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Unique phenomena associated with tungsten and plasma particles in fusion reactor

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Abstract

Unique phenomena are expected associated with interaction between tungsten (W) materials and plasma particles in fusion reactors. In the present paper, we introduce some important and interesting studies of the characteristic behaviors of the plasma particles in the W materials. In particular, abnormal stable configurations of multiple hydrogen (H) atoms trapped in a W vacancy are found in terms of first-principle calculations. We calculate binding energies of the multiple H atoms to a W vacancy. Besides, zero-point energy (ZPE) corrections are estimated according to the abnormal H configurations. We estimate binding energy difference depending on the H isotopes for the first time.

Key words : *tungsten, hydrogen isotope, fusion reactor, first-principle calculation*

1. Introduction

In the fusion reactor, divertor armor tiles are exposed to extremely intense plasma particle irradiation. In order to protect the divertor armor tiles, its surface is planning to be covered with tungsten (W) or W alloy. So, study of interaction between W and plasma particle started. W is one of promising plasma facing materials because of its high melting point, low hydrogen (H) solubility, and low sputtering erosion. Besides, it has high thermal conductivity and low induced radioactivity.

By the way, some unique phenomena are observed associated with the interaction between W and plasma particles. (1) Negative formation energy for di-vacancy in W . Di-vacancy in metals is usually more stable than mono-vacancy because the inner surface of the di-vacancy is smaller than the total inner surface of the two mono-vacancies. However, it has reported that di-vacancy in W lattice is unstable [1]. (2) Helium (He) cluster migrations more quickly than a single He atom. He clusters are nucleated in a molecular dynamics simulations and diffusion constants are estimated [2]. He clusters smoothly migrate in the W lattice. (3) Fibre-form tungsten covering surface by He irradiation. An characteristic surface morphology has been reported on the W specimens irradiated by He [3]. (4) Abnormal and stable H configurations in a W vacancy has been reported [4, 5, 6]. We will focus on the fourth topics in the present paper.

Typical interstitial sites of bcc metals are tetrahedral interstitial site (T-site) and octahedral interstitial site (O-site). According to the previous works, T-site is more favorable for an H atom than O-site in perfect bcc metals. On the other hand, an H atom trapped in a vacancy is located close to an O-site. If multiple H atoms would be trapped in the vacancy, it was reported that each H atom was also located close to an O-site. As a result, a maximum of 6 H atoms can be accommodated in a vacancy because there are 6 O-sites next to a vacancy in bcc lattice, which is standard model for multiple H atom configuration in a vacancy [7]. However, stable configurations of multiple H atoms trapped in a W vacancy are abnormal and a maximum of 12 H atoms can be accommodated.

A large amount of H atoms and H isotopes are retained in irradiation zone of W materials. The hydrogen solubility of W and W alloys is very low but lattice defects of vacancy types are nucleated in the irradiation zone. Then, two types of hydrogen isotopes coexist in fusion reactors because D-T fusion reaction takes place. It is expected that the binding energies of lighter H isotopes to a vacancy are larger than those of heavier ones due to the difference of zero-point energy (ZPE) corrections. The coexistence effects of H isotopes will be important subject associated with fusion reactors. In particular, tritium (T) retention in the W materials is a serious problem for the safety of fusion reactors because T is a radioisotope whose physical half-life is 12 years. We estimate the binding energies of multiple H isotopes trapped in a W vacancy.

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2. Simulation method

In the present simulation, we do not assume that H atoms in a W vacancy are located close to the O-sites. Instead, initial H positions for ionic relaxation are randomly generated to find unexpected and the most stable configuration. We performed first-principles calculations based on DFT using Vienna ab-initio simulation package (VASP) [8, 9] with PBE potential [10]. Plane wave cut-off energy is 350 eV. Electronic and ionic relaxations are iterated until a break condition (0.003 eV/Åfor every atom) is satisfied.

