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Effect of Chrome and Vanadium on the Behavior of Hydrogen and Helium in Tungsten

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Abstract: Tungsten is a promising material for nuclear fusion reactors, but its performance can be degraded by the accumulation of hydrogen (H) and helium (He) isotopes produced by nuclear reactions. This study investigates the effect of chrome (Cr) and vanadium (V) on the behavior of hydrogen and helium in tungsten (W) using first-principles calculations. The results show W becomes easier to process after adding Cr and V. Stability improves after adding V. Adding Cr negatively impacts H and He diffusion in W, while V promotes it. There is attraction between H and Cr or H and V for distances over 1.769 Å but repulsion below 1.583 Å. There is always attraction between He and Cr or V. The attraction between vacancies and He is stronger than that between He and Cr or V. There is no clear effect on H when vacancies and Cr or V coexist in W. Vacancies can dilute the effects of Cr and V on H and He in W.

Keywords: first-principles calculation; facing plasma materials; tungsten; fusion energy



Citation: Li, M.; Zhang, Z.; Li, Y.; Zhao, Q.; Huang, M.; Ouyang, X. Effect of Chrome and Vanadium on the Behavior of Hydrogen and Helium in Tungsten. *Math. Comput. Appl.* **2023**, *28*, 81. <https://doi.org/10.3390/mca28040081>

Academic Editors: Fuat Kara, Hargovind Soni, Uğur Köklü and Onur Özbek

Received: 17 May 2023

Revised: 25 June 2023

Accepted: 30 June 2023

Published: 3 July 2023



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1. Introduction

Tungsten (W) is considered to be one of the most promising plasma-facing materials (PFMs) for diverters and first wall materials (FWMs) in fusion power reactors [1–5] because it has a high melting point, maintains strength at high temperatures, resists neutron radiation, has high sputtering threshold energy, transfers heat well, and has a low coefficient of thermal expansion [6]. However, pure W exhibits poor radiation stability, low fracture toughness, little ductility, and a high ductile-to-brittle transition temperature (DBTT) [7–9]. These properties of W closely relate to its chemical composition and microstructural state. To improve W's physical properties, alloying is an effective approach [10]. For example, alloying W with other elements can enhance its thermal properties and improve its mechanical properties [11–16].

Here, we have reviewed relevant research on perfect body-centered cubic (bcc) tungsten (W) and W-based alloys from experimental and theoretical perspectives. In the recent years, some experiments have explored how foreign solute atoms affect hydrogen retention in W, clearly showing solute atoms significantly impact hydrogen retention in W [17–24]. Theoretical work includes molecular dynamics simulations and first-principles calculations. Some molecular dynamics simulations have investigated the formation mechanism of hydrogen and helium bubbles in W and the diffusion pattern of hydrogen and helium atoms in W [25–39]. Many first-principles studies have examined the formation energy of point defects formed by hydrogen and helium atoms in W, the diffusion of hydrogen and helium atoms in W, and how these point defects impact W and W-based alloy performance [10,40–51]. Specifically, Kong et al. [47] studied how transition metals interact with hydrogen in W, and Ma et al. [48] explored how cerium affects helium behavior in W. While experimental research requires substantial time and money, appropriate potential

functions are needed for molecular dynamics simulations of crystal systems. Compared to experiments and molecular dynamics simulations, first-principles studies have some advantages as they require no parameters, use only basic physical constants, and basic properties of ground-state crystal systems can be determined from these constants. With advances in quantum mechanics and computing, first-principles calculations will greatly aid the development of W-based alloys.

Although some studies have explored different alloying elements in W, we lack a comprehensive and reliable understanding of how chromium (Cr) and vanadium (V) affect hydrogen and helium behavior in W. In this paper, using first-principles density functional theory (DFT) calculations, we investigate how Cr and V influence hydrogen and helium behavior in W, the stability and mechanical properties of W after adding Cr and V, interactions between H-Cr, H-V, He-Cr, and He-V, and competition between vacancies and Cr or V.

