



He–He and He–metal interactions in transition metals from first-principles



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ABSTRACT

We investigated the atomistic mechanism of He–He and He–metal interactions in bcc transition metals (V, Nb, Ta, Cr, Mo, W, and Fe) using first-principles methods. We calculated formation energy and binding energy of He–He pair as function of distance within the host lattices. The strengths of He–He attraction in Cr, Mo, W, and Fe (0.37–1.11 eV) are significantly stronger than those in V, Nb, and Ta (0.06–0.17 eV). Such strong attractions mean that He atoms would spontaneously aggregate inside perfect Cr, Mo, W, and Fe host lattices in absence of defects like vacancies. The most stable configuration of He–He pair is <100> dumbbell in groups VB metals, whereas it adopts close <110> configuration in Cr, Mo, and Fe, and close <111> configuration in W. Overall speaking, the He–He equilibrium distances of 1.51–1.55 Å in the group VIB metals are shorter than 1.65–1.70 Å in the group VB metals. Moreover, the presence of interstitial He significantly facilitates vacancy formation and this effect is more pronounced in the group VIB metals. The present calculations help understand the He–metal/He–He interaction mechanism and make a prediction that He is easier to form He cluster and bubbles in the groups VIB metals and Fe.

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1. Introduction

Plasma-material interaction (PMI) is one of the major concerns in the International Thermonuclear Experimental Reactor (ITER) and the future fusion reactors [1–4] and is a key factor in the material selection and plasma-facing component (PFC) design. Under typical environment of a fusion reactor, large amounts of helium (He) impurities are produced by neutron transmutation reactions in the structural materials or come from the edge plasma in the plasma facing materials [5,6]. Experiments showed He impurities can be trapped in structural defects (such as vacancies, grain boundaries and voids), forming clusters and bubbles, and finally leading to embrittlement and swellings of the fusion materials [5,7–10]. To elucidate He effects on the mechanical and physical

properties of the metal materials facing fusion plasma or under neutron irradiation, deep understanding of the fundamental mechanism of He–He and He–metal interactions is needed.

Previously, density functional theory (DFT) calculations have been extensively performed to study He behavior in bcc transition metals [11–20]. Seletskaya [14] systematically investigated the stable position of a single He impurity in bcc transition metals of V, Nb, Ta, Mo, and W. Fu and Willaime [11] studied the stability of He and He–vacancy clusters and found the strength of He–He attraction in Fe is 0.43 eV. Becquart and Domain [12] predicted that He–He attraction energy is 1.03 eV, which can result in formation of He bubbles even without vacancies. Recently, our group investigated the stability of He and He–vacancy clusters in V [16] and found weak attraction (0.02–0.21 eV) for He–He pair in V. Despite the above mentioned efforts, until now the physical mechanism of strong attraction of He–He in W and Fe has not been clearly elucidated. For fusion reactors, V, Ta, Cr, and Fe are the main low activation elements for structural materials. Thus, atomistic simulations of He–He/He–metal interactions in bcc transition metals not only are essential for understanding the microscopic mechanism of He aggregation and He bubble formation, but also help establish more

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accurate empirical potentials [21] to simulate the kinetic evolution of the microstructure of materials in larger length/time scale.

The purpose of this paper is to perform a systematical first-principles investigation of the He–He interactions and He effects on vacancy formation in bcc transition metals of group VB (V, Nb, Ta), group VIB (Cr, Mo, W) and VIII (Fe), including formation energy, binding energy, atomic configurations. We calculated binding energy of He–He pair as a function of distance in various metal host lattices and discussed the most stable configurations. We also analyzed geometry structures, charge densities and density of states to elucidate the attractive interactions of He–He in metals. Finally, we discussed the effects of interstitial He atoms on vacancy formation.

2. Computational methods

All calculations were performed using spin polarized DFT and plane-wave pseudopotential approach [22,23], as implemented in the Vienna Ab initio Simulation Package (VASP) [24,25]. We adopted the generalized gradient approximation (GGA) with PW91 functional [26] for the exchange–correlation interaction and the projector-augmented wave (PAW) potentials [27,28] for the ion–electron interaction. A bcc supercell of 128 atoms ($4 \times 4 \times 4$ unit cells) was used and the Brillouin zones were sampled with $3 \times 3 \times 3$ k points generated by the Monkhorst-Pack scheme [29]. The energy cutoff of plane-wave was chosen as 500 eV. Due to the ferromagnetism of bcc Fe, spin polarization was considered for all DFT calculations. The electronic configurations of transition metal atoms are $3d^4 4s^1$ for V, $4d^4 5s^1$ for Nb, $5d^3 6s^2$ for Ta, $3d^5 4s^1$ for Cr, $4d^5 5s^1$ for Mo, $5d^4 6s^2$ for W, and $3d^7 4s^1$ for Fe, respectively. The equilibrium configurations at constant supercell volume were fully relaxed with the convergence criterion of the force on each atom less than 0.005 eV/Å.

