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INVESTIGATION OF THE MELTING PROCESS OF NIOBIUM USING TWO DIFFERENT POTENTIALS: A MOLECULAR DYNAMICS SIMULATION STUDY

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Abstract
This study explores the heating process of niobium (Nb) through molecular dynamics (MD) simulations employing both the embedded atom method (EAM) and tight-binding (TB) many-body potentials, with analyses conducted using structural approaches such as the pair distribution function (g(r)), volume–temperature relationship, and common neighbor analysis. Both TB and EAM potentials successfully predicted the physical properties of bcc Nb, including cohesive energy, lattice parameter, thermal expansion coefficient, and heat capacity, at and around room temperature with only minor deviations. However, during the heating process, TB-MD simulations predicted the melting point of the system significantly earlier (T_m^{TB}=800 K), whereas EAM-MD simulations (T_m^{EAM}=3100 K) provided predictions very close to the experimental results (T_m^{exp}=2750 K). For liquid Nb, the g(r) curve obtained from EAM-MD simulations shows good agreement with previously reported ab initio MD simulation results, apart from minor deviations, whereas TB-MD simulations failed to accurately describe the structural properties of liquid Nb at high temperatures. These findings are expected to contribute to future studies on Nb under different conditions

Keywords: Niobium, molecular dynamics simulation, pair distribution function, melting temperature, embedded atom method.

INTRODUCTION

It is widely recognized that the ability to rapidly, accurately, and reliably characterize various physical properties of materials such as structural, dynamic, mechanical, and thermodynamic features at the atomic scale is of critical importance [1]. The literature indicates that experimental approaches and quantum-based molecular dynamics (MD) simulations provide the most realistic, accurate, and reliable results. However, the literature also highlights that experimental methods are costly and offer limited insight at the microscale, whereas quantum-based simulations suffer from several limitations, including the treatment of relatively few atoms and slower computational performance. Consequently, researchers have increasingly turned to classical MD simulations, which enable the investigation of larger atomic systems, provide faster results, and, most importantly, entail minimal computational cost. As the number of particles in a system increases, solving the equations of motion analytically becomes increasingly challenging. In this simulation approach, atoms in the system are allowed to interact over a defined time scale, enabling complex calculations to be addressed more efficiently through numerical methods. Indeed, this method provides access to information that is difficult to obtain experimentally, representing a significant advancement in the field. Owing to these advantageous features, this method is now widely employed across diverse disciplines,

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including physics, nanotechnology, chemistry, biology, materials science, and engineering. However, the success and reliability of MD simulations critically depend on the choice of an interatomic potential that can accurately capture atomic interactions within the system and yield results consistent with experimental observations. [2, 3]. The most frequently cited interatomic potentials for metallic systems in the literature include the embedded atom method (EAM) [4], Finnis–Sinclair (FS) [5], Sutton–Chen (SC) [[6, 7], and tight-binding (TB) [8] many-body potentials.

In the present study, the evolution of the atomic structure of niobium (Nb) during the heating process has been thoroughly investigated using classical molecular dynamics (MD) simulations with EAM [4] and TB [8] potentials. Nb is a gray-metallic transition metal widely recognized as a 'superpower' in various modern engineering fields. Its excellent corrosion resistance and high melting point of 2750 K [9] make Nb a refractory metal well-suited for applications under extreme conditions [10]. Moreover, due to its exceptional corrosion resistance, Nb is used both as a base material for superconducting magnets, which exhibit zero electrical resistance, and as a refractory metal that significantly enhances the strength of steel in structural applications [11, 12].

EXPOSITION

According to the EAM formalism, the total energy is expressed as the sum of the electrostatic repulsive interactions between atoms and the embedding energy terms arising from the local electronic charge density. The total energy of an N-atom system is defined by the following expression [4]:

$$E_T = \frac{1}{2}\sum_{i,j,i\neq j}^{N}\varphi_{ij}\left(r_{ij}\right)+\sum_{i}^{N}F_i\left(\rho_i\right), \qquad (1)$$

where $\varphi_{ij}(r_{ij})$ represents the pair interaction potential between atoms i and j, and F_i denotes the embedding energy associated with placing atom i at a site characterized by the electronic charge density ρ_i. This study employed the EAM potential parameter set developed by Fellinger et al [13].

