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Molecular dynamics simulations of the characteristics of Mo/Ti interfaces

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ABSTRACT

The study of the diffusion bonding of Mo-Ti interface is of very importance to joint the composite structures. In the present work, new analytical interatomic potentials for Mo, Ti and Mo-Ti alloy have been developed. Based on those potentials, the diffusion bonding of Mo-Ti interface has been investigated, in which the temperature effect and orientation dependence are studied detailedly by using molecular dynamics (MD) simulations. The results indicated that the asymmetrical diffusion phenomenon exists in Mo-Ti interface, and temperature plays a crucial role during the diffusion. Three interfacial orientations of the Mo substrates have been discussed, and the interfaces are characterized by the fine-scale profiles and concentration distribution along the Z axis. It is found that the interface diffusion is obviously anisotropic, and (1 1 1) plane is more beneficial to atomic diffusion than the (1 0 0) and (1 1 0) planes.

1. Introduction

Mo and Mo-based alloys have been widely used in electrical and electronic equipment manufacturing, metal materials processing industry, aerospace and defense industry applications due to their thermal conductivity, electrical conductivity and high temperature strength [1]. The applications of Mo and Mo-based alloys in the above fields mainly adopt the methods of metal processing and welding [2–4]. Diffusion welding [5] has inherent advantages over conventional welding, such as low welding temperature, wide range of materials, high welding strength and small welding deformation. The key to the realization of Mo-Ti composite structure is the welding of Mo-Ti joints. He et al. [6] used Ti foil as an interlayer to realize the properties of Mo-Mo diffusion bonding in the conditions of bonding temperature (1000 °C), axial pressure (10 MPa) and holding time (60 min). Because of the atomic interdiffusion between Ti foil and Mo substrates, Mo/Ti solid solution was usually generated at the interface region. Vacuum diffusion bonding of Mo substrates with Ti foil as an interlayer could obtain solid Mo-Ti-Mo joints, with the interface bonding rate reaching to 100%. Sun et al. [7] adopted Ti as the middle layer material of Mo-Al foil, and found that the diffusion welding rate reached 100%. Wu et al. [8] used Ni or Ti foil as the middle layer material to connect Mo and graphite by diffusion method, and the results indicated that the shear strength of the joint exceeded the strength of the graphite itself. Laik et al. [9] studied the mutual diffusion between Ti and Ti/Zr/Mo (TZM) alloys in the temperature range of 1273–1373 K. The microstructure of the TZM/Ti interfaces exhibited good contact for all the samples at above 1273 K. Obviously, Ti has a strong ability of diffusion, and it is also one of the most effective active elements in active brazing.

So far, extensive experiments about the Mo-Ti interface diffusion bonding have been carried out [6,9,10]. The effects of temperature on the microstructures and the morphology of interfacial diffusion were researched by using X-ray diffraction and scanning electron microscopy [6]. By means of the backscattered scanning electron technique [9,10], the annealing of the different intermediate layer materials at the corresponding temperature was studied. However, the diffusion mechanism of Mo/Ti on the interface has not been clear up to now and needs to be explored. As is known to all, MD simulations provide a useful tool for a detailed understanding of the underlying mechanisms at atomistic scales [11,12]. However, the reliability of the MD simulations of Mo-Ti interface is mainly dependent on the accuracy of the interaction potentials between Mo and Ti. Several potentials have been developed for the pure Mo, such as the embedded-atom method (EAM) potentials obtained by Derlet et al. [13] and Starikov et al. [14], the Tersoff–Brenner potential (TBP) of Sun et al. [15] and the modified embedded-atom method (MEAM) potential developed by Park et al. [16]. Similarly, there were many potentials describing the

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physical property of the pure Ti, such as the EAM potentials constructed by Oh and Johnson [17,18], the analytic modified embedded-atom method (AMEAM) potential of Hu et al. [19] and the MEAM potentials obtained by Kim et al. [20] and Ko et al. [21]. As far as we know, no Mo-Ti alloy potential has existed up to data for MD simulations.

