Journal of Alloys and Compounds 661 (2016) 553–556

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Letter

Effects of Zr alloying on cohesion properties of Cu/W interfaces

Keywords:
CuCrZr alloy
Solution energy
Work of separation
Interface energy
Electronic structure

A B S T R A C T

First principles calculation reveals that the substitution of Cu or W atoms by Zr in the Cu/W interface is energetically favorable with big negative solution energy, suggesting that the Zr atoms in the CuCrZr alloy have the tendency to segregate to the Cu/W interface area. Calculations also show that the Zr substitution for Cu atom has only a negligible effect on cohesion properties of Cu/W interface, while the substitution of W atom by Zr could significantly increase the interface strength and interface stability of the Cu/W interface, which seems good to the performance and lifetime of the Cu/W interface. In addition, the effects of Zr alloying on interface properties are discussed in terms of electronic structures to provide a deeper understanding, and the calculated results are in excellent agreement with experimental observations in the literature.

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1. Introduction

During the past decades, tungsten (W) has been chosen as a promising candidate for plasma facing materials (PFM) in fusion reactors and has sparked great research interests due to its excellent properties such as high melting point, low tritium inventory, high strength at elevated temperature, and low erosion rate against sputtering [1–11]. Admittedly, W components in fusion reactors should be structurally bonded with heat sinks in order to remove a huge quantity of heat during thermonuclear reaction, and the CuCrZr alloy has been widely considered as an encouraging candidate of heat sinks in the design of International Thermonuclear Experimental Reactor (ITER), thanks to its high thermal conductivity, good irradiation resistance, and high fracture toughness, etc. [12].

To be used as heat sinks, the CuCrZr alloy possesses only a very small amount of Cr (0.6–0.9 wt.%) as well as Zr (0.07–0.17 wt.%), and the cohesion between W and CuCrZr alloy could be therefore regarded as mainly Cu/W interfaces [10,12]. It should be noted that the cohesion properties between W and Cu alloys have significant effects on the performance and lifetime of PFM components [13], and that interface cohesion of several W–Cu interfaces has been investigated through theoretical methods [14]. Apparently, the Zr and Cr atoms in CuCrZr alloy would probably diffuse into the W–Cu interfaces area, and influence the cohesion between W and Cu atoms. As to the detailed effects of Zr or Cr on various properties of Cu/W interfaces, however, there is no any scientific report so far in the literature.

By choosing the element of Zr as a typical example, the present study is dedicated, by means of highly accurate first principles calculation, to systematically reveal the effects of Zr on interface strength, interface energy, and electronic structures of Cu/W interfaces. Moreover, the location and stability of Zr atom at Cu/W interfaces are also discussed and compared with each other. It will be shown that the calculated results are not only in good agreement with experimental results in the literature, but also provide a deep understanding of cohesion properties of Cu/W interfaces with the doping of Zr atom.

2. Calculation method

The present first principles calculation is based on the well–established Vienna *ab initio* simulation package (VASP) within the density functional theory [15–18]. The interaction between electrons and ions is described by the projector–augmented wave (PAW) method [19]. The exchange and correlation items are treated by generalized gradient approximation (GGA) of Perdew et al. [20] and the cutoff energies are 400 eV for plane–wave basis. For the Brillouin zone sampling, the temperature smearing method of Methfessel–Paxton [21] is used for dynamical calculation and the modified tetrahedron method of Blöchl–Jepsen–Andersen [22] is performed for static calculation.

Accordingly, (111)Cu/(110)W is selected as a typical example to find out the effects of Zr on cohesion properties of Cu/W, mainly due to the stable nature and extensively experimental studies of the (111)Cu/(110)W interface [23–28]. A surface unit cell of 3×3 (9 atoms) with the optimized lattice constant of W bulk (a = 3.18 Å) [14] is chosen for each interface model, which has four Cu layers (overlayer) and six W layers (substrate) with a vacuum distance of 18 Å. To have a vivid picture of interface structure, Fig. 1 shows the atomic configurations of (111)Cu/(110)W interface, and one Zr atom is added to substitute the W or Cu atom at the positions of (1)–(5), respectively. It should be pointed out that the interstitial positions are not considered for Zr atom due to the

http://dx.doi.org/10.1016/j.jallcom.2015.11.154
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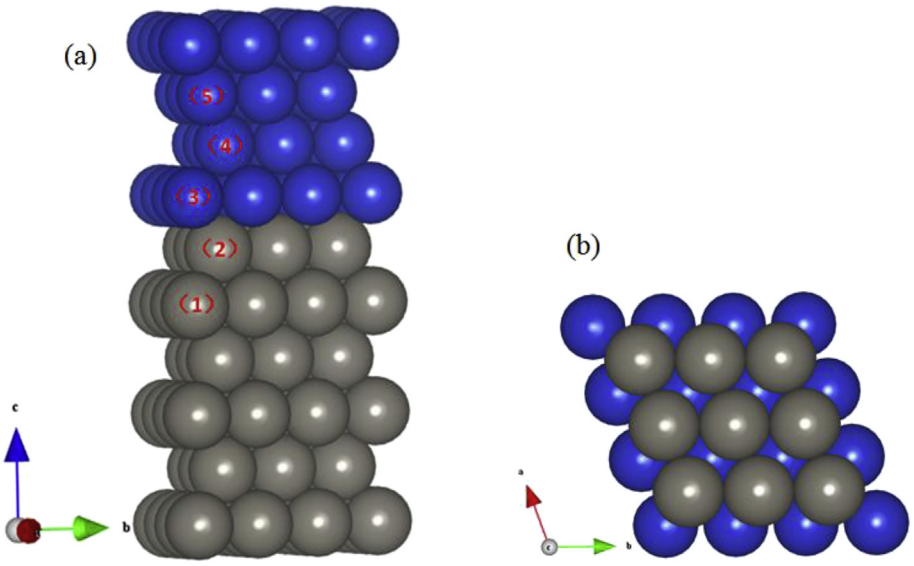

