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The effect of titanium doping on carbon behavior in tungsten: A first-principles study

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HIGHLIGHTS

- The interaction structure, solution energies, energy barriers and mechanical properties between C and the W–Ti lattice are calculated from DFT.
- The effect of titanium doping on the carbon migration behavior is small, while the migration energy barrier is quite high, and the highest energy barrier is up to 1.60 eV.
- Titanium doping tungsten can compensate the degradation of mechanical strength induced by carbon impurities.
- The ductility of pure W metal and W–Ti alloys is improved substantially by carbon impurities from the B/G ratio and the Poisson's ratio ν. The effect of the improved ductility is more obvious in pure W than that in the W–Ti alloys.
- In addition, substitutional C atom is better than interstitial C atom in terms of enhancing the ductility of pure W.

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ABSTRACT

We investigated the structural and mechanical properties, the solution and diffusion behavior of carbon atom in the W–Ti lattice from first-principles calculations. The single C atom is energetically most favorable sitting at the octahedral interstitial site (OIS) nearest neighboring to the Ti atom in the W–Ti lattice. The minimum solution energy is about 0.874 eV. It is shown that the effect of titanium doping on the carbon migration behavior is small, while the migration energy barrier is quite high, and the highest energy barrier is up to 1.60 eV. Based on the elastic constants analysis, titanium doping tungsten can compensate the degradation of mechanical strength induced by carbon impurities. On the other hand, it is found that the ductility of pure W metal and W–Ti alloys is improved substantially by carbon impurities from the B/G ratio and the Poisson's ratio ν. The effect of the improved ductility is more obvious in pure W than that in the W–Ti alloys. In addition, substitutional C atom is better than interstitial C atom in terms of enhancing the ductility of pure W.

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1. Introduction

As we know that tungsten (W) and W alloys have attracted considerable attention in a large number of industrial applications. In particular, in the International Thermonuclear Experimental Reactor (ITER), pure W and W alloys are considered to be one of the most promising candidates for plasma facing materials (PFMs) and divertor plates due to its high melting point, high strength at high temperature, high sputtering threshold energy, good thermal conductivity and low thermal expansion coefficient [1–3]. Among various alloying strategies of W metal, W–Ti alloy is the most typical one [4,5]. To our knowledge, most experimental efforts on the binary W–Ti alloys have been devoted to understanding the effect of Ti concentration on the grain growth behaviors [6–10]. Based on researches from first-principles calculations, the ductility of bcc W can be improved through Ti alloying and the metallic bonding is strengthened upon alloying higher concentration of Ti in the bcc W [11]. In addition, W and Ti exhibit complete mutual solid solubility in the β phase at temperatures between the solidus and the criti-

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cal temperature of the miscibility gap [12]. Therefore, W–Ti alloy is one of the most promising candidate materials for PFMs.

The interaction of carbon (C) with all kinds of metals is of great scientific and technological interest [13–20]. Understanding of the interaction between C and metals has a broad range of implications in material sciences. Above the C solubility limit, the carbides can be formed, which are useful for improving the strength and the hardness of metals such as steel. Below the solubility limit, even a very small amount of C impurity atoms in the interstitial site can change the mechanical and thermal characteristics significantly [21,22] due to the strong interaction between C and metal. Under plasma irradiation at high temperatures and high flux, the properties of the surface of PFMs are possibly changed because of being easily mixed with different elements [23,24], in which C is commonly considered as one of the most frequent impurity atoms, although experimental studies have shown that the concentration of C impurity in W is very small, i.e. close to several ppm [25–27]. On the one hand, C can change the microstructure of W significantly. Many experiments [28–30] have confirmed that under high flux and heat load, C atoms form surface carbides in the W surface, and can be easily trapped by some extended defects such as vacancies to form C-vacancy complexes, leading to the degradation of the mechanical properties. On the other hand, interstitial C diffusion can also give rise to some problems such as strain ageing, erosion and embrittlement [21].

So far, however, little work has been reported on the interaction between C and W–Ti alloys in the low C concentration case, especially computational simulation work. Correspondingly, many fundamental aspects underlying the interaction of C impurities with W–Ti alloys remain not well understood. In this paper, we thus investigate the interaction structure, solution energies, energy barriers and mechanical properties between C and the W–Ti lattice using the first-principles calculations. These results will be quite helpful to understand the interaction of C with W–Ti alloys, which will provide a useful database for PFMs investigation. For the above-mentioned purpose, carbon behavior has been performed on both pure W_{54} and $W_{53}Ti_1$ lattices. In addition, in pure W lattice, we also investigated the mechanical properties of W_{53}-V, W_{53}-V-C, and $W_{53}C$ by using the first-principles calculations and comparing the calculated results with the experimental results.

