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Molecular dynamics studies of body-centered cubic tungsten during melting under pressure

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ABSTRACT

A pressure-dependent embedded-atom-method (PDEAM) potential for the body-centered cubic (bcc) tungsten (W) is introduced in the pressure range of 0–400 GPa, which makes the P-V/V_0 curve of bcc W in highly consistent with the experimental data. It is found that all the pressure-dependent parameters for repulsive core-core interaction term (c_0, c_1, c_2, c_3, c_4 and c) increase first and become constants later, while the pressure-dependent parameters for n-body term (A and d) decrease first before they tend to constants. The reliability of our PDEAM potential is confirmed by studying the lattice constant, elastic constants, cohesive energy, vacancy formation energy, structural stabilities, zero pressure melting point, and the equation of states of the bcc W. With the PDEAM potential, we determined the melting curves, self-diffusion coefficients of liquid W along the melting curve, and entropies of fusion of the bcc W over a wide pressure range. Moreover, we obtained the structural properties of W including the variations of radial distribution functions $g(r)$ during melting and with increasing pressure.

1. Introduction

Transition metals like tungsten (W), molybdenum (Mo) and iron (Fe) are widely used in the syntheses of alloys with high-strength and high temperature resistance. These alloys have attracted vast attentions due to their special use in fields of rocket, guided missile, satellite, airplane, and so on [1–7]. Therefore, getting a better knowledge of the equation of states (EOS) (``pressure-density-temperature" relations) of these metals is the basis of practical applications. Melting curve, however, is an important component of the EOS. Here, we pay our attention to an important body-centered cubic (bcc) transition metal, W, due to that it has very high melting point (about 3680–3695 K [8–10]) and remains in a stable bcc structure up to extremely high pressures [11,12]. So, W is a good candidate to further explore how metals melt under pressures.

Recently, we have investigated the melting curves and entropy of fusion of the bcc W [13] using the molecular dynamics (MD) simulations with a set of constant (pressure-independent) embedded-atom-method (EAM) potential parameters, i.e. the extended Finnis–Sinclair (EFS) potential parameters introduced by Dai et al. [14]. We have simulated the melting properties of the bcc W with two methods (i.e. the hysteresis (one-phase) approach [15] and the solid-liquid coexistence (two-phase) approach [16]) using the DL_POLY program [17]. Compared with the available experimental data (3680–3695 K) [8–10], the obtained zero pressure melting point 3925 ± 25 K seems to be better than that from *ab initio* MD simulations (3465 K) [18] and those from other MD theoretical

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simulations [18,19] with the potentials of the embedded-atom-method (EAM) (4637 K) [20], the Finnis–Sinclair (FS) (4125.6 ± 8.0 K) [21] and the modified EAM (MEAM) (4389.0 ± 9.1 K) [22]. However, the obtained *P-V* relationships have obvious discrepancies from the experimental *P-V* data [23,24], which suggested that the constant EAM potential parameters can not well describe the EOS and melting processes of the bcc W.

Over the last several decades, broad varieties of empirical and semi-empirical potentials have been introduced and applied [14,20–22,26–29]. They have reproduced successfully the experimental data of crystals around the equilibrium structures, such as lattice parameters, elastic constants, and so on. Unfortunately, we note that all these attempts are confined to take the potential parameters as constants, even at extreme conditions. Accurately, such treatment is really an approximate solution and leads to a common problem in a practical simulation not only in our previous calculations [13]. That is, the produced pressure-volume (*P-V*) relationships have discrepancies with the available experimental data more or less, especially under high pressure and high temperature [27–29,30–33]. Obviously, such discrepancies should be due to the absence of consideration of the thermodynamic quantities during fitting these potential parameters. Of all the thermodynamic quantities, the *P-V* relationship is of essential importance. To obtain the good potential parameters, the produced *P-V* relationship should be in highly agreement with the available experimental *P-V* curve. In other words, the potential parameters should be dependent on pressures.

In this work, we introduced a pressure-depended EAM (PDEAM) potential to investigate the melting processes of the bcc W by molecular dynamics simulations. With MD, many properties about dynamic processes of materials have been investigated successfully [34–38]. All the calculations were performed with the DL_POLY program [17]. The paper is organized as follows: In Section 2, the theoretical methods and calculation details are described. The results and discussions are presented in Section 3. Conclusions are summarized in the last Section.

2. Theoretical methods and calculation details

The particular form of the PDEAM potential is the same as that of EFS potential [14], in which the total energy of a system is given by

$$U_{tot} = \frac{1}{2}\sum_{ij} V(r_{ij}) - \sum_{i} f(\rho_i). \tag{1}$$

The first term in Eq. (1) is the conventional central pair-potential, in which $V(r)$ is expressed by

$$V(r) = \begin{cases} (r-c)^2(c_0 + c_1 r + c_2 r^2 + c_3 r^3 + c_4 r^4), & r \le c, \\ 0, & r > c, \end{cases} \tag{2}$$

The second term in Eq. (1) is the *n*-body term. The embedding function f can be expressed by

$$f(\rho) = \sqrt{\rho_i}, \tag{3}$$

where the host electronic density ρ_i can be written as the sum of the electronic density functions $\varphi(r_{ij})$ of the individual atoms i,

$$\rho_i = \sum_{j \ne i} A^2 \varphi(r_{ij}). \tag{4}$$

The electronic density function is expressed by

$$\varphi(r) = \begin{cases} (r-d)^2 + B^2(r-d)^4, & r \le d, \\ 0, & r > d, \end{cases} \tag{5}$$

Different from those in the EFS potential, however, in the PDEAM potential, c and d are pressure-dependent cut-off parameters, c_0, c_1, c_2, c_3, c_4 and A are also pressure-dependent potential parameters. For the bcc W, these pressure-dependent parameters are determined by fitting the available experimental data (including lattice constant, cohesive energies, elastic constants, and vacancy formation energies) of the bcc W at 0 GPa and 300 K and the experimental *P-V* data of the bcc W at 300 K. Here, we obtained a set of PDEAM potential parameters for the bcc W used in an isobaric ensemble as follows.

$$c_0 = \begin{cases} 48.53524 + 4.5612 \times 10^{-4} P - 1.746 \times 10^{-6} P^2, & P \le 100\ GPa \\ 48.563391, & P > 100\ GPa \end{cases} \tag{6}$$

$$c_1 = \begin{cases} -33.79114 + 1.1562 \times 10^{-4} P + 4.0 \times 10^{-8} P^2, & P \le 100\ GPa \\ -33.779179, & P > 100\ GPa \end{cases} \tag{7}$$

$$c_2 = \begin{cases} 5.85638 + 3.508 \times 10^{-5} P + 3.52 \times 10^{-7} P^2, & P \le 100\ GPa \\ 5.863411, & P > 100\ GPa \end{cases} \tag{8}$$

$$c_3 = \begin{cases} -0.00904 + 3.238 \times 10^{-5} P - 1.132 \times 10^{-7} P^2, & P \le 100\ GPa \\ -0.00693, & P > 100\ GPa \end{cases} \tag{9}$$