



Strain-induced variation of electronic structure of helium in tungsten and its effects on dissolution and diffusion



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ABSTRACT

We have investigated the effects of strain on the dissolution and diffusion properties of helium (He) in tungsten (W) using a first-principles method. We show that the solubility and diffusion of He can be enhanced (suppressed) with increasing tensile (compressive) strain. This can be attributed to the variation of the effective volume and the *p*-projected DOS of He induced by the strain. We demonstrate that the strong electronic interaction between He and W atoms plays a key role in the poor solubility of He in W. The tetrahedral interstitial site is always the preferred site of He under all strains. The same rule is believed to hold for other inert gas elements in strained W.

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1. Introduction

The interaction of helium (He) with metal is very important in the materials design and development. In spite of its extremely low solubility, tiny amount of He can lead to significant changes in the microstructure and mechanical properties of metals, such as high-temperature He embrittlement [1,2]. Helium energetically prefers to occupy the defects with excess volume, such as vacancies, dislocations, and grain boundaries in metals [3–5], owing to its closed shell electronic structure. The accumulation of He at defects will form He bubbles, and further lead to void swelling, surface roughening, irradiation-induced hardening, and temperature intergranular embrittlement increasing [6–8], which can significantly degrade the mechanical properties of materials.

Although the He-metal interaction has been under intensive investigation, the physical mechanism for the growth of He bubbles in metals remains poorly understood. It is found that the gas pressure in He bubbles can reach several GPa [9,10]. Kajita et al. reported that the stresses induced by bubble formation and growth are responsible for fuzz formation [11]. Sharafat et al. showed that the collection of bubbles moves rapidly to the free surface with the increasing stress gradient [12]. Faiza et al. reported that He bubbles will induce significant plastic deformation of the surface ligament [7]. Apparently, the accumulation of He will cause strain to the lattice surrounding the defects, and the further He trapped by defects must pass through the strain region. Therefore, the effects of strain

on He behaviors in metals is very important for the growth of He bubbles.

Tungsten (W) and W alloys are considered as the most promising plasma facing materials (PFM) in a fusion reactor, which will be exposed to a high flux of He escaping from the plasma [13–15]. Therefore, the mechanical properties and the structural strength of W under He irradiation are some of the key concerns for W PFM and have been under intensive investigation. It has been demonstrated that a single He is energetically favorable sitting at the tetrahedral interstitial site (TIS) rather than the octahedral interstitial site (OIS) in bcc metals [16–21]. Strain can change the lattice space and the impurity-metal atoms distances, thus should have effect on the behaviors of He in metals. Lu et al. investigated the effects of strain on hydrogen (H) behaviors in W [22,23], and found that strain plays an important role in H bubble nucleation and growth. Yet the behaviors of He under strain has not been fully understood. So far little work focuses on this aspect. In order to understand the physical mechanism of strain effects on He behaviors in W, we have systematically investigated the effects of hydrostatic strain on the dissolution and diffusion of He in W using the first-principles method. Our calculations will provide a good reference for understanding He-bubble nucleation and growth mechanism in W.

2. Computational method

Calculations have been made within the plane-wave pseudo-potential method and density functional theory (DFT), which are implemented in the Vienna Ab-initio Simulation Package (VASP)

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[24,25]. The interaction between core ion and valence electron is described by the projector augmented-wave method (PAW) [24], while the exchange–correlation part of electron is described with generalized gradient approximation (GGA) by Perdew and Wang [26]. The cutoff energy was set to be 350 eV and a $3 \times 3 \times 3$ k-points mesh was built up according to the Monkhorst–Pack scheme [27]. A bcc supercell model containing 128 atoms has been utilized. The calculated equilibrium lattice constant is 3.17 Å for bcc W, which is consistent with experiment value of 3.16 Å. The convergence tests of the total energy with respect to the k-points sampling and cutoff energy have been carefully examined. Under the hydrostatic strain, the supercell size is fixed at given strain values with atomic positions relaxed. The iteration concluded when forces on all atoms reached less than 10^{-3} eV/Å.

Helium is a typical interstitial impurity in metals, because the atomic radius of He is smaller than that of a metal atom. We thus only calculate the solution energies of a single He at interstitial case to investigate the site preference of He under the hydrostatic strain. The potential occupation interstitial sites of He in the bulk W include the TIS and the OIS, as shown in Fig. 1. The hydrostatic strain is applied to the supercell by changing its dimension. The range of applied strain is between -5% and $+5\%$ with the interval of 1%. The solution energy of a single He in the bulk W is defined as

$$E_{\text{He},\varepsilon}^{\text{sol}} = E_{\text{NW,He},\varepsilon} - E_{\text{NW},\varepsilon} - E_{\text{He}}, \quad (1)$$

where $E_{\text{NW,He},\varepsilon}$ and $E_{\text{NW},\varepsilon}$ are the total energies of the supercell containing N W atoms with and without He atom, respectively. The third term E_{He} is the energy of an isolated He atom. ε is the strain.

