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Ab initio study of interaction of helium with edge and screw dislocations in tungsten

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ABSTRACT

The interaction of a single He atom with edge and screw dislocations in tungsten has been studied using *ab initio* calculations. It was revealed that He is strongly attracted to the core of both dislocations with the interaction energy of −1.3 and −3.0 eV for screw and edge dislocations, respectively, which corresponds to the detrapping temperature in thermal desorption spectroscopy experiments of about 500 K and 1050 K, respectively. The lowest energy positions for He around the dislocation cores are identified and the atomic structures are rationalized on the basis of elasticity theory considerations. Both types of dislocations exhibit a higher binding energy for He as compared to the He-He binding (known as self-trapping) and are weaker traps as compared to a single vacancy. It is, thus, concluded that the strong attraction to dislocation lines can contribute to the nucleation of He clusters in the temperature range which already excludes He self-trapping.

1. Introduction

Tungsten is an important material for fusion applications, selected for use in International Thermonuclear Experimental Reactor (ITER) and DEMOnstration Power Station (DEMO) projects for divertor armor and first wall. During operation of thermonuclear fusion devices plasma-facing components undergo exposure to high energy fast neutrons and are bombarded by plasma ions such as H isotopes and He. This process inevitably leads to subsurface damage of the material due to accumulation (the so-called trapping) of H and He which reduces the resistance to a thermo-mechanical load and as the worst-case scenario can lead to a failure of the component.

At present, significant efforts are dedicated to build up the theoretical and empirical models to assess the amount of gas atoms accumulated in the components during the operation and to estimate their storage for ITER-relevant conditions i.e. the high flux low energy plasma regime. Such a task requires deep understanding of a variety of processes including the very basic ones: the initial trapping of single H and He atoms in tungsten.

The experimental study of the problem of trapping and penetration of plasma components in tungsten-made components [1–3] is largely obstructed by the fact that the real material contains a certain density of lattice imperfections which include vacancies, dislocations and grain boundaries. The latter affect the penetration depth profile and may act as seeds for nucleation of high order clusters. In turn, the dislocations subdivide into edge and screw types which are likely traps for He (alike H [4]). Edge and screw dislocations experience different interaction with an interstitial He due to a difference in the elastic field around the core (being of larger size for edge dislocations [5]) and core structure itself. Since the real material contains not just pure straight edge and screw dislocations but rather a network of dislocations including mixed ones, it is rather difficult to deduce the actual trapping strength of particular types of dislocations using conventional experimental means (e.g. plasma exposure and thermal desorption spectroscopy), while this data is very important for numerical assessment of the H/He trapping and release. Therefore, in this work an alternative method – computational atomistic modelling – is chosen to determine the binding of He with the dislocations.

From earlier theoretical studies [6] it is known that He interacts repulsively with any host atom in transition metals including W. Two He atoms bind strongly one to another (~1 eV [7]) and this interaction vanishes at a distance of 3 Å [8]. He is strongly attracted

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to a vacancy – 4.5 eV [9] and it is positioned in the center of a vacancy, i.e. in the region with minimum of electron charge density. Also, the extended lattice defects such as grain boundaries and dislocations can play a role of trapping sites and diffusion channels thereby promoting deeper penetration of light interstitials into the material especially at a high temperature.

In this work we apply *ab initio* calculations to deduce the interaction energy of a single He atom with ½⟨1 1 1⟩ edge and screw dislocations and calculate the corresponding detrapping temperature. The energetically favourable positions around the dislocation core are identified. The contribution to the trapping of He in W from the dislocation of both screw and edge character is thus evaluated and compared with other typical trapping defects such as vacancy and grain boundaries.

2. Computational details

The *ab initio* calculations were performed using the density functional theory code Vienna Ab Initio Simulation Package (VASP) [10,11]. The projector-augmented wave (PAW) potentials [12,13] were applied. The electron exchange-correlation functional was described within the generalized gradient approximation using PW91 functionals [14], with a Vosko-Wilk-Nusair interpolation [15]. Ionic relaxation was carried out using the conjugate gradient algorithm with a force convergence criterion of 0.03 eV/Å. During the relaxation the cell shape and volume (equal to the equilibrium volume of bulk tungsten of 3.1781 Å) were kept constant. The energy cutoff equal to 450 eV was applied to get the converged values for total energy and interaction energy.