To overcome these issues, the potentials for Mo and Ti elements were firstly developed in the present work, and the Mo-Ti alloy potential was subsequently addressed. The Mo-Ti potentials were validated by comparing with some available experimental data and density functional theory (DFT) calculations. Then the characteristics of Mo/Ti interfaces were studied with MD simulations.

2. Interatomic potentials and simulation methodology

2.1. Construction of the Mo-Ti interatomic potentials

For Mo, Ti and Mo-Ti alloy potentials, the modified analytic embedded atom model (MAEAM) developed in our group was adopted. In the MAEAM, the total energy (E_{tot}) is expressed as [22–25]:

$$E_{tot(Mo)} = \frac{1}{2}\sum_{j(\neq i)}\phi_{ij}(r_{ij}) + \sum_i F_i(\rho_i) + \sum_i M_i(P_i) \tag{1}$$

$$E_{tot(Ti)} = \frac{1}{2}\sum_{j(\neq i)}\phi_{ij}(r_{ij}) + \sum_i F_i(\rho_i) + \sum_i M_i(P_i) + \sum_i H_i(Q_i) \tag{2}$$

where $F(\rho_i)$ is the embedding energy with the electron density ρ_i induced at site i by all other atoms in the system. r_{ij} and $\phi(r_{ij})$ are the distance and pair-potential between atom i and atom j, respectively. Some parameters should be introduced into the potentials to correctly describe the symmetry relations for the elasticity tensor (or the Cauchy relations) [19,26] for specific crystal. Moreover, the number of those parameters should be the same as the Cauchy relations, which are related to crystalline symmetry. There is one parameter for cubic crystal, two for tetragonal, three for orthorhombic, four for monoclinic and six for triclinic. In the present model, for Ti, the hexagonal close packed (hcp) structure has two Cauchy relations, and therefore there are correspondingly two modification terms $M_{Ti}(P_i)$ and $H_{Ti}(Q_i)$ [25]. For Mo, the body-centered cubic (bcc) structure has only one modification term $M_{Mo}(P_i)$. The arguments (P_i and Q_i) of the modification terms in the present MAEAM potentials are the sum of higher orders of electron density, which is used to correct the discrepancy of the linear superposition of spherically averaged atomic electron density in original EAM potentials. The specific expressions for above functions are empirically taken as follows:

$$\phi_{Mo}(r_{ij}) = \begin{cases} k_1 + k_2\left(\frac{r_1}{r_{ij}}\right)^2 + k_3\left(\frac{r_1}{r_{ij}}\right)^4 + k_4\left(\frac{r_1}{r_{ij}}\right)^6, & r < r_e \\ k_5 + k_6\left(\frac{r_1}{r_{ij}}\right)^2 + k_7\left(\frac{r_1}{r_{ij}}\right)^4 + k_8\left(\frac{r_1}{r_{ij}}\right)^6 + k_9\left(\frac{r_1}{r_{ij}}\right)^9, & r_e \leqslant r \leqslant r_c \end{cases} \tag{3}$$

$$\phi_{Ti}(r_{ij}) = \begin{cases} k_1 + k_2\left(\frac{r_1}{r_{ij}}\right) + k_3\left(\frac{r_1}{r_{ij}}\right)^{-1} + k_4\left(\frac{r_1}{r_{ij}}\right)^{-2}, & r < r_e \\ k_5 + k_6\left(\frac{r_1}{r_{ij}}\right)^{\frac{1}{2}} + k_7\left(\frac{r_1}{r_{ij}}\right) + k_8\left(\frac{r_1}{r_{ij}}\right)^{-\frac{1}{2}} + k_9\left(\frac{r_1}{r_{ij}}\right)^{-1} & \\ \quad + k_{10}\left(\frac{r_1}{r_{ij}}\right)^{-2} + k_{11}\left(\frac{r_1}{r_{ij}}\right)^{-3}, & r_e \leqslant r \leqslant r_c \end{cases} \tag{4}$$

