



Solution and diffusion of hydrogen isotopes in tungsten-rhenium alloy



Fei Ren ^{a, b}, Wen Yin ^{b, c, *}, Quanzhi Yu ^c, Xuejun Jia ^c, Zongfang Zhao ^{a, b}, Baotian Wang ^b

^a School of Nuclear Science and Technology, Lanzhou University, Lanzhou 730000, People's Republic of China

^b Dongguan Branch, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, People's Republic of China

^c Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China

HIGHLIGHTS

- With or without ZPE corrections, the properties of H solution and diffusion in W and W-Re alloy are investigated.
- The presence of Re in W increases the solution energy and the real normal modes of vibration, compared to H in pure W.
- The concentration of Re does not influence noticeably the properties of H solution and diffusion in W-Re alloy.
- For H in perfect W and W-Re crystals, the presence of Re would decrease the solubility and increase the diffusivity.

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ABSTRACT

Rhenium is one of the main transmutation elements forming in tungsten under neutron irradiation. Therefore, it is essential to understand the influence of rhenium impurity on hydrogen isotopes retention in tungsten. First-principle calculations were used to study the properties of hydrogen solution and diffusion in perfect tungsten-rhenium lattice. The interstitial hydrogen still prefers the tetrahedral site in presence of rhenium, and rhenium atom cannot act directly as a trapping site of hydrogen. The presence of rhenium in tungsten raises the solution energy and the real normal modes of vibration on the ground state and the transition state, compared to hydrogen in pure tungsten. Without zero point energy corrections, the presence of rhenium decreases slightly the migration barrier. It is found that although the solution energy would tend to increase slightly with the rising of the concentration of rhenium, but which does not influence noticeably the solution energy of hydrogen in tungsten-rhenium alloy. The solubility and diffusion coefficient of hydrogen in perfect tungsten and tungsten-rhenium alloy have been estimated, according to Sievert's law and harmonic transition state theory. The results show the solubility of hydrogen in tungsten agrees well the experimental data, and the presence of Re would decrease the solubility and increase the diffusivity for the perfect crystals.

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1. Introduction

Tungsten (W) and its alloys are the promising plasma-facing material (PFM) for fusion reactor because of their high melting point, low sputtering yield, good thermal conductivity and low tritium (T) retention [1–3]. The plasma-facing components must withstand high heat and high flux particle bombardment escaping from the plasma, and hydrogen (H) isotopes can congregate on the surfaces of those components or penetrate through the surface and diffuse deep into the bulk [4–6]. In particular, H isotopes can be

trapped by various defects, such as vacancies, grain boundaries and impurity atoms, thus it would affect utilization efficiency of fusion fuel [7]. On the other hand, H isotopes retention in W-based materials may lead to modification of the materials' physical and mechanical properties. For instance, H is known to have a critical influence on metal embrittlement [8,9], due to vacancy formation induced by H would play a key role in the process of embrittlement [10,11]. Besides, H in W could have an impact on the brittle to ductile transition temperature [12]. Therefore, for safety and efficiency reasons, it is very important to understand the solution and diffusion of H isotopes in W-based materials.

There are many experimental and computational methods developed to study H isotopes retention in W-based materials [2,13]. Frauenfelder [14] and Mazayev [15] measured the solubility of H in W in the temperature range of 1100 K–2400 K, which agrees

* Corresponding author. Dongguan Branch, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, People's Republic of China.

E-mail address: yinwen@ihep.ac.cn (W. Yin).

with the calculated result by the first-principle calculations [16]. The diffusion coefficient of H in W was evaluated using the harmonic transition state theory (hTST) [17], which is agreement with the experimental result by Frauenfelder [14] at temperature above 1500 K. However, the calculated result of diffusion coefficient by Heinola [17] are much higher than the experimental results below 1500 K, which had been measured by Zakharov [18], Benamati [19], Otsuka [20], Ikeda [21] and Hoshihira [22], respectively. Furthermore, there is a significant difference in migration barrier of H in W between Frauenfelder's [14] experimental value and Heinola's [17] calculated value. It is worthy of note that the migration barrier was calculated by Johnson's [6] along a higher barrier path via octahedral site, although the calculated value is in accordance with Frauenfelder's [14] experimental result. Nevertheless, if the Frauenfelder's [14] experimental data at temperatures above 1500 K is fitted, the migration barrier of H in W will decrease from 0.39 eV to 0.25 eV. Therefore, it is very possible that there is a significant influence of lattice defects on H diffusion even at temperature up to about 1500 K, and Kong [16], Fernandez [23] and Oda [24] have corroborated this by first-principle calculations and Kinetic Monte Carlo method, respectively. Thus Kong's [16] calculated results agree with those experimental results when the influence of temperature and defects on H diffusion in W are considered.