Within the present theoretical scheme, the cohesive energy of each metal is calculated by $E_{\text{coh}} = E(\text{perfect}) - NE_{\text{atom}}$, where $E(\text{perfect})$ is the energy of the supercell with perfect lattice (128 atoms), $N = 128$ is the number of atoms in the working supercell, E_{atom} is the energy of one metal atom in vacuum, here we considered spin polarization for a metal atom in the DFT calculations. We also calculated bulk modulus for the seven transition metals by fitting Birch–Murnaghan equation. The calculated equilibrium lattice constants (a), cohesive energy (E_{coh}) per atom, and bulk modulus (B) for seven bcc transition metals (V, Nb, Ta, Cr, Mo, W, and Fe) are compared with experimental data [30] in Table 1. Reasonable agreement is found between our DFT calculations and experiments. Calculated formation energies of single tetrahedral He in seven transition metals coincide well with previous DFT results (see Table 1). Besides, since He is a closed-shell atom, we discuss the effect of Van der Waals interaction of He–He and He–metal using dispersion corrected DFT method (DFT-D) [31]. It is shown that effect of Van der Waals interaction of He–He pair is quite small ($-0.02 \sim -0.05$ eV) on He–He binding energy, which is

negligible for the He–He and He–metal interactions.

3. Results and discussion

3.1. He–He interactions in transition metals

As a light element, He is a typical interstitial impurity in metal lattices due to its smaller atomic radius relative to the metal atom. In the bcc solid of transition metals, a single He atom prefers to occupy at a tetrahedral interstitial site energetically rather than an octahedral interstitial site from previous experiments and calculations [14]. To discuss the He–He interactions in bcc transition metals, we calculated the binding energies of He–He pairs as function of distance by considering two He atoms at favorable tetrahedral sites as first (1nn) to 14 nn nearest neighboring sites (about 1–6 Å). The binding energy of He–He pair in a transition metal host is defined by:

$$E^b(\text{He}, \text{He}) = E^f(2\text{He}) - E^f(2\text{farHe}_T), \quad (1)$$

$$E^f = E(m\text{He}) - E(\text{perfect}) - E(\text{He}), \quad (2)$$

where $E^f(2\text{He})$ and $E^f(2\text{farHe}_T)$ are the formation energies of the supercell with a He–He pair and two separated He atoms, respectively. In Eq. (2), $E(m\text{He})$ is the energy of the supercell with m He atoms ($m = 1, 2$); $E(\text{perfect})$ is the energy of the supercell with perfect lattice; $E(\text{He})$ is the energy of a He atom in vacuum. By definition, negative formation energy means exothermic process, and negative binding energy means attractive interaction.

The calculated binding energies of He–He pairs as function of distances in host lattices are plotted in Fig. 1. Generally speaking, He–He interactions show similar trend with their distance in host lattice for the seven metals considered: repulsion (less than 1.5 Å) → attraction → repulsion → no interaction (larger than 4.0 Å). As for the strength of attraction, we found a distinct group-specific trend: He–He pair exhibits weak attraction (less than 0.20 eV) in the group VB (V, Nb, Ta), while it is strong attraction (larger than 0.70 eV) in the group VIB metals (Cr, Mo, W). In all metals, 1nn configuration of He–He pair is unstable and would transform into 2nn configuration after relaxations. Both 3nn and 5nn He–He configurations in group VIB metals are unstable and tend to transform into 2nn configuration due to inter-helium attraction. As He–He distance exceeds 4.0 Å, the strength of He–He interaction drops to nearly zero and is negligible. Importantly, such a strong binding energy means that clustering of two single He impurities is quite probable and that the He clusters will be very stable. Namely, He in perfect Cr, Mo, W, and Fe solids can directly attract another He atoms in absence of other defects like vacancies. Previous first-principles calculations by Fu and Willaime [11] reported a He–He attractive energy of 0.43 eV in Fe, while Becquart and Domain [12] predicted that the strength of He–He attraction in W is 1.03 eV. All

Table 1
: Calculated equilibrium lattice constants a (Å), cohesive energies E_{coh} (eV), and bulk modulus B (GPa) for seven bcc transition metals (V, Nb, Ta, Cr, Mo, W, and Fe) in comparison with experimental data [30]. Single He formation energy at tetrahedral sites is compared with the present calculation and previous DFT results [11,14].

