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Ab initio calculation of helium behavior in the spallation tungsten

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ABSTRACT

The non-elastic reaction in spallation will produce many new light particles such as hydrogen and helium. At the same time, it also produces many new heavy species. In this manuscript a series of *ab initio* calculations have been performed to quantify the helium behavior in spallation tungsten, especially the effect of these spallation nuclides on the helium behavior. The following results were found: (i) The formation energies of the main spallation nuclides are positive, except tantalum; (ii) All spallation nuclides trap helium with strong positive binding energy, except tantalum; (iii) The vacancy also is the trap site for the most of spallation nuclides with the positive binding energies between vacancy and the spallation nuclides, except tantalum; (iv) Vacancy is the strong helium trap, which will not be changed with the existence of the spallation nuclides; (v) The strong binding energy between two helium atoms will not be changed by the spallation nuclides; (vi) The spallation nuclides may increase the energy barrier that a tetrahedral helium migrates between two equivalent sites.

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1. Introduction

Because of high neutron production, high melting point, and high thermal conductivity, tungsten and its alloy are the most promising candidates for spallation neutron source target such as CSNS [1,2], ISIS and KENS [3]. It also is the primary candidate for the plasma-facing material (PEM) of fusion reactors due to its low tritium retention and the reasons mentioned above [4,5]. These spallation tungsten targets are usually bombarded by protons whose energies range from 800 MeV to 1600 MeV. Under such high energies, the protons and spallation neutrons lead to the production of large amounts of helium, hydrogen and much heavier new species in forms of transmutation products. The accumulation of hydrogen and helium can lead to modification of the material's mechanical and physical properties. Hydrogen and helium build-up in cavities, voids and platelets can enhance bubble growth and blistering in the materials. Fortunately, in the case of hydrogen, the first SINQ target irradiation experiment, STIP-I, indicates that only a small amount of hydrogen remains in the spallation samples when the irradiation temperature is above 250 °C [6]. But for helium, the situation is not the same. The measured He concentrations were consistent with the calculated at the temperature above 250 °C. This means that helium does not diffuse out of the material at the temperature and helium effects should be an important issue than hydrogen effect. Recent experiments led to the conclusion that helium caused a larger increase in yield stress than that due to displacement damage and any irradiation-induced precipitation hardening. An increase in the ductile-brittle transition temperature (DBTT) had been found experimentally due to helium and there is linear relationship between ΔDBTT and helium concentration for steel irradiated over the range 2.5 ~ 18.4 dpa and 85 ~ 1530 appm helium [7,8].

Owing to the highly important role of helium in irradiated metals, especially for fusion materials, there are extensive works on helium production and much is still on the study of the behavior of helium migration, diffusion, trapping, dissolution as well as their relation with the effects on mechanical properties [9–13]. At present, no fusion reactor or intense 14 MeV neutron source exists, fusion neutron irradiation effects cannot be studied directly at the appropriate level. Special techniques such as nickel doping, boron doping, helium implantation, and spallation neutron source irradiation are used to simulate the simultaneous production of helium and displacement damage. Obviously, nickel doping, boron doping, and helium implantation experiments are not very ideal for simulating helium effects for fusion applications because they alter the materials' composition. Spallation neutron source irradiation can be used to investigate the helium and displacement damage simultaneously without introducing a large number of other atoms or implanting helium. However it will produce very small amount of spallation atoms whose atom numbers are near the spallation

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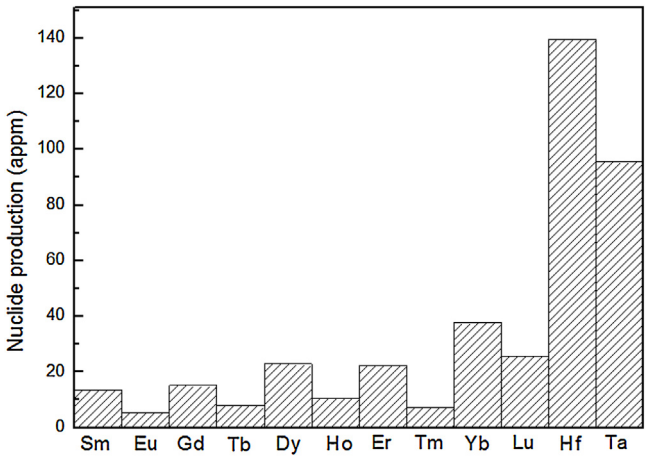

Fig. 1. The production rate of the main spallation atoms, calculated with MCNPX2.5.0 [14] and CINDER90.

material. Thus the effect of the spallation atoms on helium behavior of materials is very meaningful when we use the spallation data to investigate the material irradiation effect under fusion. This work aims at investigating the production of the heavy nuclides and the effects of these nuclides on helium behavior in tungsten.

The paper is organized as follows: Firstly, the production rate of the main spallation nuclides in tungsten target is calculated for 100 kW proton beam power and 5 years. Then the favorite positions of the spallation defects in tungsten are determined by calculating the formation energy of these defects. Finally the effects of the main spallation nuclides on the binding energy between helium and vacancy, the binding energy between two tetrahedral helium atoms, and helium migration energy barrier were discussed.