The tight-binding (TB) second-moment approximation potential model is founded on the premise that many of a metal's properties can be derived from the density of its outer d-electron states. Similar to the EAM potential, the TB potential comprises two components: an attractive term and a repulsive term. Its analytical form is presented below [8, 14]:

$$E_T = -\left\{\sum_{j\neq i}\xi^2\, exp\left[-2q\left(\frac{r_{ij}}{r_0}-1\right)\right]\right\}^{1/2} + \sum_{j\neq i}A\, exp\left[-p\left(\frac{r_{ij}}{r_0}-1\right)\right], \qquad (2)$$

where r_{ij} denotes the distance between atoms i and j, and r_0 represents the nearest-neighbor distance. The parameters A, p, ζ, and q are adjustable potential parameters, typically determined by fitting relevant physical properties of the element. The TB potential parameters employed for Nb in this study are provided in Ref [15].

The heating process simulations were conducted using the open-source DL_POLY 2.0 software package [16]. The system was initially configured in a body-centered cubic (bcc) structure, which is the most stable phase of Nb. A total of 27648 Nb atoms were positioned within the simulation box, with periodic boundary conditions applied in all three spatial directions throughout the simulation. Newton's equations of motion were integrated using the velocity Verlet algorithm. During the simulations, temperature and pressure were controlled using the Berendsen thermostat and barostat, respectively. To minimize potential stress in the system, an initial heating to 300 K was performed over 3,000,000 MD steps, followed by cooling to 0 K using the same number of MD steps. Subsequently, the system was heated from 0 K to 3800 K in increments of 50 K, exceeding the melting point (T_m=2750 K [9]) of Nb, using the isothermal-isobaric (NPT) ensemble with a

time step of 2 fs. The OVITO package was utilized for visualizations [17].

Figure 1 presents a comparison of the per-atom volume as a function of temperature for simulations carried out using EAM and TB potentials. As can be seen from the figure, the two potential models predict significantly different values for the system volume, and their melting points also differ considerably. Ab initio molecular dynamics (AIMD) simulation data for the cooling process of liquid Nb, reported by Debela et al. [18], have been included in the figure to evaluate the accuracy of our results. The volume values reported for AIMD simulations lie between those obtained from TB-MD and EAM-MD simulations, but are closer to the results produced by the EAM-MD simulation. The melting temperatures (T_m) obtained from TB-MD and EAM-MD simulations deviate from the experimental value (T_m = 2750 K[9]) by approximately −70.91% and +12.73%, respectively. It has been widely observed that melting temperatures predicted by interatomic potentials used in atomic simulations deviate by approximately ±30% from experimental values [19]. This demonstrates that the EAM potential provides a much more accurate prediction of the melting behavior of bcc Nb compared to the TB potential. Additionally, two-phase melting simulations, in which solid and liquid phases coexist, yield more reliable melting temperature predictions. Using this method, Fellinger et al. [13] found the melting temperature of Nb to be 2686 K using the same EAM potential data. Kazanc and Canbay [10] determined the melting temperature to be 2850 K based on a standard heating procedure. Additionally, an unexpected anomaly in the volume curve obtained from the TB-MD simulations was observed within the temperature range of 100 K to 150 K. This phenomenon, observed in the volume curve, will be discussed in detail in the following sections (see inset).

Table 1 presents the calculated values of cohesive energy per atom (E_c(eV/atom), lattice parameter (a(Å)), melting temperature (T_m(K)), thermal expansion coefficient ($\varepsilon(K^{-1})$), and heat capacity ($C_p(J.mol^{-1}.K^{-1})$) obtained from TB-MD and EAM-MD simulations. These results are compared with experimental data and values reported in previous simulation studies.

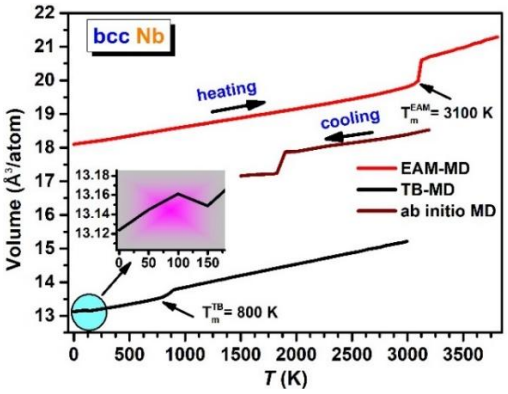

Fig. 1. *Volume curves obtained from TB-MD and EAM-MD simulations during the heating process. ab initio MD simulation results during the cooling process reported in the literature*[18].

Table 1. *Comparison of some physical properties calculated from the present study for pure Nb with experimental and other results in the literature.*

	EAM	TB	Exp.
E_c(eV/atom)	7.03	7.77	7.57[a]
a(Å)	3.31	3.00	3.30[a]
T_m(K)	3100	800	2750[a]
$\varepsilon(x10^{-6},K^{-1})$	9.29	13.83	7.10[b]
$C_p(Jmol^{-1}K^{-1})$	24.8	22.9	24.9[b]
$\rho(g/cm^3)$	8.48	11.66	8.57[b]

[a]Ref [9], [b]Ref [20].