3. Results and discussions

Fig. 2 shows the solution energies of a single He atom at both the TIS and the OIS under the hydrostatic strain. It can be found that the solution energy of He decreases for both the TIS and the OIS with the increasing tensile strain but increases with the increasing compressive strain, which may be attributed to the variation of He “effective volume” under the hydrostatic strain. It has been demonstrated that the stability of interstitial He atom in the strain-free metals mainly depends on its effective volume provided by the given interstitial site [19]. This indicates that the tensile strain is more favorable than the compressive one for He dissolution in W. Further, the solution energy of He at the TIS are always lower than that at the OIS regardless of the strain sign and value, as shown in Fig. 2. Hence, the TIS remains to be the preferred site under the hydrostatic strain.

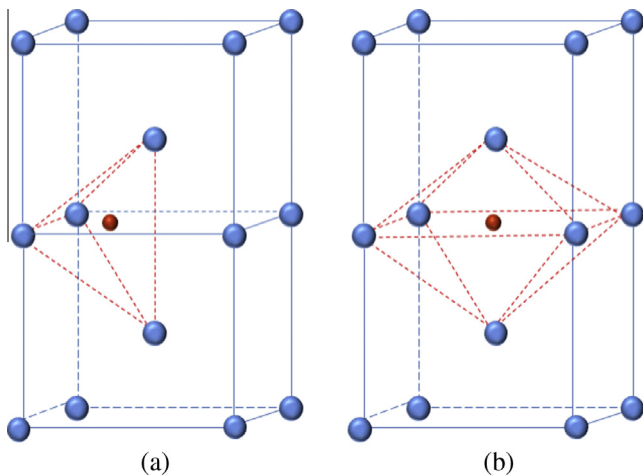


Fig. 1. The interstitial sites in bcc W, (a) TIS and (b) OIS. The smaller red spheres represent the He atoms; the larger blue spheres represent the W atoms.

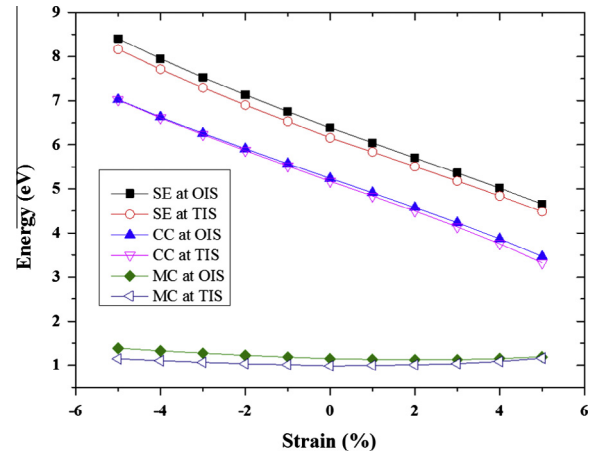


Fig. 2. The solution energy (SE) of He, the mechanical contribution (MC), and the chemical contribution (CC) at both the TIS and the OIS in W as a function of strain.

To further shed light on the physical mechanism underlying the stability of He in W under the hydrostatic strain, it is helpful to decompose the solution energies into two contributions [28]. One is the deformation energy induced by the embedded He atom, defined as the energy release during the course of W relaxation after He is removed, and called the *mechanical contribution* (MC). The other is the electronic effect (the direct interaction between He and W atoms), called the *chemical contribution* (CC).

The covalent radii of He and W atoms are ~ 0.49 Å and ~ 1.30 Å, respectively; while the initial distances between He and its first nearest neighboring (1NN) W atoms at the TIS and the OIS are 1.77 Å and 1.59 Å in the bulk W, respectively. Therefore, He will lattice distortion when it occupies the interstitial sites. The distances between He and its 1NN W atoms are found to increase 9.60% for the TIS and 15.20% for the OIS after the structure optimization. Correspondingly, the MC is calculated to be 0.99 eV and 1.15 eV for He at the TIS and the OIS, respectively. Meanwhile, the CC is equal to the difference between the MC and the solution energy, thus it is calculated to be 5.18 eV and 5.24 eV for He at the TIS and the OIS, respectively. Apparently, the CC is much larger than the MC for the solution energy of He at the interstitial sites, and takes up 84% and 82% for He solution energy at the TIS and the OIS, respectively. Therefore, the strong electronic interaction between He and W atoms is largely responsible for the poor solubility of He in W. This can be attributed to that He is characterized by its closed-shell electronic structure, and prefers to keep such structure when it goes into different environment. Any interaction with other elements which breaks such structure can elevate the system energy.

Fig. 2 shows the MC and CC for the solution energy of He at both the TIS and OIS under the hydrostatic strain. It can be found that the CC decreases for both the TIS and OIS with the increasing tensile strain but increases with the increasing compressive strain, similar to that of He solution energy under the hydrostatic strain. The MC also increases with the increasing compressive strain, but it basically increases with the increasing tensile strain. The relative stability of He at the interstitial site depends on the difference of He solution energy at the TIS and the OIS, which also consists of the MC and the CC. It can be found that the MC of He at the TIS is 0.16 eV lower than that at the OIS in the strain-free W, while the CC difference between the TIS and the OIS is only 0.06 eV. Therefore, the MC dominates in the relative stability of He in the strain-free W. The differences of He solution energy (DSE), the mechanical contribution (DMC), and the chemical contribution (DCC) between at the TIS and the OIS as a function of the hydrostatic strain are shown in Fig. 3.

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