Under neutron irradiation, many transmutation elements are produced in PFM. Among them, rhenium (Re) is one of the main products [25], and calculations by Cottrell [26] and Gilbert [27] suggest that after several years of exposure of fusion neutrons, the concentration of Re in W might reach several percent. According to the previous experimental and theoretical studies for W-Re alloy, the concentration of Re can be increased to above 25% in a body-centered cubic (bcc) structure [28–30], and the bcc structure is dynamically stable based on Federer's [28] experimental study, as well as Ekman's [29] and Chouhan's [30] calculations. Although Golubeva's [31] experimental results show the Re concentration in W–Re alloy does not influence noticeably the deuterium (D) retention in the range of 1–10%, and Tyburska [32] investigated D retention in damaged W-Re alloy, but the influence of Re on solubility of H in W is still not clear. Moreover, the solubility of the extrapolation of Frauenfelder's [14] datas and Kong's [16] calculated result are much lower than Benamati's [19] data of D in W doped with 5% Re at 850 K–885 K. Recently, Wróbel investigated Re precipitation in irradiated bcc W-Re alloy and the interactions of Re and vacancy using first-principle calculations and Monte Carlo simulations [33]. However, the interactions between H and vacancy in W-Re alloy were not studied. Therefore, in this paper, we pay attention to the influence of Re on solution and diffusion of H isotopes in W-Re alloy. We carry out a systematic first-principle calculations to investigate the solution energies, migration barriers and binding energies of Re–H for H in perfect bcc W and W-Re crystals. Furthermore, the solubility and diffusion coefficient of H in perfect W and W-Re alloy were evaluated using Sievert's law and hTST.

2. Computational methods

The solution energies of H in W or W-Re alloy can be defined by:

$$E_{\text{sol}} = E[\text{W}/(\text{W} + \text{Re}) + \text{H}] - E[\text{W}/(\text{W} + \text{Re})] - 0.5E_{\text{H}_2}, \quad (1)$$

where $E[\text{W}/(\text{W} + \text{Re}) + \text{H}]$ is the total energy of W or W-Re supercell with a single H atom, and $E[\text{W}/(\text{W} + \text{Re})]$ is the reference energy of perfect W or W-Re supercell. E_{H_2} is the total energy of H molecule, our calculated value is -6.744 eV. The binding energy of a H molecule is 4.516 eV, which agrees well with the experimental value 4.747 eV [34].

The binding energy between two entities A and B is obtained as:

$$E_b = (E_A + E_B) - (E_{\text{AB}} + E_{\text{ref}}), \quad (2)$$

where E_A and E_B are the total energies of the supercell containing A or B, respectively, E_{AB} is the total energy of the supercell containing both A and B in interaction, E_{ref} is the energy of the supercell without A and B. All the supercells contain the same number of sites. Note that a positive binding energy means attraction between A and B.

According to Sievert's law, the solubility can be given approximately by:

$$S = \sqrt{\frac{P}{P_0}} \exp\left(\frac{\Delta S T - E_{\text{sol}}}{kT}\right), \quad (3)$$

where P and P_0 represent the background pressure and the standard pressure, respectively, k is the Boltzmann constant and T is the absolute temperature, the solution entropy ΔS is equal to about $4.7k$ [35].

The diffusion coefficient of interstitial atoms in solid solutions can be evaluated by Arrhenius equation:

$$D = D_0 \times \exp\left(-E_m/kT\right), \quad (4)$$

where D_0 is usually assumed to be the temperature independent diffusion constant, E_m is the activation energy which is equal to migration energy for the interstitial atomic diffusion.

According to the interstitial atomic diffusion theory presented by Wert and Zener [36], D_0 can be written as:

$$D_0 = \frac{n}{6} \lambda^2 \nu, \quad (5)$$

where $n = 4$ is a geometrical factor of the number of equivalent jump paths for H jumping along tetrahedral site to another tetrahedral site in bcc structure metal, λ is the jump length which equals to $\sqrt{2}a/4$, and a is the lattice constant. ν is the vibration frequency, which can be approximately evaluated by:

$$\nu = \sqrt{E_m/2m\lambda^2}, \quad (6)$$

where m is the mass of a H atom.

In addition, according to reference [37] the diffusion coefficient can also be calculated as:

$$D = \frac{1}{6} \lambda^2 \Gamma, \quad (7)$$

where Γ is the jump rate, based on Eyring's theory [38,39] and hTST [40], it can be calculated by:

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