



First principles study of helium trapping by solute elements in tungsten



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ARTICLE INFO

Article history:

Available online 5 June 2014

ABSTRACT

The behavior of helium in metals is particularly important in fusion research due to the He induced degradation of materials. A small amount of impurities introduced by alloying or transmutation reactions will interact with He and lead the microstructure and mechanical properties of materials to change. In this paper, we present the results of first-principles calculations on the interactions of He with impurities in tungsten (W), including the interstitials C, N, O, and substitutional 3d, 4d and 5d transition metals. We find that the trapping radii of interstitial atoms for He are almost twice larger than those of substitutional solutes. A preliminary evaluation of the effective trapping of He is also given when considering the detrapping of He at high temperature. The binding energies between the substitutional impurities and He increase linearly with the relative charge densities at the He occupation site, implying that He atoms easily aggregate at low charge density sites. The present results suggest that Ta might be chosen as a relatively suitable alloying element compared to other possible choices.

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1. Introduction

Tungsten (W) and W alloys are most promising for use as the divertor material in the International Thermonuclear Experimental Reactor (ITER) and in future fusion reactors due to their high melting point, good thermal conductivity, low tritium inventory, and low sputtering rate [1,2]. In ITER and future fusion devices, the surface of W will be exposed to extremely large fluxes of hydrogen and helium, and special surface structures can form on the W surface by impact of low energy hydrogen and helium, which may influence the surface stability [3]. Experimental results show that exposure of W to He leads to blisters and bubbles confined to a depth of more than 140 nm [3–5]. Moreover, it was found that He irradiation generates a fuzzy structure on the surface, which consists of a very porous W network and is mechanically unstable [3,6]. Understanding these macroscopic effects requires detailed knowledge of the processes controlling microstructural evolution, such as the He atom configuration in the W lattice, diffusion of He atoms, their trapping and dissociation from other defects, as well as bubble nucleation and growth [7,8].

In addition, the practical use of W is hindered by its high ductile–brittle transition temperature (DBTT) and consequently high brittleness at the operation temperature. It has been proposed that

the ductility of W can be improved by the addition of certain alloying elements such as Re, Ta, Tc, Os, Ru, Ti and V [9–11]. Transmutation reactions during neutron irradiation also generates some new elements such as Re, Os, Ta [10,12]. These impurities will inevitably interact with the emitted He from neutron-induced reactions, consequently leading the change of microstructure and mechanical properties of materials [13]. Therefore, it is necessary to clarify the interactions of impurities with He in W. Previous results showed that the substitutional impurities such as Ag and Cu and inert gas atoms are capable of trapping He atoms in W [14]. Recently, Becquart et al. have investigated the binding energies of a series of impurities with He and He clusters, and found that most of the substitutional impurities can trap He atoms as well as small He clusters except for Re [15,16]. These investigations have certainly advanced our understanding of helium trapping by solutes in W, but as the authors of Ref. [16] pointed out the relationship between the binding energies of impurities with He and the electron densities is not clear and requires further investigations.

The results of our earlier studies by first-principles suggest that there is a linear relation between the binding energies and the relative charge densities at the He occupation site for some common alloying and transmutation impurities in W such as Re, Ta, Os and Ti [17]. The diffusion behaviors of He around these impurities were also studied. However, it should be further confirmed if the relationship between binding energies and electron densities

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exists for more alloying elements in W. Another purpose of this study is to present a quantitative comparison of the trapping radii of interstitial atoms and substitutional solutes for He. In this paper, we carry out a systematic first-principles calculation to quantify the binding energies and the trapping radii of He around impurities in W. These impurities include interstitial C, N and O atoms and substitutional 3d, 4d and 5d transition-metal (TM) solutes, which are chosen to construct an extensive first-principles database of He-solute binding and gain insight into fundamental and general trends. We believe the general conclusion of He behavior in W are also applicable to other metals.

