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Influence of carbon–vacancy interaction on carbon and vacancy diffusivity in tungsten

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We calculate the effective vacancy diffusion coefficient caused by the synergistic migrating effect of pure vacancy and C_nV complexes using first-principles calculations combined with statistical model. We demonstrate that at the lower temperature, the C_nV complexes can move hardly due to the larger dissolution energy, while with the increasing temperature, these C_nV complexes will gradually become mobile. When the temperature increase to $T = 1500$ K, the effective vacancy diffusion coefficient is equal to that of pure vacancy. When the temperature is further increased and higher than $T = 1500$ K, all the C_nV complexes will dissolve to become isolated vacancies and simultaneously form interstitial C atoms, suggesting that all the C_nV complexes do not exist anymore. Finally, by exploring the possible influence of C_nV complexes on diffusivity of interstitial C, we find that C_nV complexes will almost have no influence on the bulk diffusion of interstitial C through W crystal.

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1. Introduction

Because of scientific interest or technological importance, the interaction between impurity atom and metals or metal-alloys has many broad studies [1–4]. As the most frequent impurity atom, from the viewpoint of materials science, there are many properties on the carbon (C)–metal interaction. Above C solubility limit, the carbides can be easily formed, which are useful to improve the strength and the hardness of metals such as in metals. Below the solubility limit, even a very little amount of C impurity atoms in the interstitial site can change the thermal and mechanical characteristics significantly [5,6] due to the strong interaction between C and metal.

At present, one striking example is that in the future magnetic confinement fusion reactors in ITER (International Thermonuclear Experimental Reactor) project [7], the first wall including the divertor and plasma facing materials must withstand irradiation from low energy (0–100 eV) and high-flux (>10^{24}/m^2 s) plasma of hydrogen isotopes and helium as well as neutrons with the high energy of 14.2 MeV and high heat flux from several MW/m^2 to several hundred MW/m^2 [8–11]. This requires the first wall retains the structure integrity even at the high temperature of 1200 K [12]. Consequently, the properties and choices of the first wall have an important influence on the success of the future magnetic confinement fusion reactors.

High-Z metal tungsten (W) and molybdenum (Mo) with refractory character are considered as the most promising first walls because of their low sputtering erosion and good thermal properties such as high thermal conductivity and high melting temperature, and it has been studied broadly [13–21] and already successfully applied in the ASDEX-U tokamak [22]. For the initial ITER design [7], the first wall material was jointly made up of C and W. Then the W wall in the divertor chamber are exposed to high heat and C impurity fluxes which will in turn lead to large amount of C impurity retention in W material. While for the current ITER design in tokamak, the first wall is fully covered by the W material, as a result, the presence of C is considered as a sort of main impurity in metal material. Experimental studies show that the concentration of C impurity is close to atomic parts per million (appm) orders of magnitude in W [23,24]. Although, the C concentration is much lower, it might have a crucial influence on the energetics and kinetics of defects and thus can have a large effect on the properties of W material. Therefore, investigating the interaction of C with W not only greatly helps us to understand the effects of C on structure and properties of W, but also has a direct impact on the design of first wall material in a fusion reactor.

Up to now, there are many studies on the interaction of C with W [25–30] and other metals [31–37]. In the previous theoretical predictions and experimental measurements, C impurities have been found to interact strongly with vacancy-type defects [32–34] in some metals and metal-alloys such as iron (α-Fe). Earlier experiments showed that C impurity atom can be strongly trapped by a mono-vacancy in α-Fe, where positron-lifetime measurements observed asymmetric C-vacancy (C_1V) pairs at room

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temperature [33]. Recent first-principles calculations [6,32] have shown that C_nV complexes are energetically favorable and easily formed in α-Fe. Concerning the C–W binary system studies, the phase diagram has been investigated by Rudy [27] in terms of the constitution. The C–W system is a refractory and binary compound. Rudy et al. found that there are three different compounds forms, i.e., one simple hexagonal carbide WC which melts incongruently, the other hexagonal carbide W_2C, and the cubic carbide which is referred to as WC_{1-x}. Both of the latter carbides melt congruently and appear to have a slightly varying C content. As the most preferred carbide, the hexagonal WC is stable from room temperature up to 3049 K. Recently, Demetriou and co-workers have studied the C–W system using a dynamic computational model developed by the classic theory of phase evolution [28]. One can note that these studies mentioned above are considered for the C–W alloy, namely, much higher C concentration case. As to the interaction between C impurity (the lower C concentration case) and W, Schmid et al. [25] gave the dependent relation between diffusion coefficient and effective concentration for impurity C in W at the temperature range from 1000 to 1100 K. The results showed that the diffusion coefficients are close to the order of $10^{-19}/m^2$ s and strongly depend on the C concentration in W. Moreover, Such concentration dependence exhibits a sharp drop of approximately one order of magnitude when the C concentration is beyond 20%. Ueda et al. [26] gave detailed investigation on C ions into W substrates at the concentration from 0.1% to 0.8%. The results indicate that impurity C distributions at the temperatures less than 653 K were much broader, and most of injected C atoms formed carbide WC for C at the concentrations of both 0.1% and 0.8% cases.