2. Methodology

Tungsten has a body-centered cubic (bcc) crystal structure with space group Im-3m. We used a 24-lattice-point ($2 \times 3 \times 2$) supercell in this study. The crystal structure appears in Figure 1. We replaced one W atom with either a Cr or V atom, resulting in Cr and V mass fractions of 1.21 wt% and 1.22 wt%, respectively. Hydrogen or helium atoms can trap interstitially at three sites in bcc W. We denote these sites as H_{Sub} , H_{Tet} , H_{Oct} , He_{Sub} , He_{Tet} , and He_{Oct} for hydrogen or helium at substitutional, tetrahedral, and octahedral sites, respectively. When Cr or V replaces a W atom near the H or He atom in the supercell, we denote these point defects as $H_{\text{Sub}}^{\text{Cr}}$, $H_{\text{Tet}}^{\text{Cr}}$, $H_{\text{Oct}}^{\text{Cr}}$, $He_{\text{Sub}}^{\text{V}}$, $He_{\text{Tet}}^{\text{V}}$, and $He_{\text{Oct}}^{\text{V}}$, respectively. For simplicity, we refer to the supercells with one Cr or one V atom as W-Cr and W-V alloys in the following sections, respectively.

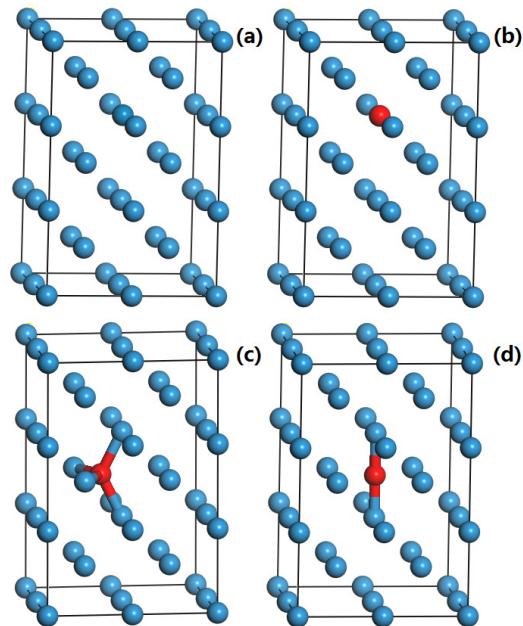


Figure 1. Color image available online. The crystal structure of tungsten, with or without a point defect, is depicted in the figure. The blue balls represent tungsten atoms, while the red ball represents either a hydrogen or helium atom, respectively. (a) The perfect W, (b) H_{Sub} or He_{Sub} , (c) H_{Tet} or He_{Tet} , (d) H_{Oct} or He_{Oct} .

We performed calculations using density functional theory (DFT) and the plane-wave pseudopotential method [52,53] as implemented in the Cambridge Sequential Total Energy Package (CASTEP) [54]. We used the generalized gradient approximation (GGA) [55–58] with the Perdew–Burke–Ernzerhof (PBE) [57] functional to describe electron-exchange-

correlation interactions. Ultrasoft pseudopotentials were employed to model ion-electron interactions. Since the H atom only has a single valence electron and the He atom is a closed-shell atom, Ortmann–Bechstedt–Schmidt (OBS) [59] dispersion correction DFT (DFT-D) was used to describe the van der Waals force. The energy cutoff was 500 eV for all calculations. We chose the following basic parameters: space representation = reciprocal, SCF tolerance = 1.0×10^{-6} eV/atom, and a $5 \times 5 \times 5$ k -point mesh in a Brillouin zone. We determined atomic positions by satisfying these conditions: (1) the maximum force on atoms was less than 0.05 eV/nm; (2) the maximum change in energy per atom was less than 1.0×10^{-5} eV; (3) the maximum displacement was less than 0.001 Å; and (4) the maximum stress of the crystal was less than 0.02 GPa.