		V	Nb	Ta	Cr	Mo	W	Fe
a	This work	2.98	3.32	3.32	2.84	3.15	3.18	2.82
	Expt.	3.03	3.30	3.30	2.88	3.15	3.16	2.87
E_{coh}	This work	5.49	7.04	8.20	4.20	6.49	8.54	5.10
	Expt.	5.31	7.57	8.10	4.10	6.82	8.90	4.28
B	This work	173.5	170.4	191.7	185.3	256.2	298.7	177.5
	Expt.	161.9	170.2	200.0	190.1	272.5	323.2	168.3
$E^f(\text{He}_T)$	This work	2.95	3.09	3.42	5.42	5.33	6.24	4.66
	Other DFT	2.94	3.05	3.16	–	5.16	6.15	4.40

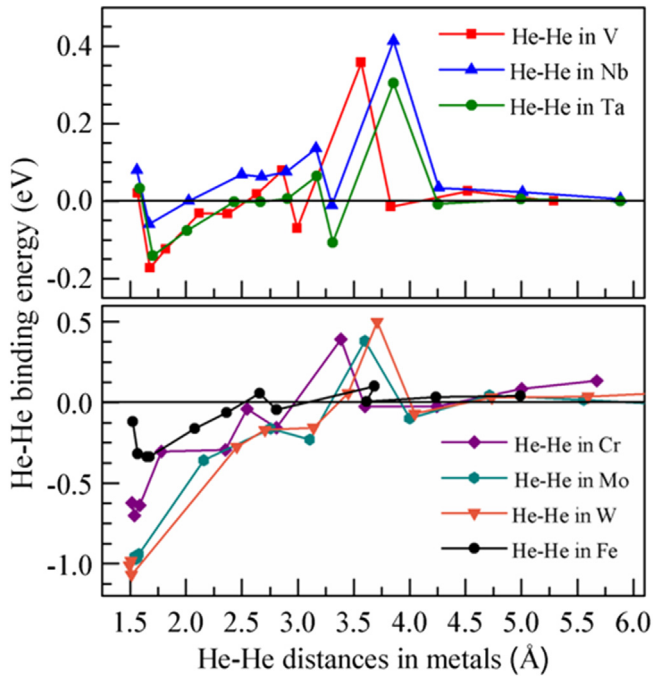


Fig. 1. Binding energies of He–He pairs as function of the distance in V, Nb, Ta, Cr, Mo, W, and Fe after full relaxation.

these values are well consistent with our results in Table 2 (0.37 eV in Fe, 1.11 eV in W).

To explain the origin of such strong He–He attraction, we compared the most stable configurations, equilibrium distances,

formation energies, and binding energies of He–He pairs in V, Nb, Ta, Cr, Mo, W, and Fe metals, as shown in Fig. 2 and Table 2. Upon full relaxation, the most stable configurations are different in the transition metals. In the group VB metals (V, Nb, Ta), the most stable configurations of He–He pairs are the same, i.e., $\langle 100 \rangle$ dumbbell. He–He pair displays the same configurations in Cr, Fe, and Mo, i.e., close $\langle 110 \rangle$ dumbbell, whereas it is close $\langle 111 \rangle$ dumbbell in W. After relaxation, He–He equilibrium distances with 1.51–1.55 Å in the group VIB metals are shorter than those of 1.65–1.70 Å in the group VB metals. He–metal equilibrium distances reach the range of 1.70–1.90 Å by outward expansion of about 4%–7%, and these values are generally greater than He–He distances. Compared to the summation of formation energies for two individual interstitial He atoms in bulk metal, the formation energy of a He–He pair inside V, Nb, or Ta is nearly equal, while the formation energy of He–He pair inside Cr, Mo, W, or Fe is significantly smaller (see Table 2). This suggests that He impurities prefer to aggregate in metal hosts of Cr, Mo, W, and Fe due to stronger He–He attractions. Table 2 shows the sequence of He–He attraction strength from strong to weak: W, Mo, Cr, Fe, V, Nb, Ta. Attraction of He–He pair in the group VIB metals (Cr, Mo, W) is significantly stronger than other metals by over twice of magnitude.