Fig. 1. Atomic configurations of (a) three dimensional model and (b) x–y projection of (111)Cu/(110)W interface. One Zr atom is added to substitute W or Cu atom at the positions of (1)–(5), respectively. The gray and blue balls represent W and Cu atoms, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

similar atomic radius of Zr as W or Cu atoms.

After the test calculation, the k–meshes of $3 \times 3 \times 1$ and $5 \times 5 \times 1$ are adopted for relaxation and static calculations, respectively. In each calculation, periodic boundary conditions are added in three directions, and the atoms in the interface are allowed to fully relax, while the bottom layer of W substrate is fixed as the reference of the relaxation of other interface atoms. The force criterion acting on each atom during relaxation is 0.025 eV/Å, and the energy criteria are 0.1 and 0.01 meV for the static and density of states calculations, respectively. The calculated results are discussed in terms of electronic structures [29–32].

3. Results and discussion

We first investigate the possible location of Zr atom at the Cu/W interface. As shown in Fig. 1, five possible positions are purposely selected for Zr atom to substitute W or Cu atoms, i.e., the positions of (1) and (2) for substitution of W, and the positions of (3), (4), and (5) for Cu. Accordingly, the symbols of Cu/W–Zr(i) (i = 1,2, 3, 4, 5) are used to represent the five interface models in the following text, table, and figures, e.g., the Cu/W–Zr(2) interface signifies that the Zr atom substitute the W atom at the position of (2) in the (111) Cu/(110)W interface.

To investigate the thermodynamic stability of Zr atom in the Cu/W interface, the solution energy (E_{sol}) of one Zr atom to substitute one W or Cu atoms in the Cu/W interface is calculated according to the following formula [33]:

$$E_{sol} = E_{Cu/W-Zr} - E_{Cu/W} + E_X - E_{Zr}, \quad (1)$$

where $E_{Cu/W\text{-}Zr}$ and $E_{Cu/W}$ are total energies of the Cu/W interface with and without Zr alloying, respectively, E_X is total energy of one substituted W or Cu atom in BCC W or FCC Cu bulk, and E_{Zr} is energy per atom of HCP Zr bulk. It should be pointed out that a negative solution energy corresponds to an exothermic reaction, and that the lower solution energy, the more stable substitution.

Consequently, the solution energies of Zr alloying in the five positions of the Cu/W interface are calculated, and the results are listed in Table 1. Several characteristics could be observed from this table. Firstly, the Cu/W–Zr(3) interface has the lowest solution energy of −1.660 eV among the five interface models. Such a big negative solution energy suggests that the Zr atom to substitute the Cu atom at the interface layer is energetically more favorable than other substitution positions.

Secondly, the solution energy of Zr atom in the Cu/W–Zr(2) interface is a negative value of −1.162 eV, implying that the Zr atom is also thermodynamically stable to substitute the W atom in the interface layer of Cu/W interface. Considering that the Zr atom is originally located at the Cu lattice of the CuCrZr alloy, the above big negative solution energy suggests that the Zr atom would probably diffuse across the Cu/W interface and energetically enter the W lattice. It should be pointed out that the negative solution energies of Zr in Cu/W interfaces revealed from the present study are in excellent agreement with the dissolution of Zr atoms in both Cu and W lattices of the Cu/W interface from experimental observations [34].

Thirdly, the four interfaces of Cu/W–Zr(2), Cu/W–Zr(3), Cu/W–Zr(4), and Cu/W–Zr(5) possess the very low solution energy of less than −1.1 eV. From the point view of thermodynamics, the above feature indicates that the Zr atom has the tendency to segregate to the Cu/W interface area. Such a kind of Zr segregation would probably influence the cohesion properties of Cu/W interfaces, which will be discussed in the following paragraphs.

It is of interest to discuss about the fundamental reason why the substitution of Zr in the Cu/W interface is thermodynamically stable with negative solution energy. When one Cu (or W) atom in the interface is replaced by the Zr atom, several Cu–W bonds in the interface have been changed to the W–Zr (or Cu–Zr) bonds. According to the well-known thermodynamic model of Miedema [35], the heats of formation of binary Cu–W, W–Zr, and Cu–Zr systems are +33, −14, and −34 kJ/mol, respectively. Note that the W–Zr and Cu–Zr bonds are energetically more favorable than the Cu–W bonds, it is the W–Zr or Cu–Zr bonds substituting the W–Cu bonds, which should fundamentally bring about the negative solution energy of Zr in the Cu/W interfaces.

We now turn to investigate the effects of Zr alloying on the

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