects from the classical simulation can reproduce the *ab initio* results.

In this work, we employ three interatomic potentials to investigate the core structures and static properties of ½<1 1 1> screw dislocations. Considering the important effect of vacancies on H bubble nucleation in both W bulk [20–23], and extended defects such as dislocations [24], grain boundaries [25], and sub-surfaces [26], the energetics of vacancy segregation to the screw dislocation

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has also been examined. Some of the results from the present atomistic simulations have been compared with *ab initio* calculations and elasticity theory predictions.

2. Computational method

Atomistic simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code, based on three interatomic potentials including an embedded atom method (EAM) potential developed by Marinica et al. [27], a modified version [28] of the original EAM potential developed by Ackland et al. [29] and a bond order potential (BOP) developed by Li and coworkers [30]. These potentials give bulk and defect properties in good agreement with *ab initio* and experimental results. In the following sections, the two EAM potentials are thus denoted as EAM I and EAM II, by Marinica and Ackland, respectively. In the coordinate system shown in Fig. 1, an initial 1/2 <1 1 1> screw dislocation model of a cylindrical configuration with a height of 27 Å and a radius of 102 Å was constructed by placing W atoms into the system based on dislocation elasticity theory, after which a low temperature annealing for 1 ps and a steepest descent minimization using the potentials mentioned above were performed. The modeled dislocation system, which is periodic along the dislocation line, contains 57900 atoms with 13500 atoms at the outmost region remaining fixed during the annealing and minimization process. Vacancies were introduced by iteratively removing an atom around the screw dislocation core. The size of the system is large enough that the interaction of vacancy with its periodic images can be neglected.

3. Results and discussion

3.1. Core structures

Fig. 2 shows the differential displacement map of the ½<1 1 1> screw dislocations obtained by the three interatomic potentials. Atoms with different colors denote different adjacent (1 1 1) atomic layers perpendicular to the dislocation line. Displacement differences of neighboring atoms parallel to the dislocation line (the direction of the Burgers vector $\boldsymbol{b}$) are depicted by the length of the arrows, which is the largest when the displacement difference equals $b/3$. All the other displacement differences are normalized by the largest length. Note that arrows are drawn from the atoms with smaller displacements to the ones with larger displacements. As was also revealed by Grigorev et al. [14], the EAM I gives a non-degenerate core structure (Fig. 2a), which is invariant with respect to the $[10\bar{1}]$ two-fold symmetry operation and agrees with *ab initio* results [4–7], while both the EAM II and the BOP yield similar degenerate core structures (Fig. 2b and c).

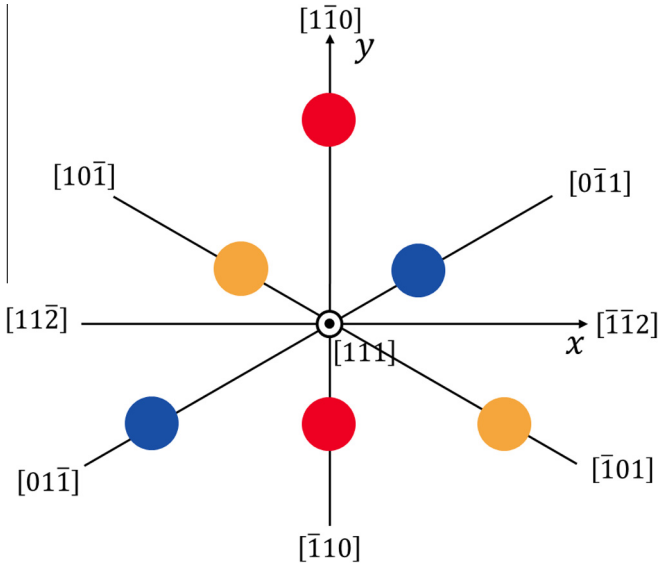

Fig. 1. The coordinate system used to present the dislocation core projection at the (1 1 1) plane in this paper. The Burgers vector $\boldsymbol{b}$ and the dislocation line ξ point towards the *z*-axis, corresponding to the [1 1 1] direction. Circles of different colors represent atoms at different layers close to the dislocation core in the (1 1 1) plane.

To find out how these two types of core structures are formed, we further examined the component of atomic displacement in the (1 1 1) plane during the relaxation, as shown in Fig. 3. For the displacement map from EAM I, both atoms moving towards and away from the core are present, and there is tendency of displacement magnitude decay as a function of the distance from the core, in distinct contrast to those from the EAM II and the BOP, in which all atoms move away from the core and the magnitude of atomic displacement increase by the distance from the core. Based on these results, we demonstrate that, unlike non-degenerate core structure formation, the formation of degenerate core structures involves significant structural rearrangement.

3.2. Strain energy and stress

The strain energy of an atom reflects the activity of it, and a higher strain energy means less energy is needed to move away the atom from its position. Thus the total strain energy of a structure may reflect its ability to get itself changed. We define the strain energy as the difference between the total energy of equilibrium dislocation structure and the total energy of the corresponding perfect lattice, which is equivalent to the energy needed to create a screw dislocation in a perfect crystal. The total strain energy of a dislocation can be expressed as

$$E_{total} = E_{core} + E_{elastic\ strain} \tag{1}$$

where E_{core} and $E_{elastic\ strain}$ represent the contributions from the core field and from the long range elastic strain field, respectively. Assuming the core region has a radius of r_0, we can thus calculate, according to elasticity theory, the elastic strain energy per unit length in the cylindrical region with radius of R as

$$E_{elastic\ strain}(R) = \frac{\mu b^2}{4\pi} \ln\left(\frac{R}{r_0}\right) (R > r_0) \tag{2}$$

where the μ stands for the shear modulus of W. Therefore, the total strain energy per unit length can be numerically described as

$$E_{total}(R) = \left[E_{core} - \frac{\mu b^2}{4\pi} \ln(r_0)\right] + \frac{\mu b^2}{4\pi} \ln(R)\ (R > r_0) \tag{3}$$

Fig. 4 illustrates the total strain energy as a function of distance from the core center from atomistic simulations. E_{total} linearly increases with the increase of natural logarithmic distance $\ln(R)$ at the elastic region ($R > r_0$). We can detect that the elastic region starts at $\ln(R) = 1.75$ Å, indicating the radius of the core region is approximately 3.16 Å, which contains 18 atoms per unit Burgers vector b. The slopes at the elastic region of three structures are similar, which correspond to the factor $\frac{\mu b^2}{4\pi}$ in formula (3). According to the fitted slopes we may obtain the shear modulus of W, i.e. the μ, for three interatomic potentials. These are 164.20 GPa for EAM I, 159.82 GPa for EAM II, and 159.95 GPa for BOP, consistent with the values of 160 Gpa [27] for EAM I, 161 GPa [31] for EAM II, and 161 GPa [30] for BOP calculated in the bulk of W. Among the results the one obtained by EAM I is very close to the experimental value of 164.00 GPa [32] at the temperature of 4 K.

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