In brief, shorter distance and higher formation energy of He–He pair in metals correspond to stronger He–He attraction. Indeed, the apparent attraction between He atoms relies most probably on its very low solubility in transition metals and high repulsion with group VIB metals specifically, as shown in Table 2. It is no surprise to see in Table 2 a clear correlation between the He–He binding energy and the formation energy of an interstitial He in the metal. Expectedly, the binding energy is the highest for W, which has the lowest solubility for He. This suggests smaller repulsion in the He–He pair than in the He–W one. The structural changes cannot account for the strong attraction of He–He in the group VIB metals

Table 2

The formation energies E^f (eV), binding energies E^b (eV) and equilibrium distances d_1 (Å) of He–He pair in bulk solids of V, Nb, Ta, Cr, Mo, W, and Fe, respectively. He–metal equilibrium distances d_2 (Å) and the electronegativity for each metal are also given.

	$E^f(1\text{He})$	$E^f(2\text{He})$	$E^b(\text{He–He})$	$d_1(\text{He–He})$	$d_2(\text{He–metal})$	Electronegativity
V	2.95	5.88	−0.17	1.68	1.88	1.63
Nb	3.09	6.13	−0.14	1.70	2.04	1.59
Ta	3.42	6.79	−0.06	1.67	2.04	1.51
Cr	5.42	9.78	−0.70	1.54	1.70	1.66
Mo	5.33	9.69	−0.97	1.55	1.90	2.16
W	6.24	11.42	−1.11	1.51	1.89	2.36
Fe	4.66	8.99	−0.37	1.65	1.76	1.83

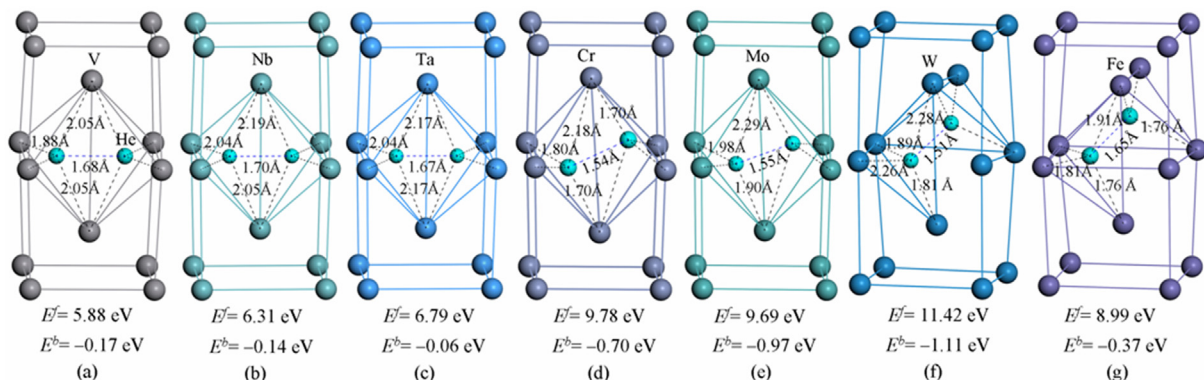


Fig. 2. The most stable configurations, equilibrium distances, formation and binding energies of He–He pairs in V, Nb, Ta, Cr, Mo, W, and Fe, respectively.

and Fe, implying that the electronic factors must play an important role here, as discussed below.

3.2. Charge density and density of states of He–He pair in transition metals

To gain deeper insight into physical origin of He–He attraction in transition metals, we calculated charge density difference of He–He pair in V, Nb, Ta, Cr, Mo, W, and Fe hosts, as shown in Fig. 3. The presence of interstitial He–He pair in bulk metal induces strong perturbation of local charge density distributions, forming the low electron-density area surrounding He. This low electron-density region can act as a preferable site for He. He–He pair also causes distortions of charge densities, which are more pronounced in the Cr, Mo, W, and Fe hosts. Since noble He atoms have a closed-shell structure, larger polarization of charge densities would cost more extra energy. This picture can well explain higher formation energy of interstitial He–He in group VIB metals (Cr, Mo, W) and Fe than group VB metals (V, Nb, Ta).