3. Results and Discussion

3.1. The Energetics and Stability of the Binary W-Cr and W-V Alloys

To evaluate alloy stability, we calculated the formation energy and binding energy of W-Cr and W-V alloys as follows:

$$E_f = E_{nWxCr yV} - nE_W - xE_{Cr} - yE_V \quad (1)$$

$$E_b = E_{nWxCr yV} - nE_W^i - xE_{Cr}^i - yE_V^i \quad (2)$$

Here, E_f and E_b are the formation energy and binding energy of the alloys, respectively. $E_{nWxCr yV}$ is the total energy of alloys containing n W atoms, x Cr atoms, and y V atoms. E_W is the energy of a W atom in perfect bcc W. E_{Cr} is the energy of a Cr atom in perfect Cr crystal. E_V is the energy of a V atom in perfect V crystal. E_W^i , E_{Cr}^i , and E_V^i are the energies of isolated W, Cr, and V atoms, respectively. Lower formation energy indicates easier alloy formation. Higher absolute binding energy indicates a more stable crystal structure. Table 1 shows the formation energy and binding energy of W-Cr and W-V alloys. From Table 1, the formation energy of W-Cr alloy is larger than that of perfect bcc W, so W-Cr alloy formation requires more energy than perfect bcc W. W-V alloy has the lowest formation energy, indicating it forms most easily among perfect W, W-Cr alloy, and W-V alloy. It is worth mentioning that we have calculated the formation energy of W-Re to be -0.526 eV [41], which falls between that of W-Cr and W-V. The absolute value of W-Cr alloy's binding energy is the smallest, while W-V alloy's is the largest. Thus, W-V alloy has the most stable crystal structure, and W-Cr alloy has the least stable structure among these three.

Table 1. The formation energies (in eV) and binding energies (in eV) of bcc W, W-Cr alloy, and W-V alloy.

Crystal	E_f	E_b
W	0	−270.531
W-Cr	3.683	−268.780
W-V	−0.973	−780.043

3.2. Mechanical Properties of the W-Cr and W-V Alloys

As the most promising PFMs and FWMs, W and its alloys' mechanical properties are crucial. The bcc crystal structure has three independent elastic constants: C_{11} , C_{12} , and C_{44} . When $C_{11} + 2C_{12} > 0$, $C_{44} > 0$, and $C_{11} - C_{12} > 0$, the W can exist stably with a bcc structure. The mechanical properties of the W and W-based alloys, such as bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio (ν), are calculated as follows:

$$B = (C_{11} + 2C_{12})/3 \quad (3)$$

$$G = (C_{11} - C_{12} + 3C_{44})/5 \quad (4)$$

$$E = 9BG / (3B + G) \quad (5)$$

$$\nu = (3B - 2G) / 2(3B + G) \quad (6)$$

Tables 2 and 3 show the elastic constants and moduli for perfect bcc W and W-Cr and W-V alloys. Our calculated elastic constants and moduli for perfect W agree well with experimental [60] and other theoretical [61] results. From Table 2 and Figure 2, the C_{11} and C_{44} elastic constants of W-Cr alloy are smaller than those of perfect W, while C_{12} is larger. All elastic constants of W-V alloy are smaller than those of perfect W and W-Cr alloy. These changes agree with Hu et al.'s calculations [46]. From Table 3 and Figure 3, we find that the Young's modulus, bulk modulus, and shear modulus of the W-Cr alloy and the W-V alloy are smaller than that of perfect W, and all these elastic moduli of the W-V alloy are smaller than those of the W-Cr moduli. From Table 3 and Figure 3, the Young's, bulk, and shear moduli of W-Cr and W-V alloys are lower than those of perfect W, and all W-V alloy moduli are lower than those of W-Cr alloy. The elastic properties of metals are mainly related to the bond strength between their atoms. On the other hand, the diffusion coefficient of doping elements mainly depends on their mobility in the host metal. Although the relationship between the two is not direct, to some extent, they may affect each other. For example, if the diffusion of doping elements causes a significant structural change in the metal lattice, this may affect the metal's elastic properties. Similarly, the elastic properties of metal may also affect the diffusion behavior of doping elements, especially under stress or pressure. There have been many studies on the influence of element doping on the elastic properties of tungsten and the resulting impact on its processing properties, especially in the study of W-Re alloys doped with Re element [18,40,41,62].