2. Computation method

The present calculations are performed within density functional theory as implemented in the Vienna Ab-initio Simulation Package (VASP) [18,19]. The interaction between ions and electrons is described by the projector augmented wave potential (PAW) method [20]. Exchange and correlation functions are taken in a form proposed by Perdew and Wang within the generalized gradient approximation (GGA) [21,22]. The supercell composed of 128 lattice points ($4 \times 4 \times 4$) is used. The plane wave cutoff and k-point density are both checked for convergence for each system to be within 0.001 eV per atom. Following a series of test calculations a plane wave cutoff of 500 eV is used and a k-point grid density of $3 \times 3 \times 3$ is employed. The structural optimization is truncated when the forces converge to less than $0.01 \text{ eV } \text{Å}^{-1}$. In order to accurately account for the dilation effects of He in the W lattice [23], the supercell shape and volume are allowed to fully relax in our calculations. It should be noted that the constant volume relaxation is also found acceptable to describe helium trapping by solutes in W by Becquart et al. [16,24], because these two different strategies to relax the system will approach the same value when the system is large enough to reach the asymptotic behavior [24,25]. To test the validity of the size of supercell, a larger supercell containing 250 atoms ($5 \times 5 \times 5$) with $2 \times 2 \times 2$ k-points is calculated for comparison. The binding energies between He and the impurities such as vacancy, N, O and V are nearly the same to those by using the $4 \times 4 \times 4$ supercell, which means that the 128 atom supercell is big enough for this investigation.

The binding energy of two defects (A_1, A_2) is calculated as follows:

$$E_b^{A_1-A_2} = E_{tot}^{A_1} + E_{tot}^{A_2} - E_{tot}^{A_1+A_2} - E_{tot}^{bulk}$$

where $E_{tot}^{A_1}$ and $E_{tot}^{A_2}$ are total energies of the supercell with A_1 and A_2 , respectively, $E_{tot}^{A_1+A_2}$ is total energy of the supercell containing both A_1 and A_2 , and E_{tot}^{bulk} is total energy of perfect W bulk in supercell.

3. Results

The site preference of impurities in bulk W is considered first before studying their influence on trapping He. We examine the substitutional site and two interstitial sites of the W lattice, i.e., tetrahedral (t) and octahedral (o) site. The calculations of W with impurities at different sites show that transition elements prefer substitutional sites, and small elements C and N favor to occupy the o -site, while He and O prefer the t -site. These results are in good agreement with previous theoretical results [23,26]. Further calculations show that these individual equilibrium sites do not change when impurities and He form a stable pair. In order to determine the lowest energy configurations of a solute-He pair, a number of possible configurations are investigated, which are as follows: a solute is first placed on its most stable interstitial/substitutional site and then a He atom is placed on the tetrahedral/

octahedral site surrounding the solute. The obtained binding energies between the solutes and He as a function of their separation distances are shown in Fig. 1. For all the solutes considered, the binding energies are positive within a certain separation distance, implying that there exists an attractive interaction between the solutes and He. Such attraction may lead to the accumulation of He around impurities and an increase of the local He concentration. It should be noted that the binding energies between the interstitial C/N/O atom and He have different values at the same distance due to their different arrangements, as shown in Fig. 1a. The most stable solute-He pair separation distance is about 2.1 Å for the interstitial C, N or O atom. The distances (r_t) within which He spontaneously migrates to the most stable position are 3.9 Å for O and 3.3 Å for C/N. The trapping radius is the distance beyond which the attraction of He towards impurities is considered negligible. From the stable separation distance, the positive binding energies between the solutes and He decrease with increasing separation distance and ultimately decrease to almost zero at a certain distance (~ 9 Å). The small negative binding energies at larger distances indicate that there is no attractive interactions between the interstitial atoms and He. So the trapping radius of interstitial atoms on He is ~ 9 Å. For the substitutional atoms shown in Fig. 1b, the trapping radius is ~ 5 Å because the positive binding energies decrease to zero when the separation distance of the solute-He pair reaches ~ 5 Å. There is an exception for Re, where the binding energy is always low at about 0.01 eV. The binding energies of