On the other hands, within electronic environment of transition metal, why two noble He atoms prefer to get together with lower system energy, especially Cr, Mo, and W metals. We compared total density of states (DOS) for the system containing He–He pair or two separated He atoms (5 Å), as shown in Fig. 4. Total DOS of V, Nb, and Ta systems are very similar, while Cr, Mo, and W have a similar

trend. For V, Nb, and Ta, the values of total DOS of the system with He–He pair are nearly same (slightly lower) with the case of two separated He at the Fermi level. By comparison, for Cr, Mo, and W, the values of DOS of the system with He–He pair are obviously lower than that of two separated He at the Fermi level. In fact, for a given system, higher values of total DOS at Fermi level means less energetically favorable. Therefore, in group VIB metals He–He pair is significantly more stable than two separated He atoms, namely He–He pair have a strong attraction. For the group VB metals, He–He pair is slightly more favorable than that of two separated He atoms, indicating that He–He pair have a weak attraction.

Fig. 5 presents the s- and d-projected DOS of the metal atom closest to the He–He pair for V, Ta, Cr, and W, and the s- and p-projected DOS of one He atom. We can see that the hybridization between metal d states and He p states. The He atom acquires some s and p states near the Fermi energy level. Though the absolute values of He DOS are relatively small, they cannot be neglected. By comparison, the hybridization between Cr (W) d states and He p states is stronger than V (Ta) d states and He p states. We suggest that the hybridization between transition metals d states and He p states is responsible for larger formation energies and stronger attraction for He–He pairs.

Furthermore, we discuss relationship between electronegativity and binding energy, as presented in Table 2. In the periodic table, the electronegativity shows a reduction trend in the group VB

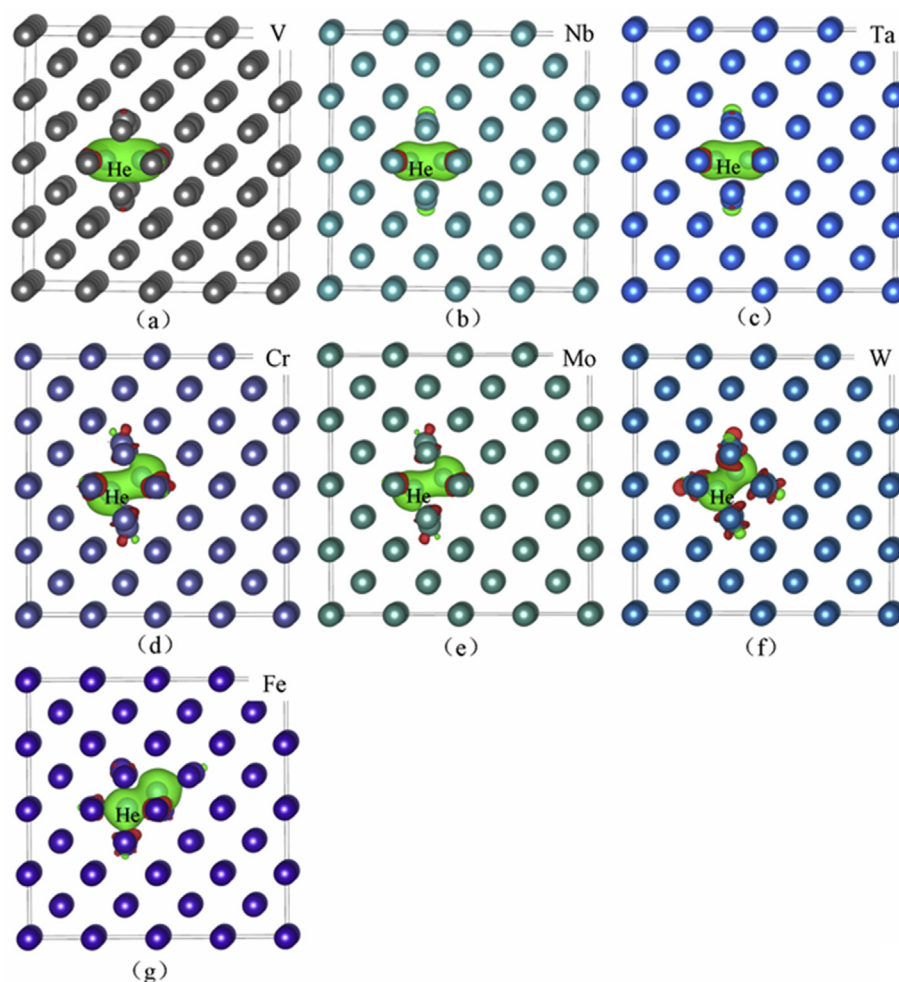


Fig. 3. Charge density difference for He–He pair in V, Nb, Ta, Cr, Mo, W, and Fe, respectively. Green contour denotes regions of charge depletion, and Red contour denotes regions of charge accumulation (isovalue is $0.004 \text{ e}/\text{\AA}^3$). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