Pugh presents an empirical relation that can predict the brittleness and ductility of the bcc metal [63]. The empirical formula is the ratio of shear modulus and bulk modulus. The metal is ductile when the ratio is lower than 0.57, and the metal is brittle when the ratio is higher than 0.57. The Poisson's ratios of W-Cr and W-V alloys exceed that of perfect W's, and W-V alloy's ratio is larger than W-Cr alloy's. The G/B values of W-Cr and W-V alloys are smaller than that of perfect W's, indicating W-Cr and W-V alloys are more ductile. Adding Cr or V makes W-based alloys easier to process.

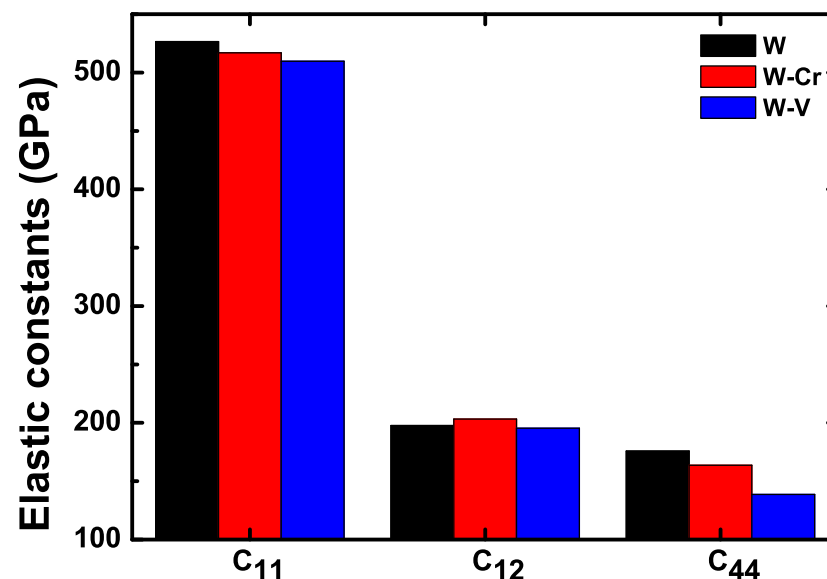


Figure 2. The elastic constants of perfect W and W-Cr and W-V alloys.

Table 2. Calculated and experimental lattice constants (a in Å) and elastic constants (C_{ij} in GPa) of bcc W and W-Cr and W-V alloys. The values in parentheses represent the percentage error relative to the experimental values.

Parameters	a	C_{11}	C_{12}	C_{44}
W	3.15 (0.3%)	526.48 (1.2%)	197.60 (3.6%)	175.80 (7.8%)
Cal [61]	3.17 (0.3%)	536.32 (0.6%)	202.25 (1.3%)	138.70 (14.9%)
Exp [60]	3.16	533	205	163
W-Cr	3.17	516.92	203.25	153.68
W-V	3.17	509.75	195.39	138.62