When H atoms trapped in a W vacancy are assumed to be classical particles without ZPE corrections, the binding energies for the classical H atoms are estimated to be

$$e_k = E[\mathrm{W}_{n-1}\mathrm{V}] - E[\mathrm{W}_{n-1}\mathrm{V}(\mathrm{H}_k)] + k(E[\mathrm{W}_n\mathrm{H}^{\mathrm{I}}] - E[\mathrm{W}_n]), \quad (1)$$

where E is cohesive energies of supercells; $\mathrm{W}_{n-1}\mathrm{V}$ is a supercell composed of $(n-1)$W and a vacancy; $\mathrm{W}_{n-1}\mathrm{V}(\mathrm{H}_k)$ is a supercell containing a vacancy trapping k classical H atoms; $\mathrm{W}_n\mathrm{H}^{\mathrm{I}}$ is that composed of nW and an interstitial H atom in W; and W_n is a supercell of perfect W lattice. Positive sign of e_k means an attractive interaction between H and W vacancy. H isotopes are represented by ${}^a\mathrm{H}$ (${}^1\mathrm{H}$ = H, ^{2} H = D, ^{3} H = T). The superscript indicates mass number. If the same type of H isotopes ${}^a\mathrm{H}$ are trapped in a W vacancy, the binding energies including ZPE corrections are

$$e_k^a = e_k + \frac{\{kZ_{\mathrm{I}}({}^1\mathrm{H}) - Z_{\mathrm{V}}({}^1\mathrm{H}_k)\}}{\sqrt{a}}, \quad (2)$$

where $Z_{\mathrm{I}}({}^1\mathrm{H})$ is the total ZPE for an interstitial ^{1}H atom located at a T-site in perfect W lattice, which is estimated to be 0.259 (eV). $Z_{\mathrm{V}}({}^1\mathrm{H}_k)$ is the total ZPE for $k{}^1$H atoms trapped in a W vacancy. The ZPE corrections are calculated by harmonic approximation assuming that the force acting on a ^{1}H is proportional to the displacement from the equilibrium position [11].

3. Results

Figure 1 shows typical abnormal but stable configurations of H atoms in a W vacancy. Stable configuration of 4 H atoms is tetrahedral structure, Fig. 1 (a), but planar one, Fig. 1 (b). Stable configuration of 6 H atoms is more complicated, as shown in Fig. 1 (c). Symmetric 6 H structure Fig. 1 (d) is unstable in the case of H atoms trapped in a W vacancy. But the symmetric structure of 6 H atoms is usually stable for other bcc transition metals. A maximum of 12 H atoms can be accommodated in a W vacancy and the H atoms are located close to T-sites, as shown in Fig. 1 (e).

Figure 2 shows the total binding energies of single and multiple H atoms (classical H atoms without ZPE correction) to a vacancy in bcc transition metals. A vacancy in W and Mo can accommodate 12 H atoms. However, 6 H atoms are trapped in a vacancy in other bcc metals, which is good agreement with the standard model [7].

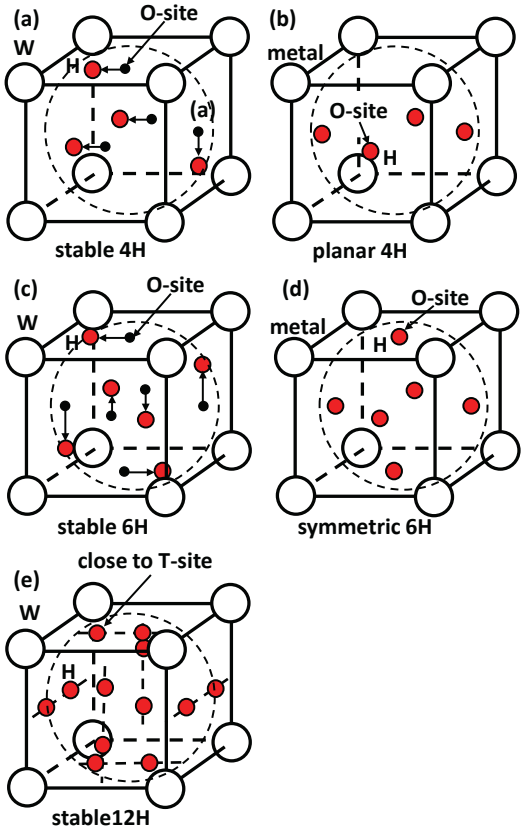

Fig. 1 Schematic view of stable H configuration in vacancy in W and BCC metals.