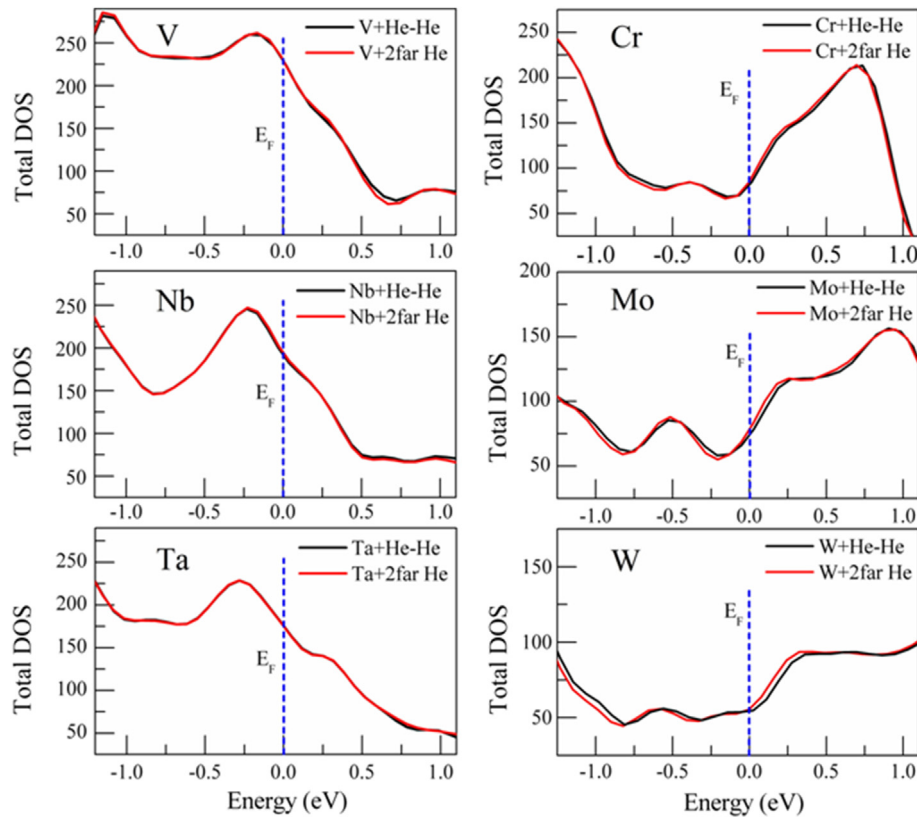


Fig. 4. Total DOS for the systems containing He–He pair and two separated He atoms (5 Å) for V, Nb, Ta, Cr, Mo, and W, respectively. The black solid line denotes the system with an interstitial He–He pair, and red solid line denotes the system with two far interstitial He atoms. The Fermi energy of the supercell with the He–He pair is 0.00 eV. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

metals (1.63 for V, 1.59 for Nb, 1.51 for Ta), while those for the groups VIB metals (1.66 for Cr, 2.16 for Mo, 2.36 for W) shows an increasing trend. We found that the trend of He–He binding energies perfectly coincide the trend of electronegativity.

3.3. Effect of interstitial He atom on vacancy formation

Previous DFT results [11,12,14,32–34] predicted that local lattice expansions after He insertion are about 10% (0.3–0.37 Å) for seven metals. Helium in metal hosts causes a local expansion (local stress) of the lattice host and may induce formation of a new vacancy [19]. To investigate this possible effect in different metals, we investigated formation of a vacancy surrounding an interstitial He in the tetrahedral site by removing a lattice atom in the bcc host lattices. The corresponding formation energy can be approximated by Ref. [35]:

$$E^f(\text{VA}) = E(\text{He}_1\text{VA}) - (N-1)E(\text{perfect})/N - [E(\text{He}_1) - E(\text{perfect})], \quad (3)$$

where $E(\text{VA}, \text{He})$ is the energy of the supercell with a vacancy and an interstitial He atom near the vacancy, $E(\text{He}_1)$ is the energy of the supercell with an interstitial He atom.