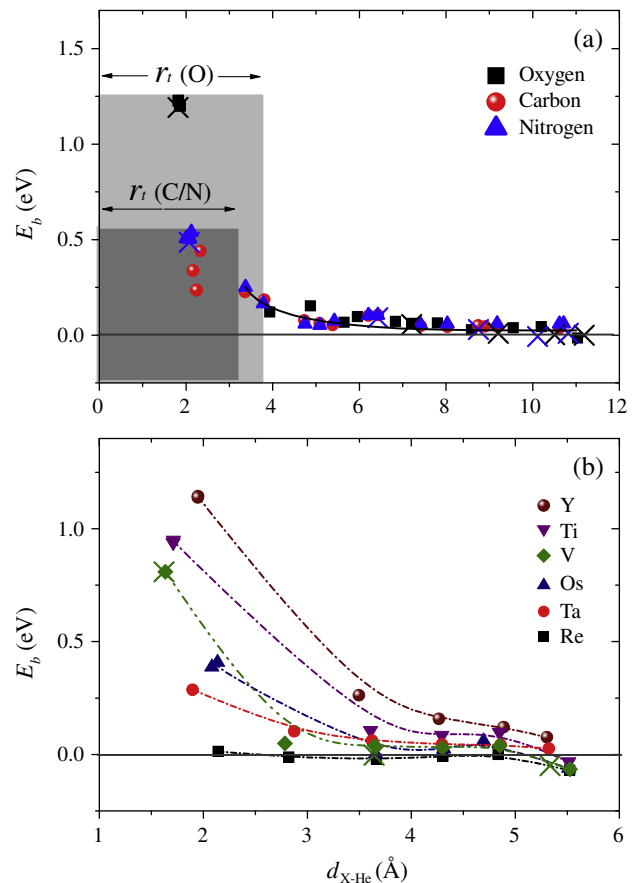


Fig. 1. Variation in the binding energy of (a) the interstitial C, N and O and (b) the substitutional Y, Ti, V, Os, Ta and Re with He as a function of the separation distance between He and the solutes. r_t is the distance within which He spontaneously migrates to its most stable position around the solutes without any energy barrier. The symbol (\times) represents the calculation results using 250 atom supercell and others represent the results using 128 atom supercell.

the impurities N/O/V with He are also calculated using a 250 atom supercell at different separation distances, and the results agree well with those obtained using the 128 atom supercell (see Fig. 1). On the whole, all the interstitial atoms and most of the substitutional solutes considered can trap He atoms. However, the He trapping radii of interstitial atoms are much larger than those of substitutional atoms. So the effect of interstitial atoms on trapping He seems to be more significant at a larger spatial scale.

We would like to stress the present binding energy results and the trapping radii of impurities for He are obtained at 0 K using the first-principles calculations based on the density functional theory, which have limitations and in particular the effect of temperature on the data needs to be carefully assessed. In Demo, the operation temperature of W is in the range of 800–1600 K [2]. In this temperature range, He atoms will not be trapped at any sink unless the binding energy exceeds ~ 0.1 eV. Considering the detrapping of He at high temperature, we can give a preliminary evaluation of the effective trapping of He based on our binding energy results (see Fig. 1). At high temperature, the He trapping radii of interstitial atoms are comparable to substitutional atoms, and in some cases the trapping radius of a few substitutional atoms appears to be greater than any of the interstitial atoms (e.g., Y and Ti). With the reliable interatomic potentials, the molecular dynamics and kinetic Monte Carlo methods should be employed to further accurately probe the temperature effects on the results.