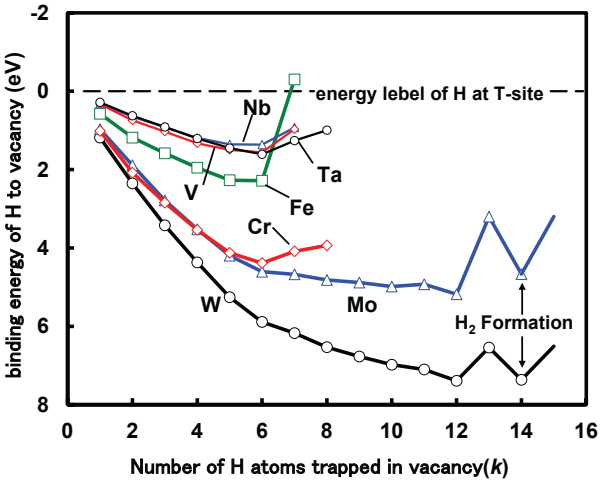

Fig. 2 Total binding energies of single and multiple hydrogen atoms trapped in vacancy in bcc transition metals.

Table 1 Total binding energies of classical H atom e_k and H isotopes, e_k^1, e_k^2, and e_k^3 to a W monovacancy (eV). $Z_V(^1H_k)$ is the total ZPE of k ^{1}H trapped in the W vacancy.

k	e_k^1 (H)	e_k^2 (D)	e_k^3 (T)	e_k	$Z_V(^1H_k)$
1	1.381	1.334	1.314	1.223	0.101
2	2.731	2.639	2.598	2.415	0.201
3	3.800	3.710	3.670	3.492	0.468
4	4.816	4.709	4.662	4.450	0.669
5	5.727	5.604	5.550	5.309	0.876
6	6.408	6.276	6.218	5.957	1.102
7	6.623	6.499	6.444	6.200	1.390
8	6.913	6.794	6.741	6.506	1.664
9	7.129	7.002	6.946	6.697	1.898
10	7.294	7.173	7.120	6.881	2.176
11	7.334	7.202	7.144	6.885	2.399
12	7.725	7.587	7.525	7.252	2.634
13	6.890	6.736	6.667	6.363	2.838
14	7.465	7.361	7.315	7.110	3.270
15	6.466	6.325	6.263	5.986	3.403

Table 1 exhibits the total binding energies for H isotopes (H, D, T) and classical H atoms without ZPE corrections to a W vacancy calculated in Eq. (2). As our expectation, the binding energies for the lighter H isotopes are larger than those for heavier ones.

4. Discussion

W and W alloys are promising plasma facing materials in fusion reactors due to their very low H solubility. However, it has been reported that large amounts of H isotopes are retained in W specimen of irradiated zone [12]. Figure 3 shows energy landscape of H atom in BCC transition metals, W, Mo, and Fe. Energy levels of H at interstitial site in W and Mo are very high, which is good agreement with the low H solubility of these metals. However, the difference between energy levels for an H at interstitial site and vacancy is very large. Therefore, vacancy type lattice defects introduced by irradiation are expected to be strong H trapping sites.

The binding energies of H isotopes depend on the types of H isotopes, according to Table 1. The amount of T retention in the plasma facing materials is serious problem for safety operation of actual fusion reactors. The results of the present work indicate that the binding energies of T to a W vacancy are smaller than those of H and D. Therefore, T retention is expected to be reduced by coexistence of other H isotopes in the W materials. We are planning to estimate the amounts of H isotopes trapped in a W vacancy in the coexistence circumstance on the basis of a thermodynamic model in the future [6].

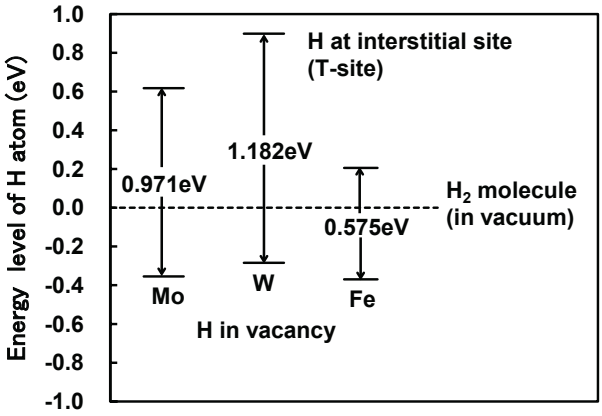

Fig. 3 Energy level of H atom at interstitial site and vacancy in W, Mo and Fe.

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