The results indicate that, considering the differences between experimental and simulation conditions, both EAM and TB potentials can accurately predict the physical properties of bcc Nb at low temperatures, except for minor deviations. However, the results obtained with the EAM potential are closer to the experimental data compared to those of the TB potential. Typically, interatomic potential parameters are optimized to match the low-temperature physical properties of the element under study. It is important to note that successful predictions at low temperatures do not

necessarily guarantee the accuracy and reliability of the potential across a wide temperature range. Although the TB potential can produce acceptable results for bcc Nb at low temperatures, it fails to achieve the same level of success in describing the melting process.

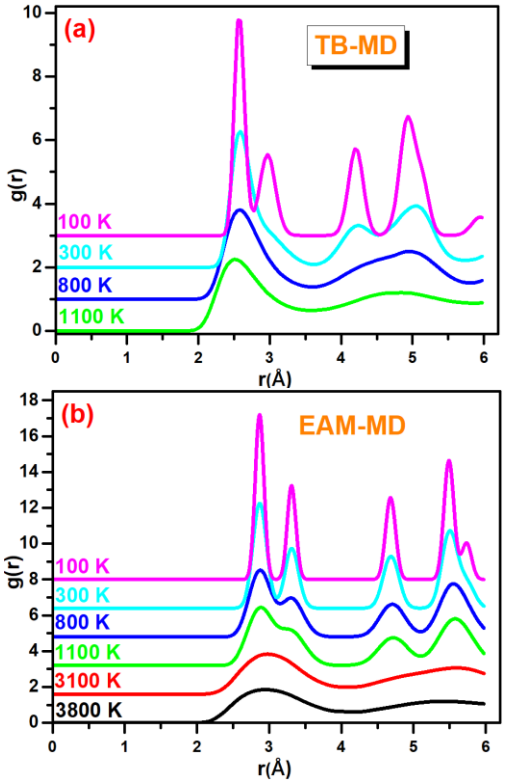

Fig. 2. *g(r) curves obtained from (a) TB-MD and (b) EAM-MD simulations at different temperatures.*

Figures 2(a) and 2(b) show the g(*r*) curves obtained at different temperatures from TB-MD and EAM-MD simulations, respectively. Figure 2(a) shows that while the g(*r*) curve obtained from TB-MD simulations at 100 K exhibits the characteristic peaks of bcc crystal structures, at 300 K it abruptly transforms into softer and more disordered peaks. Such behavior is unusual for a high-melting-point element and is attributed to the inability of the present TB potential parameter set to adequately describe the melting process of bcc Nb. In Figure 2(b), it is observed that although the g(*r*) curves obtained from EAM-MD simulations gradually soften as the temperature increases, they preserve the bcc peaks and the system exhibits stability throughout the melting process. The peaks of the g(*r*) curves generated from both potentials exhibit typical liquid-like behavior at temperatures above the melting point.

Furthermore, to evaluate the reliability of the results, we present in Figure 3 a comparison between the TB-MD and EAM-MD simulation data and the AIMD results previously reported in the literature for liquid Nb. The position and height of the first peak of the g(r) curve obtained from EAM-MD simulations show good agreement with AIMD simulation results. However, from the first minimum onward, slight shifts are observed at the positions of the other main peaks. In contrast, the g(*r*) curves obtained from TB-MD simulations exhibit larger deviations compared to both EAM-MD and AIMD simulation results. This further evidences that the current TB potential parameters fail to accurately predict the structural properties of Nb at high temperatures.

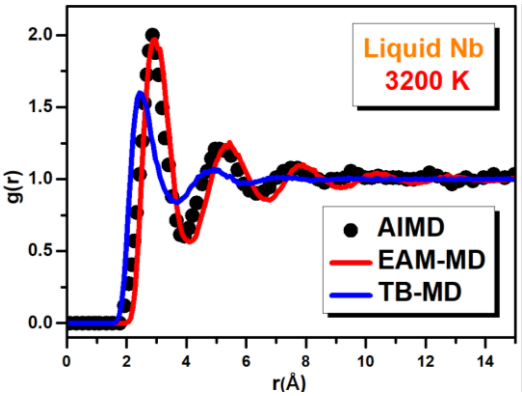

Fig. 3. *Comparison of TB-MD and EAM-MD simulation results with AIMD data for liquid Nb at 3200 K.*

To provide a more detailed insight into both simulation results, the common neighbor analysis [21] at different temperatures is presented in Figure 4(a) for TB-MD simulations and in Figure 4(b) for EAM-MD simulations. As seen in Figure 4(a), at temperatures between 0 and 100 K, the 1441 and 1661 bonded pairs have the highest fractions, indicating that the system is stable in the bcc crystal structure. However, when the temperature rises to 150

