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The nucleation and growth of H blisters in dislocation loops in W{110}

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HIGHLIGHTS

- The vacancy-type dislocation loops are energetically preferred to be present on W{110} planes.
- The nucleation and growth of H blisters on dislocation loops in W{110} planes are thoroughly addressed.
- H_2 molecules are observed in the H blisters, and the corresponding physical insight is revealed.

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ABSTRACT

We propose a mechanism for nucleation and growth of H blisters in vacancy-type dislocation loops (DLs) in tungsten (W), based on the first principles calculations. We find that vacancy-type DLs are energetically preferred to form on {110} planes. The H atoms nearby are readily to migrate to and accumulate in the DLs with energy cost less than 0.24 eV. With the increasing number of the trapped H atoms, the DL expands rapidly, consequently, the nucleation and growth of H blisters is completed in the DL gradually. In addition, H_2 molecules are observed in the H blisters when the H areal density in DL reaches to be of 6.3×10^{15} atoms/cm^2 (the number of H atoms per the cross-sectional area of the DL). Our proposed formation mechanism for H blisters in W material may also be applicable to other metals and metal alloys.

1. Introduction

In the application of fusion energy, exploration and design of plasma-facing materials (PFMs) is an important issue [1]. The metal tungsten, with high melting point, high thermal conductivity as well as low sputtering yield for light elements, is considered to be one of the most promising candidates for PFMs in fusion reactors [2,3]. However, in the fusion environments, W suffers the irradiation from high-flux plasma of hydrogen (H) isotopes and helium (He) ions, as well as 14 MeV neutrons, which causes the damage of structure and degradation of properties of this material.

The typical structural damages, H blisters (or bubbles) on W surfaces, were clearly observed after H plasma irradiation under different experimental conditions [4–7]. Such surface blisters readily lead to the ejection of W atoms in plasma, and consequently degrade the performance of fusion device [8,9]. To improve the serving properties of W as the PFM, many efforts have been paid to reveal the formation mechanism of H blisters [10–19]. Generally, formation of bubbles in metals involves two main steps: bubble nucleation and bubble growth [20]. Physically, the defects in W, such as vacancies, stacking faults, dislocations and grain boundaries, are believed to be the most possible nucleation sites for H bubbles. By using first-principles calculations, Liu et al. [10] reported that a monovacancy in W can only trap up to 10 H atoms, in which H bubbles are hard to grow up. Stacking faults in W were reported to act as traps to attract H atoms, serving as nucleation and growth sites for H bubbles [15]. Recently, it was confirmed that nucleation and growth of H bubbles can be formed on dislocation networks in W [16,17].

In addition to the defects mentioned above, vacancy-type dislocation loops (DLs) commonly exist in metals [21–26]. Providing more space for H atoms to accommodate, the vacancy-type DLs may also act as the nucleation of H bubbles. So far, there are only few reports about the interaction between H and vacancy-type DLs in W at atomic scale. These studies were performed with

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the loop planes on {100} [14] or {111} [15]. However, in experiment, the majority of vacancy-type DLs was found on {110} planes [25].

In this work, on the basis of the first-principles calculations, we reveal that the vacancy-type DL is preferred to be present in W{110} planes energetically. Furthermore, the accumulation behaviors of H in the vacancy-type DLs in W{110} planes are explored. The results depict that vacancy-type DLs can trap H atoms, serving as nucleation sites of H bubbles. With increasing the trapped H atoms, H bubbles grow up gradually. When the areal density (the number of H atoms per the cross-sectional area of the DL) of the trapped H is up to 6.3×10^{15} atoms/cm^2, H_2 molecules are observed in the bubbles.

2. Methodology

The first-principles calculations are performed using Vienna ab initio simulation package (VASP) [27] based on the density functional theory (DFT). The interaction between ions and valence electrons is described with using projector augmented wave (PAW) potentials [28], and the exchange-correlation between electrons is described with using the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) form [29]. The kinetic energy cutoff for the plane-wave basis set is 400 eV. A supercell consisting of 135 W atoms ($3 \times 3 \times 15$ unit cell) is employed in our calculations, and its Brillouin zone is sampled with $5 \times 5 \times 1$ k points within the Monkhorst-Pack scheme [30]. In our optimization, energy minimization is converged until the forces on all the atoms are less than 0.02 eV Å^{-1}. The lattice constant of the body-centered cubic (bcc) W bulk is calculated to be 3.172 Å, being in good agreement with the experimental value of 3.165 Å [31].

The climbing image nudged elastic band (CI-NEB) method [32] is used to determine minimum energy paths for diffusion of a monovacancy and H atoms. Since an H atom is a light-mass particle, the zero-point energy (ZPE) of H is taken into account in the evaluation of the diffusion barriers [33].