Fig. 2 displays the maximum binding energies between the substitutional solutes and a He atom. Also included in the figure are literature results from *ab initio* calculations of Becquart and Domain [16]. The data show that the effect of 3d TM solutes in trapping a He atom is always larger than that of the bigger 4d and 5d TM solutes. In addition, the curves have an “S” shape with minima at V for the 3d solutes, Mo for the 4d and Re for the 5d. And the late TM solutes Co, Pd and Pt have the highest binding energies with He. Note that our binding energy results are approximately in agreement with those by Becquart and Domain [16], although their calculations were done at constant volume. However, the mechanism of these observations is not clear and the correlation of binding energies with the electronic structures requires further investigations [16]. In Fig. 3 we plot the total charge densities for representative solutes Re, Y and O with He in W. The bonding between the solutes and the He atom has a covalent character via a strong hybridization of He *p* states and the metal *d* states [23,27], which is also responsible for He *t*-site preference over the *o*-site. By comparison of charge densities around Re and Y, a broader region of low charge density near Y is seen while the

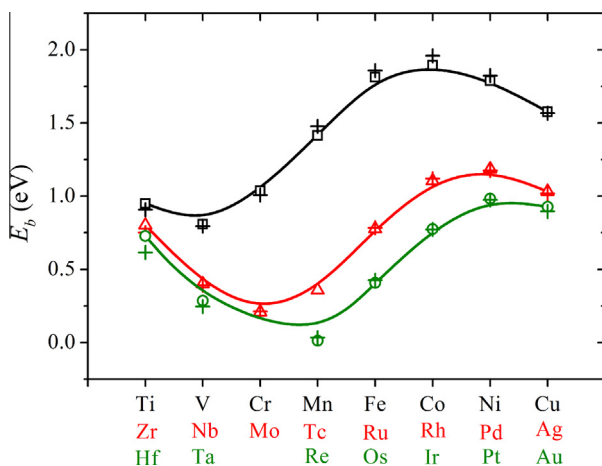


Fig. 2. Binding energies between substitutional TM solute atoms and He in W. All the solute elements were found to be nonmagnetic. Also included in the figure are other DFT results (+) from Ref. [16].

density around Re is relatively high. Besides, a strong bond between the neighboring W atoms and the O atom is observed in Fig. 3c. It should be noted that a similar trend is seen for the charge densities around other solutes with He. These facts indicate that the attraction of He towards impurities is due to the valence electron depletion around the solutes, and He prefers to occupy the low-charge-density regions. This is understandable since He is a closed-shell atom and any hybridization is energetically unfavorable for it [23].

To get further insight into the relationship between the binding energies and the local charge densities around the He atom, we calculated the charge densities at the location site of the He atom in W alloys. In Fig. 4 is plotted the dependence of He-Sol binding energies on the relative charge density rates $(1 - \rho_e^x/\rho_e^W)$, where ρ_e^W and ρ_e^x are charge densities at the favorable He occupation site in pure W and W alloys. The quantity $(1 - \rho_e^x/\rho_e^W)$ is introduced to justify the relative variation degree of charge density due to the addition of impurities. For all substitutional TM solutes, the binding energies rise linearly with the increase of $(1 - \rho_e^x/\rho_e^W)$. This indicates that the lower the charge density due to the introduction of impurities, the higher the binding energy and the easier the He atoms aggregate around the impurities. Note that the binding energy (4.55 eV) between He and the vacancy is much higher than those for the impurities, suggesting that energetically it is easy for He to aggregate around the vacancy. In addition, as shown in Fig. 4, the impurities Re, Mo, Ta, Nb, Os and Tc exhibit lower binding energies with lower charge densities. This implies that they may be chosen as possible alloying elements compared to others.

Besides the charge density, the site-projected electronic densities of states (DOS) are shown in Fig. 5 for *d*-states of the neighboring W atom, *d*-states of the substitutional impurities, *p*-states of the interstitial solutes, and *p*-states of the He atom. In Fig. 5a–c, the DOS of the adjacent W, Re and He in W–Re system are very similar to those of pure W with He. This indicates that the impurity Re has little effect on the electronic structures of the neighboring W and He atoms. In Fig. 5d–f, the impurity Ti has a slight influence on the *d*-states of the impurity and *p*-states of the He atom. The corresponding DOS are slightly reshaped and shifted to higher energies. The change of DOS may originate from the hybridization of the *d*-Ti states and He *p*-states. The He atom acquires some *p*-state near the Fermi energy level. In addition, in the case of N and O shown in Fig. 5g–i, there is a hybridization around -8 eV for N and -9 eV for O of the W *d*-state with the impurity *p*-state, exhibiting the formation of an interaction between the interstitials and He.