The diffusion properties are quite important for us to understand the behavior of impurity in metal materials. On the one hand, the diffusion coefficient, as one of the most fundamental properties in a meal, will affect the retention and migration of impurity in metal materials. On the other hand, the diffusion coefficient is also an important index to determine the diffusion rate of impurity, which can help us to further understand the diffusion properties quantitatively. In intrinsic (pure) W as well as other metal, vacancy only migrate along its own diffusion path in a single way. However, if impurity C atoms are present, the C_n–vacancy (C_nV) complexes are obviously formed due to the large binding energy between C and vacancy [38]. Then, besides the pure vacancy diffusing, C_nV complexes also migrate with the change of temperature in W. Therefore there exists the synergistic diffusion behavior between pure vacancy and C_nV complexes in W. Similarly, the C_nV complexes might also have the distinct consequence for the diffusion of interstitial C through W crystal.

In view of this mentioned above, we investigate the effect of C_nV complexes on migration of interstitial C and vacancy using first-principles calculations in junction with statistical model in W. We demonstrate that the C_nV complexes can move hardly due to the larger dissolution energy at the lower temperature, while with the increasing temperature, these C_nV complexes will gradually become mobile. When the temperature is further increased and beyond a critical value, all the C_nV complexes will dissolve to become isolated vacancies and simultaneously form interstitial C atoms, suggesting that all the C_nV complexes do not exist anymore.

2. Computational method

Our first-principles calculations were performed using the Vienna Ab-initio Simulation Package (VASP) code [39,40] based on the density functional theory (DFT). We used the generalized gradient approximation of Perdew and Wang [41]. The 5*d*6*s* and 2*p*2*s* electrons were treated as valence electrons for W and C, respectively. The ionic cores were represented by the projector augmented wave potentials [42]. The plane wave energy cutoff is 350 eV, which is sufficient for the total energy and geometry of W supercells. During geometry optimization, we used the 128-atom supercell containing (4 × 4 × 4) unit cells with the lengths of 12.69 Å in [100], [010], and [001] directions, respectively. The Brillouin zone of 128-atom supercell was sampled with the Monkhorst–Pack scheme [43] using a (3 × 3 × 3) *k*-points mesh. The Methfessel–Paxton [44] smearing method was used to integrate the Brillouin zone and account for partial occupancies of the metals near the Fermi level with a smearing width of 0.1 eV, which keeps the convergence of total energy errors below 1 meV. The calculated equilibrium lattice constant is 3.17 Å for bcc W, in good agreement with the corresponding experimental value of 3.16 Å [45]. Both supercell size, atomic positions, and shape were relaxed to equilibrium, and energy minimization was converged until the forces on all the atoms are less than 10^{-3} eV Å^{-1}.

3. Results and discussion

3.1. Reviews of previous studies on the interaction between C and W

In the previous studies [38,46,47], we have given a series of studies on the interaction between impurity C and W. A single C is shown to be energetically favorable for occupying the octahedral interstitial site (O-site) in bulk W. Two C atoms can be paired up at the two neighboring O-sites along the $\langle 210\rangle$ directions with a binding energy of 0.50 eV and the equilibrium distance of ~3.57 Å. As to the trapping properties of C in W [46], impurity C atoms are easily trapped by vacancy. A single C prefers to stay at a position of ~1.31 Å off vacancy center close to an O-site. With the C atoms further added, both of them are preferred to bind with each other to form covalent-like bond despite the metallic W environment. A mono-vacancy is ultimately capable of trapping as many as 4 C atoms to form C_nV (n = 1,2,3,4) complexes. Among the C_nV complex in W, C_2V is the major one due to its largest binding energy (1.97 eV). Based on first-principles calculations combined with statistical model [47], we further predict point defect concentrations of impurity C in W and find that the concentration of vacancy in the form of C_nV complexes notably increase due to the stimulating by C, although the concentration of interstitial C is still higher than that of C_nV complexes in W.

3.2. Influence of C_nV complexes on diffusivity of vacancy

In intrinsic (pure) W, vacancy only migrate along its own diffusion path in a single way. However, the previous results have shown that C_nV complexes are obviously formed due to the large binding energy between C and vacancy when the impurity C atoms enter the W matrix. Thus, besides the pure vacancy diffusing, C_nV complexes also migrate with the change of temperature in W. We therefore infer that there exists the synergistic diffusion behavior between pure vacancy and C_nV complexes in W. In order to investigate such a possibility, we calculate the effective vacancy diffusion coefficient caused by the synergistic migrating effect of pure vacancy and C_nV complexes.

In the case of the coexistence of pure vacancy and C_nV complexes in W, the effective vacancy diffusion coefficient [34] can be expressed as

$$D_V^{eff} = D_V \frac{C_V}{C_V^T} \tag{1}$$

where D_V is the diffusion coefficient of pure vacancy calculated with a diffusion energy barrier of 1.66 eV and pre-exponential factor of

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