2. Computational details

Calculations in the present work were done within the density-functional theory (DFT) and the plane-wave pseudopotential method, which were implemented in the Vienna *ab initio* simulation package (VASP) [31,32]. The core ion and valence electron interaction was described by the projector augmented wave method (PAW) [33]. The valence electrons included in the PAW potential for W, Ti and C atoms are W-$6s^2 5d^4$, Ti-$3d^3 4s^1$ and C-$2s^2 2p^2$, respectively. The exchange-correlation part was described with the generalized gradient approximation (GGA) by Perdew and Wang (PW91) [34]. The plane wave cut-off energy was 450 eV for all calculations. The bcc W $3 \times 3 \times 3$ supercells containing 54 atoms have been used. For the substitutional Ti case, we consider the high symmetric structure, in other words, the W atom was replaced by one Ti atom at the center of the substitutional site and denoted as $W_{53}Ti_1$. The Brillouin zones were sampled with $5 \times 5 \times 5$ k-points by the Monkhorst-Pack scheme [35]. The equilibrium lattice constant of the bcc W was first optimized to be 3.17 Å, in good agreement with other theoretical and experimental studies [36,37]. All lattice parameters and atomic positions were relaxed to equilibrium, and the energy minimization was converged until the forces on all the atoms are less than 10^{-3} eV Å^{-1}. Gaussian smearing method with a smearing width of 0.05 eV is applied in all calculations in this study.

The solution energy of C atoms in different positions in *bcc* bulk W is defined as:

$$E^s_C = E_{NW+C} - E_{NW} - \mu_C$$

where E_{NW+C} is the total energy of the W bulk containing N W atoms and one interstitial C atom, E_{NW} is the total energy of the ideal W bulk with N atoms and μ_C is the chemical potential of a C atom, which is chosen as the energy per atom in the graphite structure. Here, we directly adopted $\mu_C = -8.01$ eV from the first-principle result [38].

The solution energy of C atoms in different positions in *bcc* bulk W–Ti alloy is:

$$E^s_C = E_{(N-1)W+Ti+C} - E_{(N-1)W+Ti} - \mu_C$$

where $E_{(N-1)W+Ti+C}$ is the total energy of the W bulk containing $(N-1)$ W atoms, one Ti atom and one interstitial C atom.

Within the framework of the continuum elasticity theory [39,40], for the cubic structure, there are three independent elastic constants, i.e. C_{11}, C_{12} and C_{44}. In order to calculate these elastic constants, three sets of specific strains (δ) along different directions are applied to the cubic supercell, and the changes of the total energy are calculated as a function of the applied strains. Then, the elastic constants can be obtained through fitting the energy changes (ΔE) vs the applied strains (δ). The mechanical properties can be calculated from these single crystal elastic constants, according to the Voigt-Reuss-Hill scheme [41–44]. The bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (ν) and Cauchy pressure (C') of the cubic W–Ti alloys are calculated with C_{11}, C_{12} and C_{44} and given by the following formula:

$$B = \frac{C_{11} + 2C_{12}}{3}, G = \frac{3C_{44} + C_{11} - C_{12}}{5},$$

$$E = \frac{9BG}{3B + G}, \nu = -1 + \frac{E}{2G}, C' = \frac{C_{12} - C_{44}}{2}$$

Here we mention that the cubic symmetry will be broken if C impurity is introduced. However, and the cubic lattice is also used in our calculation to compare with the cubic W and W–Ti systems. Our consideration is based on the following reasons. Firstly, the solubility of carbon atom is very small in the W–Ti system. Thus, only one carbon atom in the $3 \times 3 \times 3$ supercell was considered, which will not change much to the lattice constant. Secondly, in real systems, if more C atoms are randomly distributed in a large supercell (with small concentration), the stress on each direction will tend to be equal and the equilibrium lattice will be cubic. Finally, with the current $3 \times 3 \times 3$ supercell, we tested the values of C_{11} and C_{22} and we found that the difference is very small and comparable to the theoretical error (difference between calculated results and experimental observations).

3. Results and discussion

3.1. Mechanical properties of bcc W and solution energy of C atom in bcc bulk W

The calculated single crystal elastic constants and mechanical property parameters of W and the solution energies of C atoms in *bcc* bulk W are listed in Tables 1–3 . For comparison purpose, we also list the data from experiments, as well as other theoretical results in the tables. Notice that the elastic constants, the mechanical parameters and the solution energies of the *bcc* W metal from our calculations are in good agreement with the experimental results and other theoretical results. This confirms that the

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