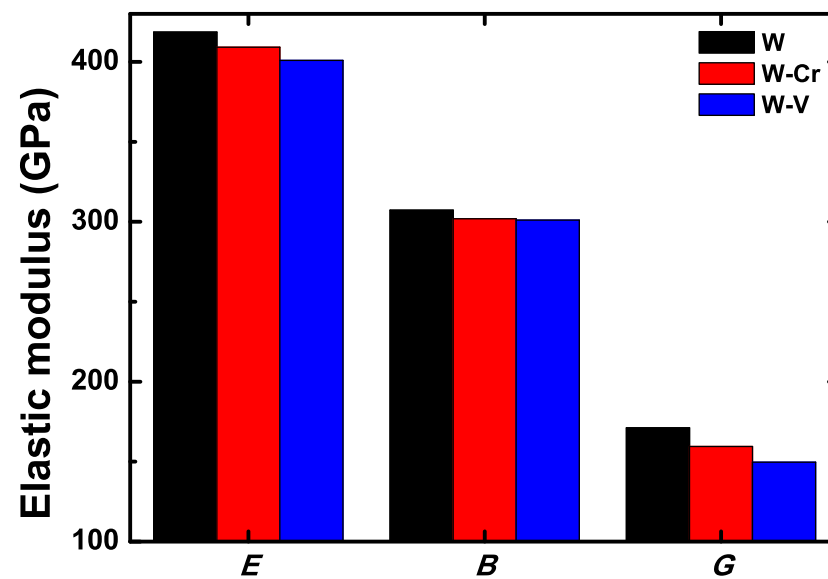


Figure 3. The elastic modulus of perfect W and W-Cr and W-V alloys.

Table 3. Calculated and experimental values for the bulk modulus (B in GPa), Young's modulus (E in GPa), shear modulus (G in GPa), Poisson's ratio (ν), and G/B of bcc W and W-Cr and W-V alloys. The values in parentheses represent the percentage error relative to the experimental values.

Parameters	B	E	G	ν	G/B
W	307.23 (2.2%)	418.63 (0.2%)	171.16 (4.7%)	0.27 (3.6%)	0.56 (3.6%)
Cal [61]	313.61 (0.2%)	386.83 (7.4%)	149.42 (8.5%)	0.29 (3.6%)	0.48 (12.5%)
Exp [60]	314.33	417.80	163.40	0.28	0.54
W-Cr	301.86	409.11	159.44	0.27	0.53
W-V	301.05	400.89	149.69	0.28	0.50

3.3. The Formation Energies of H and He in W

To investigate how Cr and V affect hydrogen and helium behavior in bcc W, we calculated the formation energies of hydrogen and helium in bcc W with and without Cr or V. Tables 4 and 5 and Figure 4 show the results. Our calculated formation energies for hydrogen and helium in perfect bcc W agree well with other studies [44,61,64]. For helium, the substitutional site is most favorable, while for hydrogen, the tetrahedral site is. Table 4 and Figure 4 show the formation energies of hydrogen and helium in bcc W containing Cr or V near the hydrogen or helium atom. Figure 4 shows that the formation energy of hydrogen or helium in W-Cr alloy is much higher than in bcc W, while in W-V alloy, it is lower. This indicates adding Cr to W reduces hydrogen and helium diffusion, while adding V promotes it. Although the formation energies change, the tetrahedral site remains most favorable for hydrogen and the substitutional site for helium. In short, added Cr or V

atoms do not change the favorable sites of hydrogen and helium in bcc W but do alter their diffusion behavior.

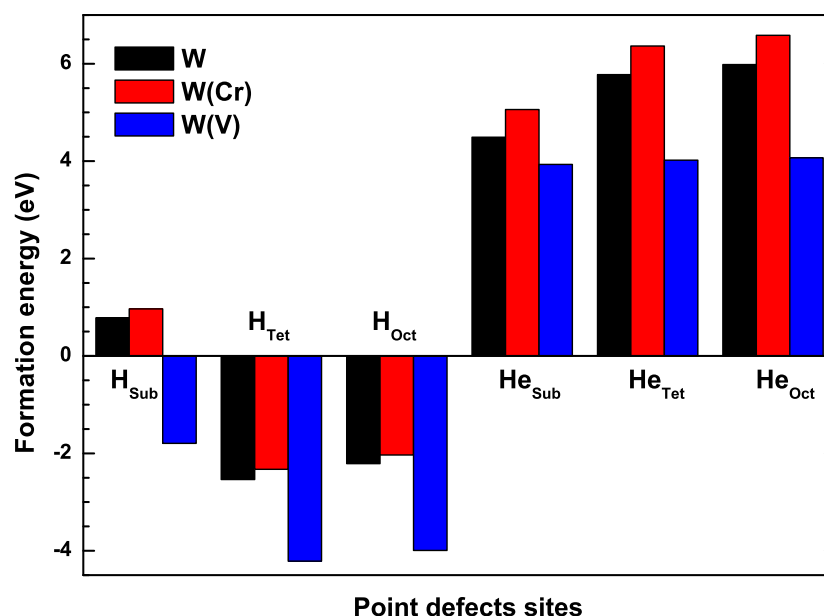


Figure 4. The formation energies of H and He in perfect W and in W-Cr and W-V alloys.

