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Atomistic simulations for the non-equilibrium surface premelting and melting of Nb(1 1 0) plane

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ABSTRACT

In the present paper molecular dynamics (MD) simulations have been preformed to investigate the surface melting process and microscopic mechanism of Nb(1 1 0) plane in the atomic scale with a modified analytic embedded atom method (MAEAM). On the basis of the MD relaxation dependence of averaged internal energy and layer structure factor at given temperatures, the melting point of the sample has been estimated to be 2510 K. Then by the above results the Nb(1 1 0) plane melting process has been approximately divided into two stages: first the layer-by-layer premelting phase in the surface region and then a simultaneous abrupt melting transition for the inner layers. According to the variation of the averaged internal energy of the inner atomic layer, the melting latent heat has been calculated and the result is in good agreement with the experimental value. The simulated snapshots of atomic configuration for Nb(1 1 0) plane have indicated that the dynamically microscopic mechanism of melting nucleation during the melting transition.

1. Introduction

Melting, one of the well-known first-order phase transitions [1], always presents some very fantastic characteristics [2]. The theoretical and experimental aspects of how the melting transition occurs have been investigated a lot but their mechanisms are still deficiently known [2,3]. As phase transitions of a material system depend on its structural, dynamic and energetic properties, it is important to probe the melting transition on the basis of micromechanics. Structural defects, particularly those on a surface [2,4–6], play a dominant role in the meting process. Hence, the impacts of surface characteristics on the melting process are worth being further studied.

Surface melting has been theoretically studied for several decades. Till 1985 was it experimentally verified by the medium-energy ion scattering designed by Frenken et al. [3,4]. Since then the melting process on different surfaces has been extensively observed with different experimental techniques [7–10]. However, some of those experimental results could not sufficiently be theoretically accounted for. Although an appropriate framework [4,9] has been established for surface melting micromechanics, it is still insufficient to give the account.

Recently, the rapid development of computational technologies makes it possible to investigate the surface melting at the atomic level. Ab initio dynamics has been successful in the computational surface melting researches [11] and the results agree with the corresponding experiments. As well known, such quantum-mechanics-based method is only applicable to smaller systems of about several hundreds atoms. For larger systems, the semi-empirical-potential-based molecular dynamics (MD) simulations [12–17] were the substitution for the surface melting researches. Han et al. [18] have studied the melting process of two dimensional tunable-diameter colloidal crystals, where the two-step melting mechanics from the crystal to a hexatic phase and then to the liquid phase was found to be a function of the temperature-tunable volume fraction. Many other researchers [19–26] also employed MD to study the structural transitions, thermodynamic and kinetic properties of the crystal-melted interface in detail and found the influence of the surface on the melting mechanism was more prominent. Ivanov and Zhigilei [27,28] made great efforts to

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explore the kinetic evolution of melting for metallic material. Their results indicated that the melting transition was strongly affected by the local drop of the lattice temperature. Additionally, Stegilov [29,30] also discussed the temperature dependence of the melting process and the kinetic coefficient of melting. Supported by experiments and theories, these results can accurately describe several aspects of the melting process.

Unfortunately, those works on surface melting have still been controversial. For instance, at superheated temperatures ($T \geqslant 1810$ K) the kinetic coefficient of melting obtained by Stegilov [30] was significantly larger than what have been obtained in the literatures [20,22]. Moreover, it is well known that the simulation (or experiment) process of surface melting evidently depends on the selected conditions. Some results prove that the premelting and melting of metal materials can occur under the melting point [31,32], while others insist that there is a superheating phenomenon of surface melting [33]. In addition, as a refractory metal, niobium is widely processed as FeNb alloys in the steel industry, where niobium is used as alloying element for the improvement of hot strength and non-scaling properties of hot working steels. The unique combination of material properties of niobium and niobium alloys is also used in the aerospace industry, where extreme working conditions are demanded [34]. Therefore, taking niobium material as an example, we further study the inherent mechanics of surface melting in order to eliminate the controversy.