$$F(\rho_i) = -F_0\left[1 - n\ln\left(\frac{\rho_i}{\rho_e}\right)\right]\left(\frac{\rho_i}{\rho_e}\right)^n \tag{5}$$

$$M_{Mo}(P_i) = \alpha\left[1 - \cos\left(10\pi\frac{p_i - p_e}{p_e}\right)\right] \tag{6}$$

$$M_{Ti}(P_i) = \alpha_1\left[1 - \cos\left(20\pi\frac{p_i - p_e}{p_e}\right)\right] \tag{7}$$

$$H_{Ti}(Q_i) = \alpha_2\left[1 - \cos\left(15\pi\frac{q_i - q_e}{q_e}\right)\right] \tag{8}$$

The expressions for ρ_i, P_i and Q_i are as follows:

$$\rho_i = \sum_{j\neq i} f_e\left(\frac{r_1}{r_{ij}}\right)^{\beta}\left(\frac{r_{ce} - r_{ij}}{r_{ce} - r_1}\right)^2 \tag{9}$$

$$P_i = \sum_{j\neq i} g_e\left(\frac{r_1}{r_{ij}}\right)^{\gamma_1}\left(\frac{r_{ce} - r_{ij}}{r_{ce} - r_1}\right)^2 \tag{10}$$

$$Q_i = \sum_{j\neq i} h_e\left(\frac{r_1}{r_{ij}}\right)^{\gamma_2}\left(\frac{r_{ce} - r_{ij}}{r_{ce} - r_1}\right)^2 \tag{11}$$

where r_c and r_{ce} are the cut-off distances of pair potential and electronic density, respectively. For Mo:

$$r_c = r_4 + 0.75(r_5 - r_4) \tag{12}$$

$$r_{ce} = r_4 + 0.5(r_5 - r_4). \tag{13}$$

For Ti:

$$r_c = r_7 + 0.75(r_8 - r_7), \tag{14}$$

$$r_{ce} = r_7 + 0.75(r_8 - r_7). \tag{15}$$

The cross-potential for Mo-Ti alloy takes a combination of Mo and Ti potentials, the same as used in our previous paper [27]:

$$\phi_{MoTi}(r_{ij}) = \frac{1}{2}\mu\left[\phi_{Mo}\left(r_{ij}\frac{r^a}{r^c}\right) + \phi_{Ti}\left(r_{ij}\frac{r^b}{r^c}\right)\right] \tag{16}$$

$$r^c = \frac{1}{2}\left(r_1^a + r_1^b\right) \tag{17}$$

where $\phi_{Mo}\left(r_{ij}\frac{r^a}{r^c}\right)$ and $\phi_{Ti}\left(r_{ij}\frac{r^b}{r^c}\right)$ are the pair potentials for pure Mo and pure Ti, respectively. In the above formulas, r_i denotes the ith near-neighbor distance, $r_1{}^a$ and $r_1{}^b$ represent the nearest-neighbor distance for elements a and b, respectively. The model parameters are obtained by fitting the properties of Mo and Ti elements and Mo-Ti alloys, such as the lattice constant (a and c), elastic constants (C_{ij}), vacancy formation energy (E_f^v), cohesive energy (E_c). The potential parameters of Mo-Ti alloy are obtained by fitting the formation enthalpy of substitutional solid solution (ΔH) in whole composition range calculated from Miedema's theory [28]. It should be noted that, although it was developed in 1980s, the Miedema's theory has still been used recently to predict the mixing properties of various binary and, especially, multi-component alloys [29–33]. The optimized parameters of Mo-Ti binary alloy potential are displayed in Table 1.

2.2. Simulation details

The initial configurations of Mo-Ti interface sample consisted of two separate parts, the single crystal Ti (top) and the single crystal Mo (bottom). As illustrated in Fig. 1. The bottom part has three different crystallographic orientations for bcc Mo, namely (1 0 0), (1 1 0) and (1 1 1) planes, respectively. For the (1 0 0) interface model, a cubic sample of Mo block containing 31,200 atoms with the size of $30a \times 26a \times 20a$ (here a = 3.1443 Å is the lattice con-