Previous experimental studies show that the impurity-interstitial binding energy could be related to the volume dilatation of the host lattice caused by the introduction of the foreign element [28], although a strictly obeyed correlation has not been found by Wollenberger [29]. To test this relation, the volume dilatation (ΔV) dependence of the binding energy for substitutional impurities is shown in Fig. 6, where ΔV is the supercell volume difference between the crystal containing an impurity and a He atom and that containing a single He atom. For most of the substitutional impurities, the binding energy shows a weak positive correlation with the volume dilatation, which implies that the local lattice relaxation around the impurities may be the primary contribution to the He-Sol binding energy. Note that the elements Re, Mo, Ta, Nb, Os and Tc also exhibit lower binding energies with lower volume changes, which further confirms the above prediction that they might be chosen as possible alloying elements in W.

4. Discussion

As mentioned in the introduction, a drawback of W for the divertor plate in ITER includes its high ductile-to-brittle transition

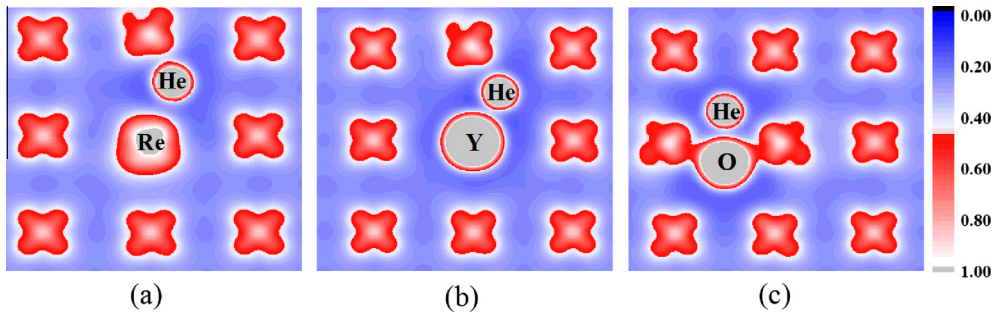


Fig. 3. Total charge densities for He-solute defects in W. (a) and (b) are He–Re and He–Y in (010) plane, respectively. (c) is He–O in (001) plane. The unmarked atoms are W atoms. The units are $e\text{Å}^{-3}$.

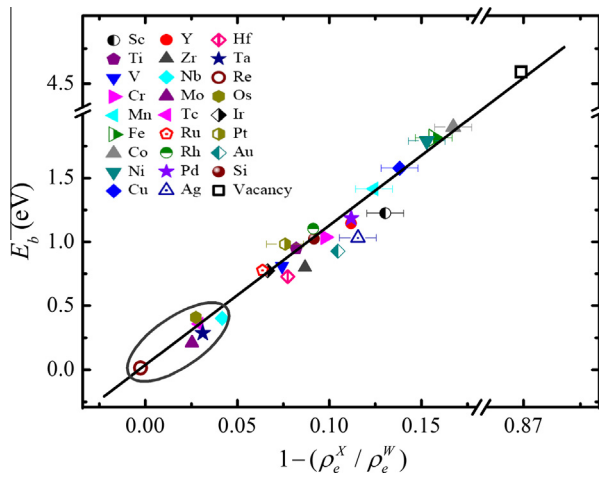


Fig. 4. Relationship between the He-Sol binding energy and the relative charge density ($1 - \rho_e^x / \rho_e^W$).