Table 4. Summary of the formation energies (in eV) of single defects in perfect bcc W. The values in parentheses represent the percentage difference relative to other calculated values.

Configuration	H _{Sub}	H _{Tet}	H _{Oct}	He _{Sub}	He _{Tet}	He _{Oct}
This paper	0.782	−2.536	−2.212	4.49	5.775	5.984
Cal [44]	0.92 (16.2%)	−2.47 (2.6%)	−2.07 (6.6%)	5.00 (10.8%)	6.23 (7.6%)	6.48 (8.0%)
Cal [61,64]	0.78 (0.3%)	−2.44 (3.9%)	−2.06 (7.1%)	4.70 (4.6%)	6.16 (6.5%)	6.38 (6.4%)

Table 5. The formation energies (in eV) of single defects in bcc W containing one Cr or V atom.

Configuration	H _{Sub} ^{Cr}	H _{Tet} ^{Cr}	H _{Oct} ^{Cr}	He _{Sub} ^{Cr}	He _{Tet} ^{Cr}	He _{Oct} ^{Cr}
E_f	0.965	−2.327	−2.034	5.059	6.365	6.583
Configuration	H _{Sub} ^V	H _{Tet} ^V	H _{Oct} ^V	He _{Sub} ^V	He _{Tet} ^V	He _{Oct} ^V
E_f	−1.795	−4.214	−3.994	3.93	4.02	4.07

3.4. The Interaction of H-Cr, H-V, He-Cr, and He-V

Figure 5 shows how the distances between H-Cr, H-V, He-Cr, and He-V change before and after relaxation. After relaxation, the H-Cr distance becomes shorter than the initial value when the initial H position is substitutional or tetrahedral but slightly longer when it is octahedral. This indicates attraction between H and Cr for initial distances over 1.769 Å but repulsion below 1.583 Å. The He-Cr distance always becomes shorter, indicating attraction regardless of initial distance. Changes in H-V and He-V distances show the same tendencies but smaller magnitudes than for Cr. Interestingly, the He-V distance increases slightly when the initial He position is substitutional. These results reflect competition between elastic and chemical interactions, primarily elastic due to the small atomic volumes and high electronegativities of Cr and V. There is attraction between H and Cr or V for distances over 1.769 Å but repulsion below 1.583 Å. There is always attraction between He and Cr or V. Cr and V solute atoms are nucleation centers for point defects near them in W, including those formed by H and He.

It is worth noting that in first-principles calculations, the precision of the results is affected by the imposition of a limited range (e.g., 0.001 Å) on the variation of atomic displacements. Hydrogen and helium atoms in tungsten alloys can interact through strain fields generated by dislocations, such as pinning. These interactions encompass intricate physical processes at the atomic scale, which can be influenced by the imposed displacement limitations. As a result, certain significant interactions involving hydrogen and helium in tungsten alloys can be unintentionally disregarded, including their interactions with dislocations and vacancies. To achieve more accurate simulations of these complex physical processes, it may be necessary to employ more flexible displacement limitations in simulations of this nature.