Fig. 6 shows that the vacancy formation energies surrounding a tetrahedral He atom remarkably decrease by 0.9–4.6 eV with regard to the value in perfect metals, namely, He insertion greatly facilitates formation of vacancy defects. For V, Nb, Ta, and Fe, after the interstitial He atom is incorporated, the vacancy formation energy reduces from 2.14, 2.66, 2.82 and 2.14 eV to 1.20, 1.30, 1.08 and 0.54 eV, respectively. On the other hand, for Cr, Mo, and W,

vacancy formation energy near tetrahedral He becomes negative with –0.49, –0.98 and –1.45 eV as compared to the positive values of 2.45, 2.65 and 3.21 eV without He; namely, the vacancy formation is an exothermic process. In general, creation of a new vacancy near interstitial He in the group VIB metals is more easily than that in the group VB and VIII metals. We also found that vacancy formation energy in W solid is the lowest (–1.45 eV) in presence of a nearby interstitial He, though it is the highest one (3.21 eV) without He (see Fig. 6). Therefore, we conclude that presence of interstitial He significantly facilitates the formation of vacancy and this effect is more pronounced in the group VIB metals.

In the realistic fusion environments, large amounts of He impurities are generated by transmutation reactions in reactor materials along with irradiation-induced defects, which would lead to formation of additional defects like vacancies. In turn, these vacancy defects provide aggregation locations for accommodating more He impurities. On the other hand, the present atomistic simulations show that the vacancy formation energy surrounding interstitial He becomes negative for Cr, Mo, and W hosts, and He–He equilibrium distance is less than the dimension of lattice spacing. This can be related to the phenomenon of supervacancy formation in metals observed in experiment [36]. We thus inferred that He bubble formation in the group VIB metals are more easily than in the group VB and VIIB metals under the irradiation environment in a fusion reactor.

4. Conclusions

First-principles calculations have been carried out to study the He–He and He–metal interactions as well as He effect on vacancy