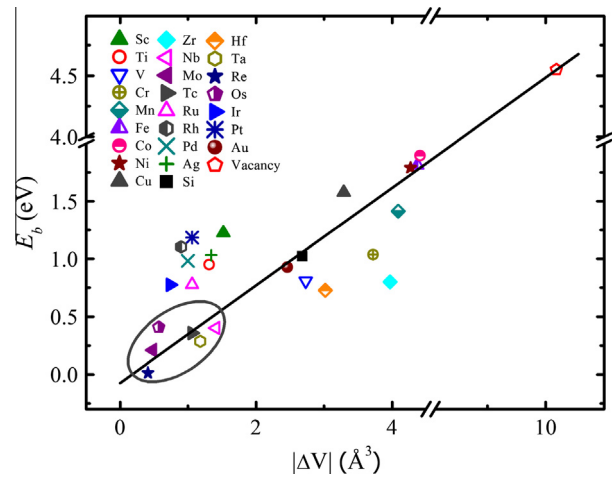


Fig. 6. The volume dilation dependence of the binding energy for substitutional TM solutes. The line is a guide for the eyes.

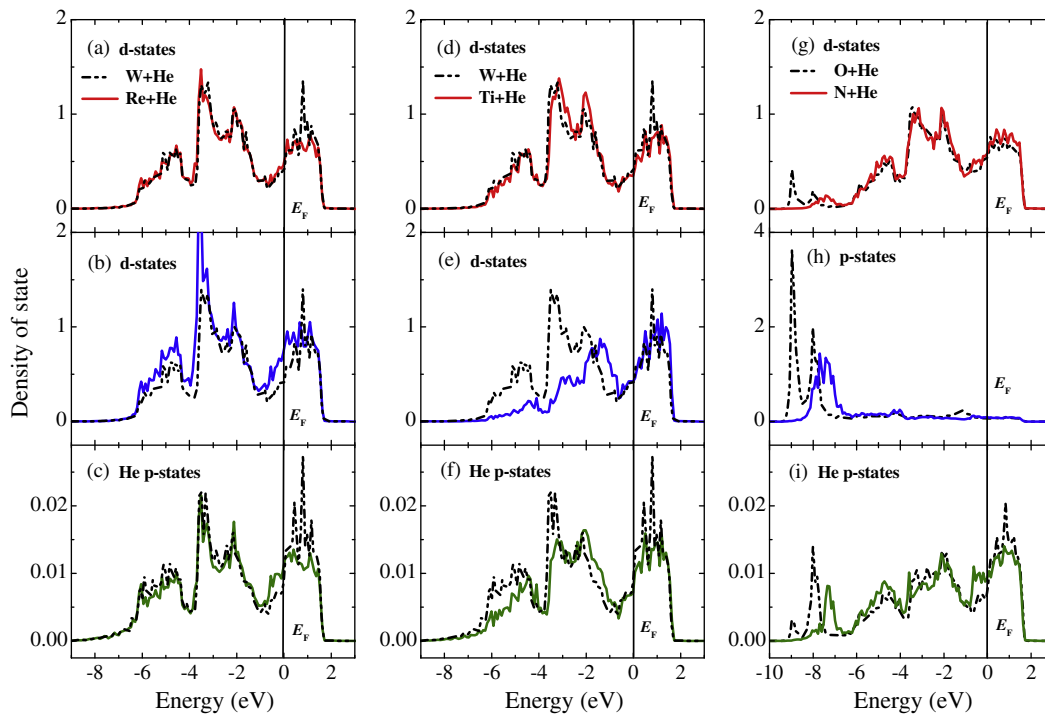


Fig. 5. Local DOS for the substitutional impurities Re (left) and Ti (middle) and the interstitials O and N (right) compared with that of the system without an impurity. (a), (d) and (g) show the *d*-states for the neighboring W atoms; (b), (e) and (h) show the *d*-states for the substitutional impurities and *p*-states for the interstitial solutes; (c), (f) and (i) show the *p*-state for the He atom. The zero energy point (solid lines) indicates the Fermi level of the supercell with the He defect.

temperature and a significant degree of irradiation embrittlement. To improve material ductility, the alloying of W with some ductile elements such as Re, Ta, Tc, Os, Ru, Ti and V has been proposed [9–11]. Some of these, such as Re, have been found to reduce the DBTT of W and significantly improve ductility [30]. Unfortunately, Re and Os are rare elements. For fusion application, the introduction of Re has to be restricted to meet low activation requirements [31] and to prevent the formation of brittle phases due to significant transmutation of W into Re [32]. Therefore, the question is whether there are other promising elements with a ductilizing effect on W.