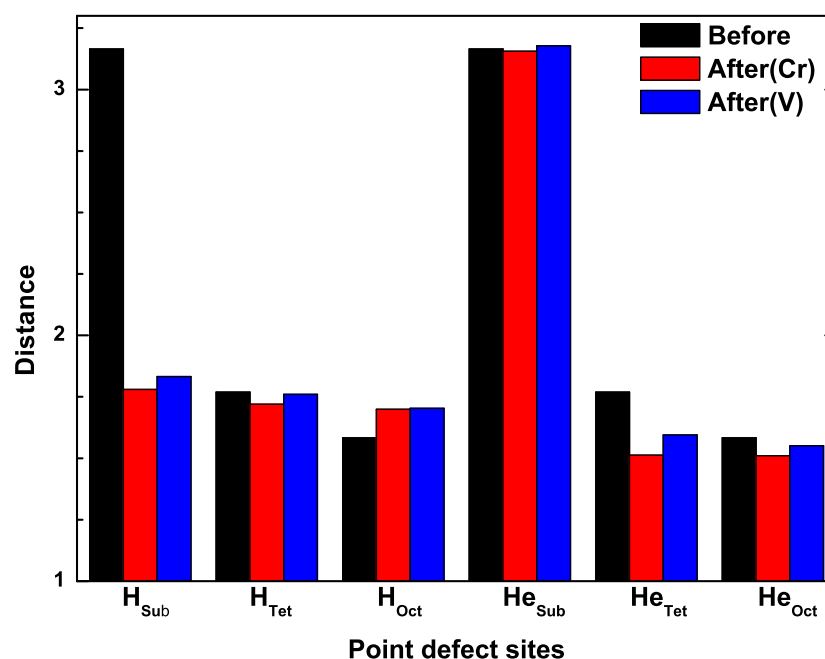


Figure 5. Distances between hydrogen or helium atoms and Cr or V atoms after structural relaxation.

3.5. The Competition between Vacancy and Cr or Vacancy and V Atoms

Figure 6 shows the sites of H and He atoms in bcc W near a vacancy after relaxation. The He atom occupies the original vacancy site, while the H atom position changes little. Our results agree with Lee's [44] results. Here, H and He behavior near vacancies is explained energetically. Figures 7 and 8 show the sites of H and He atoms in W near Cr and V atoms after relaxation. The effects of Cr and V on H and He are not obvious; the attraction between vacancies and He is stronger than that between Cr/V and He. There is no obvious attraction between H and vacancies or changes when vacancies and Cr/V are together. The effects of Cr and V on H and He behavior are not stronger than vacancies' effects. These results show vacancies can dilute the effects of Cr and V on H and He in W.

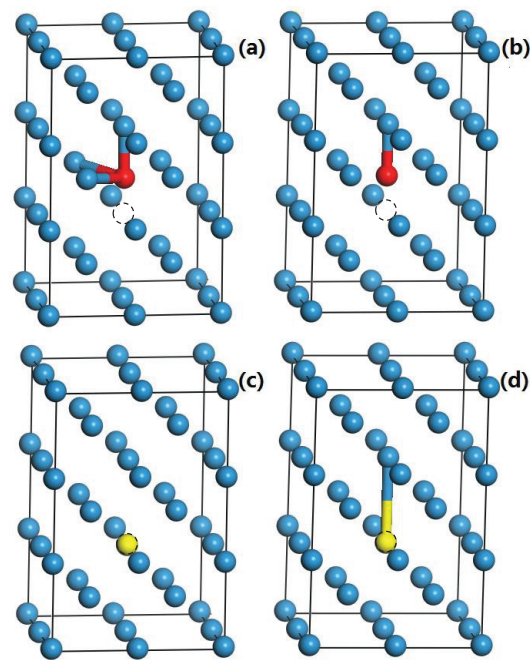


Figure 6. Color image available online. The sites of a hydrogen atom or helium atom in the tungsten with a vacancy near the hydrogen or helium atom after relaxation. The blue balls stand for W, the red ball stands for H, the yellow ball stands for He, and the dotted circle stands for the vacancy. (a) H_{Tet} , (b) H_{Oct} , (c) He_{Tet} , and (d) He_{Oct} .