K, an unexpected sudden decrease is observed in the number of these pairs, while, conversely, there is a sharp increase in the number of 1541 and 1431 disorder bonded pairs, which are more common in liquid and amorphous structures, as well as 1421 bonded pairs representing the fcc structure. The increase in these bonded pairs causes the system to melt much earlier than expected. In EAM-MD simulations, the number of dominant 1441 and 1661 bonded pairs gradually decreases with increasing temperature, leading first to a gradual increase in the 1541 and 1431 bonded pairs, followed by a gradual rise in other pairs, and finally, the system melts around the expected melting point. All of this highlights the critical importance of the chosen potential in accurately describing the system's properties and ensuring the reliability of the results.

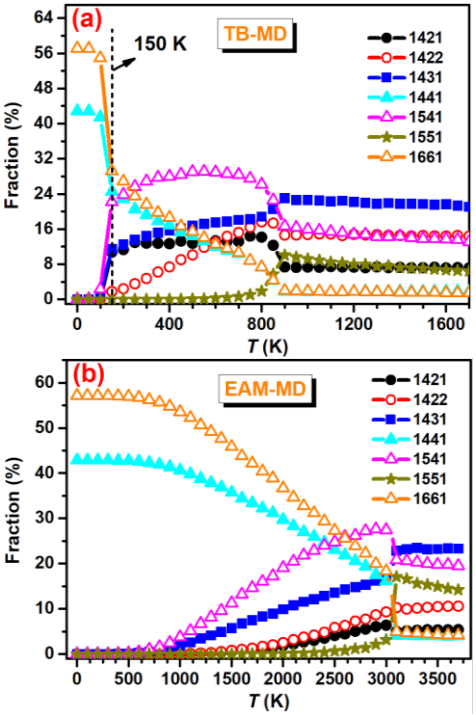

Fig. 4. *Variation of the fractions of the most dominant bonded pairs obtained from TB-MD and EAM-MD simulations as a function of temperature.*

To provide a visual perspective, the simulation boxes at different temperatures for both simulations, together with their corresponding common neighbor analysis results, are presented in Figures 5 and 6.

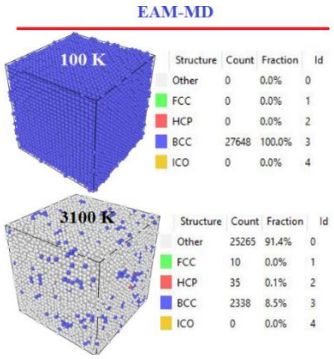

Fig. 5. *Snapshots of the simulation box and common neighbor analysis results from EAM-MD simulations at temperatures of 100 K and 3100 K.*

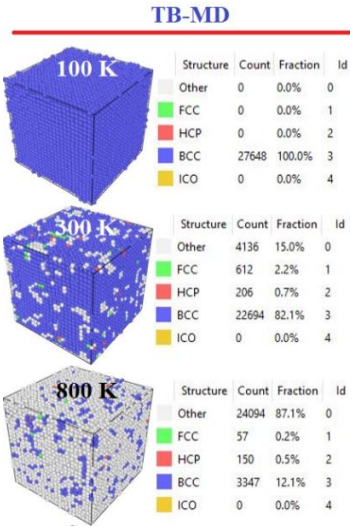

Fig. 6. *Snapshots of the simulation box and common neighbor analysis results obtained from TB-MD simulations at different temperatures (100 K, 300 K and 800 K).*

At 100 K, the atoms in the simulation boxes of both methods are clearly arranged in a crystal-like structure, and the analysis results further confirm that this corresponds to a 100% bcc crystal structure. For the TB-MD simulations at 300 K, the snapshots and analysis results show that although the number of bcc structures decreases, they still remain the most dominant type. Along with this decrease, a significant increase in fcc, hcp, and other structures is observed (see Figure 6). These findings are in agreement with the results discussed in the previous sections. For both simulations, the snapshots and analyses at the melting points indicate a

significant decrease in the number of crystal structures, accompanied by a substantial increase in the number of other structures. This is consistent with the fact that the crystal phase and the liquid phase coexist at the melting point.

CONCLUSION

The melting process of bcc Nb has been investigated using MD simulations with EAM and TB potentials. In the present study, it has been reaffirmed that the EAM potential is sufficiently capable of predicting the physical properties of Nb at both low and high temperatures. Although the existing TB potential parameter set can partly describe the physical properties of Nb at low temperatures, it fails to adequately capture the structural characteristics and the melting process of the system at higher temperatures. Therefore, a re-evaluation of the TB potential parameters for such systems is recommended.

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