As we know, only a few metals have significant solubility in W at room temperature. Ta, V, Nb and Mo can form solid solutes in the complete fraction range. While Ti and Re show a limited solubility, and their applicability is restricted to fractions of about 12% and 27%, respectively, due to the formation of intermetallic phases [33,34]. Nb and Mo cannot be used for fusion applications due to their transmutation to very long-lived radioactive isotopes [32]. So this leaves Ta, V and Ti as possible candidates. However, recent studies show that additions in W with Ta, V and Ti did not induce big changes to the dislocation-core structure leading to the ductilizing effect [32,35]. Fortunately, the DFT calculations of transition metals on W grain boundary cohesion exhibit that Ta strengthens the cohesion of the $\Sigma 27$ GB, which can explain the superior Charpy energy of W–1%Ta compared to pure W [32,36]. Furthermore, recent experimental studies of W and W–5%Ta exposed to a high-flux deuterium plasma show that blisters on the W–Ta surface are considerably smaller in size and number compared to pure W [37]. Deuterium retention is also found to be systematically lower in W–Ta than in W [37]. On the other hand, the investigation of the transmutation behaviors of possible W alloys shows that the levels of He and H production in W alloyed with Ti or V are at least an order of magnitude greater than that alloyed with Re or Ta [10]. So the ability of W alloys with Ti or V to withstand the effects of the embrittlement mechanisms activated by He must be carefully considered [35]. In the case of Re, a high amount of Os production is harmful for the structural and mechanical properties of the material. But for Ta, the primary transmutation product of W is an unexpected benefit [10]. In our previous work, the diffusion of He with a few impurities has been studied [34]. Generally there is a down-hill drift diffusion of He towards most of the elements such as Ti or V, but the migration and transport behaviors of He in W are seldom affected by the introduction of Re or Ta [17]. In this work by investigating the binding energies between He and solutes as well as He trapping radii over a wide range of element types, we find that the introduction of solutes Re or Ta has little effect of He aggregation in W. Therefore, taking into account the above effects, Ta seems to be a promising alloying element relative to other possible ones. However, as mentioned in Ref. [16], before predicting the materials behavior with confidence, the calculation results must be validated using dedicated experiments.

5. Conclusions

In summary, we use first-principles calculations to study He trapping by solute elements in tungsten. Our calculations demonstrate that all the interstitials and most of the substitutional elements except Re can trap He atoms, but the trapping radii of interstitial atoms on He are nearly twice larger than those of substitutional solutes. It should be noted that the present calculations did not consider the effect of temperature on detrapping of He atoms. Our results suggest that if detrapping of He is taken into account at fusion relevant operating temperatures, then the trapping radii of interstitial atoms are more comparable to substitutional atoms. Further studies on the charge densities show that

the binding energies between the substitutional impurities and He follow a linear relationship with the relative charge densities at the He occupation site, implying that He atoms easily aggregate at the low charge density site. The correlation of the binding energy with the volume dilatation shows that the local lattice relaxation around the impurities plays a major contribution to the binding energy. Finally, the suitability of promising alloying elements in W has been examined and Ta is considered to be an interesting alloying element compared to others.

Acknowledgments

This work was supported by the National Magnetic Confinement Fusion Program (Grant No.: 2011GB108004), the National Natural Science Foundation of China (No.: 91026002) and the Strategic Priority Research Program of Chinese Academy of Sciences (Grant No.: XDA03010303), and by the Center for Computation Science, Hefei Institutes of Physical Sciences.

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