2. Theory and methodology

The embedded atom method (EAM) [35,36] provides a suitable framework to study the metallic configuration and properties at the atomistic scale. Modified in analytical forms for different purposes, MAEAM has been successfully applied to investigate the structure and physical properties of metallic materials [37–39]. To depict atom–atom interactions for niobium, the total energy of the system is defined as

$$E_{tot} = \sum E_i, \tag{1}$$

$$E_i = F(\rho_i) + \frac{1}{2}\sum_{i \neq j} \phi(r_{ij}) + M(P_i), \tag{2}$$

where E_i stands for the associated energies with a single atom. The first term $F(\rho_i)$ represents the embedding energy for an atom and ρ_i is the sum of the electron densities of the near neighbor atoms around the ith atom. The term $\phi(r_{ij})$ shows the atom–atom pair potential as a function of the separated distance r_{ij} between atoms i and j. $M(P_i)$ plays as the modified term which is based on the non-spherical distribution of electron and deviation from the linear superposition of electronic density. Similar to ρ_i, P_i is the sum of the second order item of the electronic densities for the considered neighbor atoms. The physical implications and expressions for all these terms, including the atomic electron density distribution function $f(r_{ij})$, have been explicitly described in the literatures [38,39]. The corresponding MAEAM parameters of Nb atomic system are listed in Table 1.

The Nb(1 1 0) plane here has 31 atomic layers with 96 atoms per layer. The dimensions of the constructed cell in MD are $8a_0 \times 7a_0 \times 16a_0$, where the input lattice parameter a_0 is 0.3302 nm for niobium at 0 K. A two dimensional (2D) periodic boundary conditions have been used in $x[0\,0\,1]$ and $y[1\,\bar{1}\,0]$ directions. The $z[1\,1\,0]$ direction has been kept free. The x–y and x–z atomic planar configurations of Nb(1 1 0) plane are shown in Fig. 1a and b, respectively. As labeled in Fig. 1b the ordinal num-

Table 1
The model parameters of MAEAM for niobium.

F_0/eV	n	α/μeV	k_{-1}/eV	k_0/eV	k_1/eV	k_2/eV	k_3/eV	k_4/eV
4.96937	0.70	−6.8908	184.9418	−851.4054	1568.1679	−1442.3027	660.1191	−119.8974

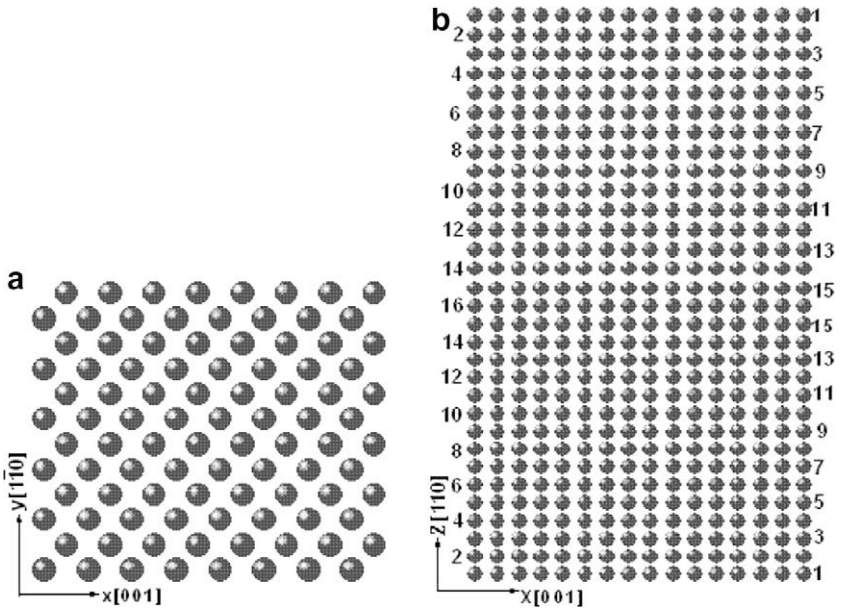

Fig. 1. (a) The planar configuration of a atomic layer for Nb(1 1 0) plane in $x[0\,0\,1]$ and $y[1\,\bar{1}\,0]$ direction. (b) The crystalline geometry of the symmetrical Nb(1 1 0) plane alone $x[0\,0\,1]$ and $z[1\,1\,0]$ direction. The outmost layer (i.e. the surface layer) has been numbered 1 in the both margins of this figure. The next layer is, then, numbered 2, and so on and so forth.