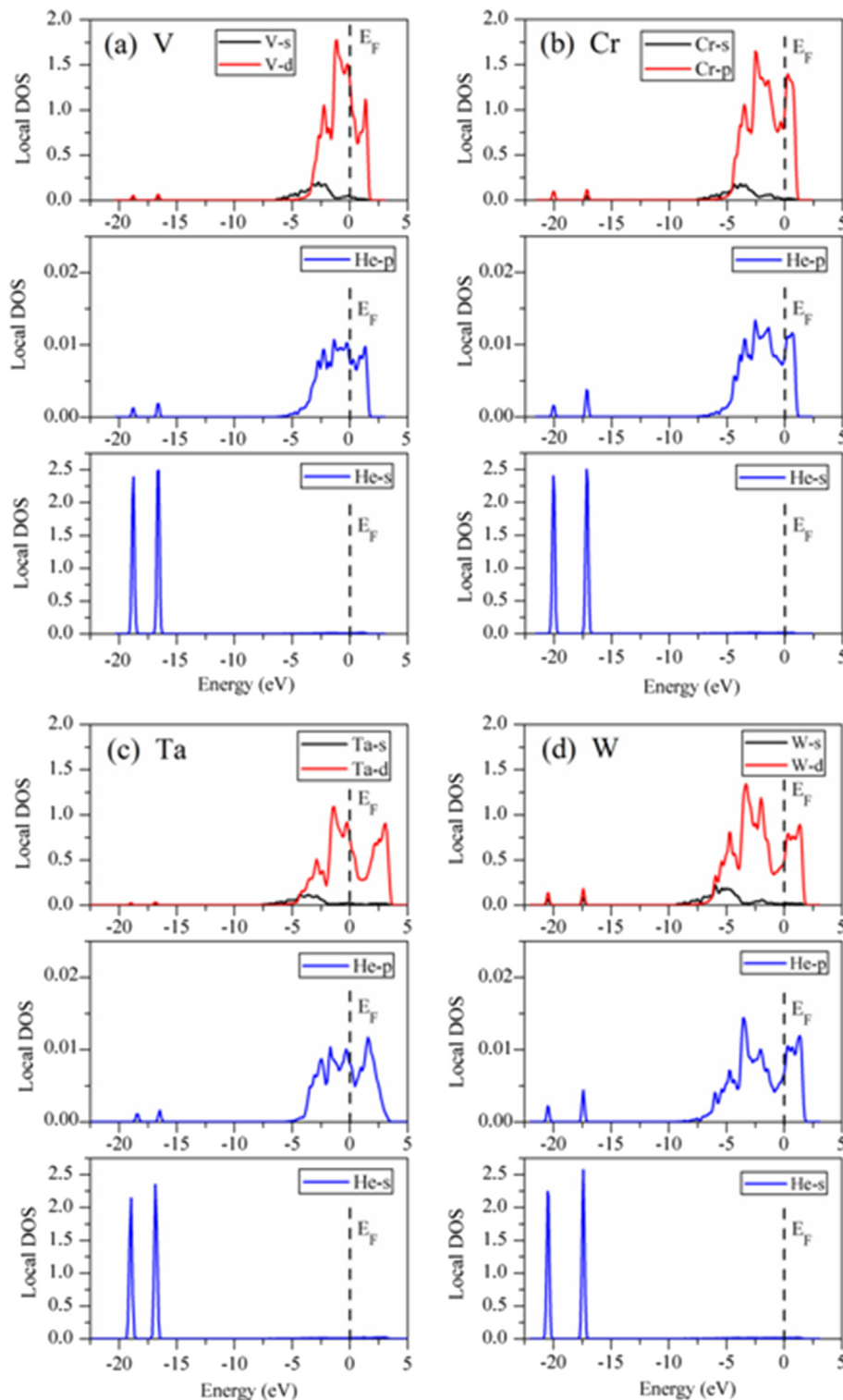


Fig. 5. Local DOS for (a) V, (b) Cr, (c) Ta, and (d) W atom with He–He pair. The black and red lines denote metal s states and d states, blue lines denote He s states and p states, respectively. The Fermi energy of the supercell with the He–He pair is 0.00 eV. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

formation in bcc transition metals (V, Nb, Ta, Cr, Mo, W, and Fe). We found that the He–He binding energy in Cr, Mo, W, and Fe hosts (0.37–1.11 eV) is significantly larger than that in groups VB metals of V, Nb, and Ta (0.06–0.17 eV). Such a strong binding energy means that He can easily attract other He impurities in absence of structural defect like vacancy, further forming He clusters inside Cr, Mo,

W, and Fe metals. The most stable of He–He pair is $\langle 100 \rangle$ dumbbell configuration in groups VB metals and close to $\langle 110 \rangle$ configuration in Cr, Mo, and Fe and close to $\langle 111 \rangle$ configuration in W. The He–He equilibrium distances (1.51–1.55 Å) in the group VIB metals are generally shorter than those in the group VB metals (1.65–1.70 Å), and the He–He distances are always shorter than

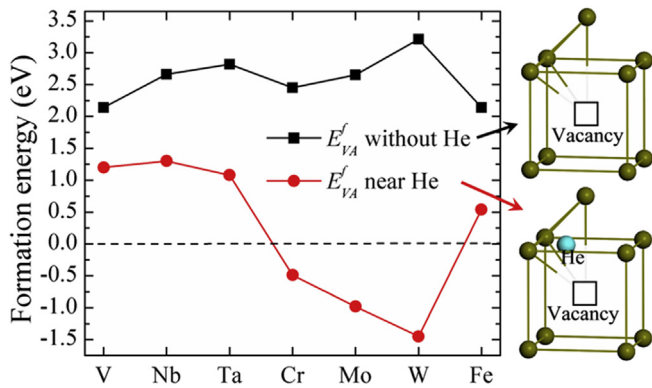


Fig. 6. Comparison of vacancy formation energies surrounding the tetrahedral He impurity and without He in bcc transition metals of V, Nb, Ta, Cr, Mo, W, and Fe. Right panel gives schematic diagram of two initial structures with and without He.

He–metal distances. He–He interactions largely depend on electronic structures. Moreover, the presence of interstitial He atom significantly facilitates vacancy formation, and this effect is more pronounced in the group VIB metals. The present calculations give a reasonable explanation for He–He attraction and He aggregation in transition metals and predict that He is easier to form He cluster and bubbles in the groups VIB metals and Fe.

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