2. The production rate and formation energies of the spallation atoms in tungsten

2.1. Spallation atoms production rate in tungsten target

Although hydrogen, helium and spallation atoms are relatively rare in metals compared with vacancies and dislocations under fission or fusions, they are plentiful and very important in spallation environment. For example, tantalum can be produced by (n, p) reaction and helium can be produced by (n, α) reaction in tungsten.

The helium and hydrogen production rate had been calculated in 100 kW CSNS target [1]. Thus in this section, we just give the main spallation atoms production. This work is performed with Monte-Carlo calculation code MCNPX2.5.0 [14] and CINDER90. Fig. 1 gives the results which is based on 100 kW power, 1.6 GeV proton beam and 5 operating years. The productions of the tantalum and hafnium atoms approach or exceed 100appm; and those of the lanthanide range from 5 to 40 appm. In this manuscript we do not consider other spallation atoms because of the minimal production rate.

2.2. Defect formation energy in tungsten

The defect formation energy is the energy required to place a defect at a certain site in the tungsten. It is defined by

$$E^f_{He/H} = \mathrm{E(NW, He/H)} - \mathrm{E(N)} - \mathrm{E(He/}H_{isolated}\mathrm{)},$$
$$E^f_I = E_{total}(\mathrm{N}+1) - \frac{N+1}{N}E_{total}, \quad (1)$$
$$E^f_V = E_{total}(\mathrm{N}-1) - \frac{N-1}{N}E_{total}(\mathrm{N}).$$

Table 1
Formation energies (eV) of He, H, Vacancy and self-interstitial defects with the different configurations in tungsten.

Conf.	Octa.	Tetra.	Sub.	<111>	<110>	<100>
He	6.34	6.11	4.92			
He [10]	6.38	6.16	4.70			
H	−0.48	−0.79	3.51			
H [18]	−2.07	−2.45	0.76			
H [19]		0.95				
SIA	12.41	11.43		10.17	10.46	12.23
SIA [20]				9.68	10.00	11.67
SIA [21]				9.94	10.20	11.88
SIA [22]				10.09	10.55	12.20
Vac.	3.64	3.11 ~ 3.57 [19–23]		3.1 ~ 4.0 [24]		

The data marked [] are from the corresponding reference.

Here $E(NW+He/H)$ is the energy of the super-cell containing N tungsten atoms and one helium or hydrogen atom, and $E(N)$ is the reference energy of tungsten in a perfect body-centered cubic structure, $E(He/H_{isolated})$ is the energy of an isolated atom, $E_{total}(N+1)$, $E_{total}(N-1)$ are the total energies of the super-cell with a self-interstitial and with a vacancy, respectively.

The energy in the above expression is computed by DFT with the generalized gradient approximation and projector augmented wave potentials within the Vienna *ab initio* Simulation Package VASP [15–17]. In this work, Perdew-Burke-Ernzerhof (PBE) exchange correlation function is used. For the plane-wave set, a cut off energy of 350 eV is used [10]. Except when otherwise mentioned, all the results presented below are obtained using 128 atoms and a $3 \times 3 \times 3$ k-points grid. The super-cell contains 128 atoms are fully relaxed until the Hellmann-Feynman forces become less than 0.001 eV/Å. The equilibrium lattice parameters obtained for tungsten is 3.1701 Å, which is a little higher than the experimental data 3.1652 Å.

Table 1 gives the formation energy of He, H, and self-interstitial atom (SIA) defects within the different configurations in tungsten. The crowdion SIA is nearly degenerate with the ⟨111⟩ configuration and not represented here. Table 1 gives the calculation results from the other group works as a comparison. The predicted favored interstitial site of helium in tungsten is tetrahedral site and the energy difference between octahedral and tetrahedral is 0.22 eV. Consequently in the following calculation, the helium is always located in its tetrahedral interstitial site.

Our results agree well with most of the previous results. For an example, the vacancy formation energies in tungsten are 3.1 ~ 4.0 eV (experimental value), 3.11 eV [18], 3.20 eV [4], 3.11 eV [21], 3.33 eV [22], 3.57 eV [22], 3.25 eV [23],and 3.64. The small differences may come from the choice for the energy cutoff, the pseudopotential, the exchange correlation energy, the relaxation mode and so on. For tetrahedral interstitial hydrogen formation energy, the formation energies in tungsten are −2.45 eV [18], 0.95 eV [19], −0.79 eV. The differences may come from the reference energy of pure tungsten and hydrogen. For the Heinola results, the reference hydrogen energy is expressed by $1/2E_{H2}$, whereE_{H2} is the energy of the hydrogen dimer in vacuum. In our calculation, the hydrogen is treated as an isolated atom, i.e. a single hydrogen atom in a large supercell. Nevertheless, the formation energy differences of octahedral and tetrahedral interstitial hydrogen atoms are 0.38 eV [18], 0.38 eV [19] and 0.31 eV; these results are in good agreement. For clarify the difference between the previous and our results, When the energy cut off is increased from 350 eV to 500 eV, and the formation energy difference of octahedral and tetrahedral interstitial hydrogen atoms is 0.38 eV; the binding energy between two nearest neighbor is −0.46 eV, and the migration energy of hydrogen is 0.23 eV, which are consistent with the results −0.45 eV [18] and 0.21 eV [19].

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