3. Results and discussion

3.1. Formation of vacancy-type dislocation loops in W bulk

Structurally, vacancy-type DLs can be regarded as line-up of the vacancies in a material, which corresponds to the gathering of monovacancies via diffusion. However, the calculated diffusion barrier of a monovacancy in W bulk is up to 1.68 eV, indicating that monovacancies are hard to migrate at low temperatures. As we know, strain commonly exists in W as the PFM in the fusion reactor, due to thermal effect and the irradiation of neutrons, hydrogen isotopes, as well as other energetic particles. We thus concern the diffusion behaviors of a monovacancy in W bulk under the applied strains.

Fig. 1 displays the energy barriers for the diffusion of a monovacancy as a function of the applied strains. From Fig. 1, one can see that when the isotropic strain (blue solid line in Fig. 1) is applied, the diffusion barrier for a monovacancy decreases monotonically with the increasing tensile strain, and increases with the increasing compressive strain. For the compressive strain of 6%, the barrier reaches to be 1.87 eV, and for tensile strain of 6%, the barrier lowers to be 1.38 eV. We then further consider the influence of the anisotropic (biaxial and uniaxial) strain on the diffusion behavior of a monovacancy. Under biaxial strain, the lattice constants along both a and b are fixed at a given strain, and the lattice constant along c direction is fully relaxed. Under uniaxial strain, the lattice constant along c direction is fixed at a given strain, and the lattice constants along both a and b are fully relaxed. Our calculations reveal that the diffusion barrier of the monovacancy decreases

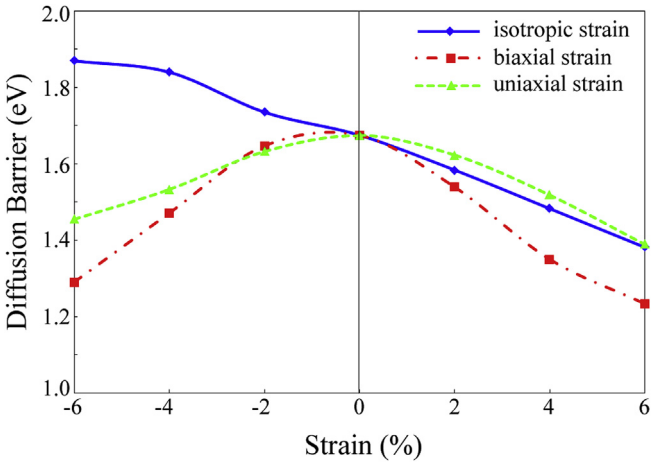

Fig. 1. The energy barrier for the diffusion of monovacancy as a function of the applied strain.

under both compressive and tensile biaxial strain, exhibiting hyperbolic feature (red dot-dashed line in Fig. 1). The diffusion barrier can be lowered to be about 1.23 eV for the tensile biaxial strain of 6%. Similar to the case under biaxial strain, the diffusion energy curve of a monovacancy under uniaxial strain also displays hyperbolic feature (green dashed line in Fig. 1). The energy barrier can be lowered to be about 1.40 eV under the applied tensile strain of 6%. This implies anisotropic strains in W are beneficial for vacancies to migrate and gather together in W bulk. Although the energy barrier above 1.0 eV is a little high, monovacancies may have large possibilities to migrate in W serving as the PFM, concerning the condition of fusion reactor.

Since the monovacancies can migrate in W as the PFM, vacancy-type dislocation loops may be generated when the vacancies diffuse and eventually accumulate on a specific plane. In our computational simulations, it is extremely hard to treat a DL with hundreds of atoms at the DFT level. It is noted that the local structure at the center of DLs is quite the same as an intrinsic stacking fault (ISF). So, for convenience, we use ISF to mimic a vacancy-type DL in our DFT calculations.

We now investigate the favorite orientation for vacancy-type DLs to be present in W bulk. In bcc lattice, there are several typical crystal orientations, for example <100>, <110>, <111> and <112>. In our structural model, the ISF is obtained by removing one atomic layer from the perfect stacking sequence along a specified direction. For example, the stacking sequence along <110> is changed from ... *ABABAB* ... to ... *AB|BAB* ..., and that along <112> is changed from ... *ABCDEFABCDEF* ... to ... *ABCDEF|BCDEF* ... et al.

We suppose that the vacancies are homogeneously distributed in W bulk initially, and thus define the formation energy of ISF in W bulk as:

$$E_f(isf) = \left(E_{isf} - n \cdot E_W - m \cdot E_f^V\right) / S, \quad (1)$$

where E_{isf} is the energy of the ISF system, E_W is the energy of a W atom in perfect bcc W, E_f^V is the formation energy of the monovacancy, S is the cross-sectional area of the ISF, n and m are the number of W atoms and vacancies in the ISF system, respectively. E_f^V is calculated with a $4 \times 4 \times 4$ supercell of the bcc W and the resulting value is 3.34 eV, being in good agreement with the experimental value of 3.1–4.0 eV [34]. Here, we remove one atomic layer in an 18-layers supercell ($1 \times 1 \times 17$) to construct an ISF and fixed the supercell size to simulate the DL with strain in the local