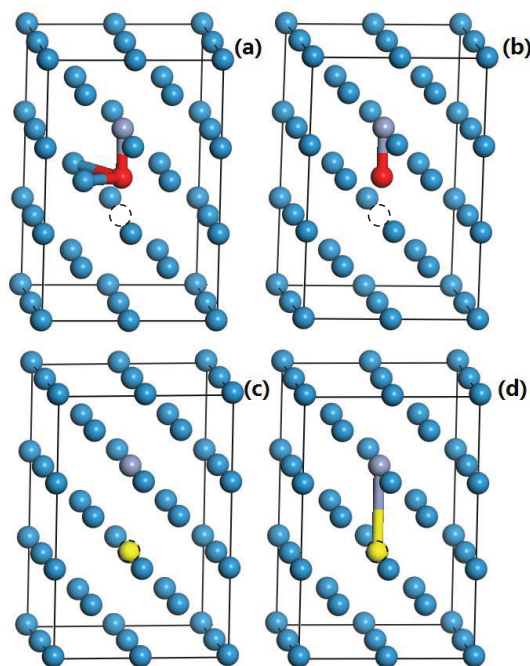


Figure 7. Color image available online. The sites of a hydrogen atom or helium atom in the tungsten with a chromium atom near the hydrogen or helium atom after relaxation. The blue balls stand for W, the red ball stands for H, the yellow ball stands for He, the gray ball stands for Cr, and the dotted circle stands for the vacancy. (a) H_{Tet} , (b) H_{Oct} , (c) He_{Tet} , and (d) He_{Oct} .

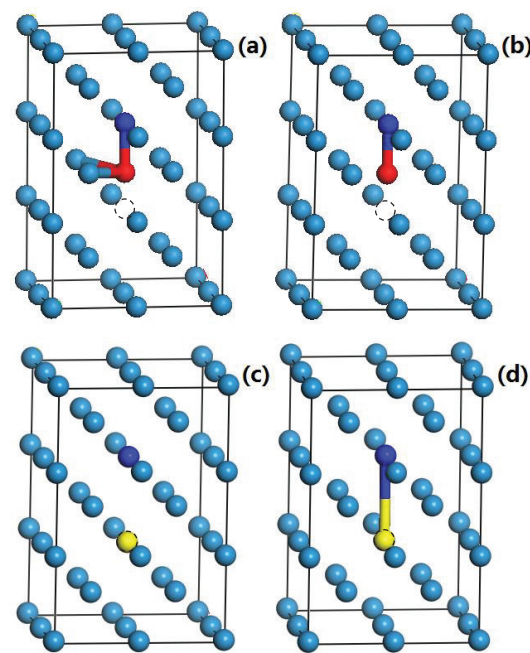


Figure 8. Color image available online. The sites of a hydrogen atom or helium atom in the tungsten with a vanadium atom near the hydrogen or helium atom after relaxation. The blue balls stand for W, the red ball stands for H, the yellow ball stands for He, the dark blue ball stands for V, and the dotted circle stands for the vacancy. (a) H_{Tet} , (b) H_{Oct} , (c) He_{Tet} , and (d) He_{Oct} .

4. Conclusions

This study investigated the effect of chrome and vanadium on the behavior of hydrogen and helium in tungsten using first-principles calculations. The results show that both elements can enhance the trapping of hydrogen and helium but through different mechanisms. Chrome affects the formation energy and binding strength of hydrogen–vacancy complexes, while vanadium affects the migration barrier and binding energy of helium–vacancy complexes. It should be noted that this study is preliminary, and, as such, there is room for more systematic research in the future. Further experimental validation is needed to confirm these theoretical predictions. In addition, future research could explore other alloying elements or dopants that can further enhance the trapping or diffusion properties of hydrogen and helium in tungsten. Overall, this study contributes to our understanding of the fundamental processes that govern radiation damage in materials and provides guidance for developing more durable materials for nuclear energy applications.

Author Contributions: Conceptualization, M.L. and Z.Z.; methodology, M.L.; software, Q.Z.; validation, Y.L. and Z.Z.; formal analysis, M.H.; investigation, M.L.; writing—original draft preparation, M.L. and Z.Z.; writing—review and editing, Q.Z.; supervision, X.O.; funding acquisition, Q.Z. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China, grant number 12275083.

Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest.

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