The screw and edge dislocations were studied by two different crystals and approaches. The screw dislocation was simulated in the model box with a square-like periodic array of dislocation quadrupoles as described in Ref. [16]. The supercell vectors {$\mathbf{C_1}$, $\mathbf{C_2}$, $\mathbf{C_3}$} are not orthogonal and are given by $\mathbf{C_1} = n \times \mathbf{a_1}$; $\mathbf{C_2} = ½n \times \mathbf{a_1} + m \times \mathbf{a_2} + ½\mathbf{a_3}$; $\mathbf{C_3} = \mathbf{a_3}$, where $\mathbf{a_1} = 1/3[-1\,1\,2]$; $\mathbf{a_2} = 1/2[1\,-1\,0]$; $\mathbf{a_3} = [1\,1\,1]$ and (n, m) = (15, 9). Two components were added to $\mathbf{C_1}$ and $\mathbf{C_2}$ along $\mathbf{a_3}$ (−1/(3m) and −1/(6m), respectively) to account for the shift along [1 −1 0] direction of the centers of gravity of the upward- and downward-pointing triangles, on which the two dislocations constituting the dipole are centered. The resulting box had 270 atoms and the dimensions of $41.01 \times 38.82 \times 5.50$ Å^3. The k-point mesh of $1 \times 3 \times 11$ was used. The length of the dislocation line was $2 \times \boldsymbol{b}$, where $\boldsymbol{b} = ½⟨1\,1\,1⟩$. Such a box size along the (z) direction was selected intentionally to minimize the self-interaction for He atoms (which is strongest at the distance of 1.5 Å) which was described in Refs. [7,8]. The edge dislocation was simulated by introducing the single edge dislocation with $\boldsymbol{b} = ½⟨1\,1\,1⟩$ in the center of the crystal with rigid boundary conditions (periodic along the dislocation line only) as described in Ref. [17]. The box with 246 atoms was dimensioned as $24.82 \times 7.78 \times 22.51$ Å^3 along [−1 −1 1] (x), [1 −1 0] (y) and [1 1 2] (z) axes. A k-point mesh of $1 \times 7 \times 1$ was applied.

In order to find the lowest energy positions for a single He atom next to the dislocation, we have identified the tetrahedral positions (the lowest energy interstitial positions for He in bulk W [8]) around the dislocation core as is visualized in the Fig 1a and b for screw and edge dislocations, respectively. Such positions were used as initial configuration for the further relaxation.

The interaction energy between an interstitial He atom and the dislocation E_I was assessed following the standard definition applied in other DFT works [18–20]:

$$E_I = [E_{disl-He} + E_{bulk}] - [E_{disl} + E_{He}], \quad (1)$$

where E_{disl} and E_{He} are the total energies of the box with the dislocation or He atom in the tetrahedral position only, respectively, $E_{disl\text{-}He}$ is the energy of the system with He and dislocation and E_{bulk} refers to the total energy of the bulk tungsten. Following this notation, a negative value implies an attractive interaction and vice versa.

3. Results and discussion

3.1. Interaction of He with screw dislocations

The results of the calculations show (see Fig. 2a) that the screw dislocation attracts strongly a single He atom with the maximum interaction energy of −1.3 eV, occurring in the vicinity of the dislocation core. Note that this value is by 0.3 eV lower that the interaction energy for a He-He pair equal to −1.0 eV. Such a value for the He-screw dislocation interaction implies that the screw dislocation can further enhance clustering of He atoms and facilitate the formation of He clusters on dislocation lines even at temperatures which already exclude He self-trapping.

Unlike the case of hydrogen [4], the equilibrium positions (corresponding to the lowest energy state configuration) for He near the screw dislocation core do not coincide with the charge density depleted zones. On the contrary, the interaction between He and neighboring tungsten atoms is purely elastic and the formation of bonding is energetically unfavorable [6]. In Fig 2a one can easily identify a set of three zones extended along non-equivalent ⟨1 1 0⟩ directions (contained in non-equivalent {1 1 1} planes) with the lowest energy positions (i.e. strong attraction) for He. Whereas,

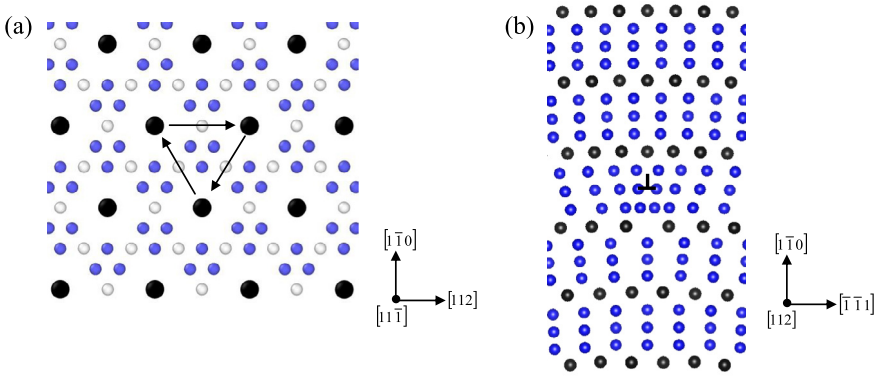

Fig. 1. The initial tetrahedral positions for He (blue) and for W atoms (black) next to screw (a) and edge (b) dislocations. The dislocation is oriented perpendicular to the image plane and its location can be identified by arrows (a) and by the sign ⊥ (b). The octahedral interstitial positions (gray) are also shown in (a). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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