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MOLECULAR DYNAMICS STUDY OF THERMAL AND STRUCTURAL PROPERTIES OF COPPER NANOWIRES DURING MELTING PROCESS

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Abstract

Nanometer-scale metallic nanowires have been extensively researched in recent years due to their diverse physical and chemical behaviors. As the wire size decreases, the proportion of surface atoms within the total number of atoms increases significantly, causing these materials to exhibit properties not observed in bulk metals. This size effect results in metallic nanowires acquiring unique mechanical, electronic, optical, catalytic, and thermodynamic properties, making them a functional group of materials for various applications in nanotechnology and materials science. In this study, the thermal and structural behaviors of copper (Cu) nanowires during the melting process were investigated using molecular dynamics (MD) simulations performed with Embedded Atom Method (EAM) potential. The results show that the nanowire diameter has a decisive effect on the melting behavior of Cu nanowires. Furthermore, a significant structural change, defined as neck formation, is observed in the central region of the nanowire as the melting temperature rises. After reaching a critical temperature, the nanowire structure loses its stability and transforms into a nanoparticle form.

Keywords: Copper, nanowire, MD simulations, size effect.

INTRODUCTION

Nanowires (NWs) have been extensively researched in recent years due to their unique mechanical and thermal properties [1]. Among the fundamental thermal characteristics of these structures, melting behavior and thermal stability are of significant importance [2]. Their high surface area relative to their volume allows NWs to be used in applications aimed at increasing reaction rates in chemical processes [3]. In this context, the thermal properties of NWs, which vary depending on their size, can directly affect the behavior of the chemical processes in which they are used. Furthermore, metallic NWs are also used in applications requiring electrical conductivity, and their small size and related thermal properties play a significant role in determining their performance in these applications [2]. Many researchers have demonstrated the size-dependent and unusual melting behavior exhibited by NWs as a result of their high surface-to-volume ratios, using MD simulations [2,4–11]. Since the proportion of surface atoms increases as the characteristic dimension decreases, the melting temperature of free-standing NWs is also expected to decrease with shrinking size. One of the fundamental reasons for this behavior is that surface atoms possess a lower coordination number. A low coordination number leads to a reduction in the cohesive energy between atoms and a consequent decline in the system's thermal stability [12,13]. Therefore, it is generally accepted that the melting process in nanowires initiates at the surface and proceeds toward the interior regions. Its high electrical conductivity and economic

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advantages have made Cu a widely preferred material for electrical interconnects in electronic systems [8,14]. With technological advancements aimed at designing electronic devices in increasingly smaller sizes, numerous studies have been conducted on the electrical and thermal properties of Cu NWs [15–17]. The results obtained have demonstrated that significant changes in electrical and thermal conduction properties can occur as characteristic dimensions decrease, and that this situation may adversely affect the reliability of electronic components due to an increased tendency for heating during operation [8]. Therefore, determining the thermal stability of Cu NWs, as well as their thermal properties, which vary depending on size reduction, is crucial for the reliability of nanoscale electronic applications. However, it is evident that the number of studies in the literature systematically addressing the size-dependent melting behavior of Cu nanowires, and specifically the changes in melting temperature, remains limited [2,6,8]. For instance, Granberg et al [8]. investigated the melting behavior of Cu NWs using MD simulations and reported that the melting temperature increases with wire diameter, the effect of the cross-sectional shape is limited, and the interatomic potential employed plays a significant role in the results. Javanbakht et al. [2] examined the melting behavior of Cu NWs using a phase-field model and demonstrated that the melting temperature decreases as the radius and length decrease. Furthermore, the obtained results were found to be consistent with existing MD simulations. In this context, the systematic investigation of the size-dependent melting behavior of Cu NWs via MD simulations is significant for understanding the thermal stability and melting mechanism of these structures at the atomic scale. Motivated by this, the thermal and structural evolution of cylindrical Cu NWs with varying diameters during the heating process has been comprehensively investigated in this study using MD simulations.

EXPOSITION

The EAM, used for modeling metallic materials at the atomic scale, enables the description of the system's energy and interatomic interactions by accounting for many-body effects. Due to this characteristic, EAM-based potentials are widely employed in MD simulations of metals. Within the framework of the EAM formalism, the total energy of a system containing N atoms is given by the following expression [18,19]:

$$E_{tot} = \sum_{i=1}^{N}\left[\frac{1}{2}\sum_{i\neq j}^{N} V(r_{ij}) + F_i(\rho_i)\right]. \qquad (1)$$

Here, the $V(r_{ij})$ term describes the pairwise interaction between atoms i and j, while the $F_i(\rho_i)$ term represents the embedding energy required to place atom i at a position with an electron density of ρ_i. ρ_i denotes the total electron density generated by neighboring atoms surrounding atom i, and r_{ij} represents the distance between atoms i and j. In this study, the EAM potential set proposed by Sheng [20] was used to model Cu–Cu atomic interactions. MD simulations of Cu NWs were performed using the DLPOLY [21] MD simulation package, which supports parallel computing. To investigate the effect of nanowire size on melting behavior, three different cylindrical Cu NWs were modeled with diameters of 2.5 nm (NW-1), 4.0 nm (NW-2), and 6.0 nm (NW-3), containing 6525, 16785, and 39105 atoms, respectively. For all NWs, the length was kept constant at 16.25 nm, and the wire axis was defined along the z-direction. The cylindrical nanowire model used in the MD simulations was obtained by cutting a cylindrical wire from a face-centered cubic (fcc) crystal. To preserve surface effects in Cu NWs, periodic boundary conditions were applied only in the [001] z-direction. Initial structures formed from an ideal fcc lattice were relaxed by heating to 300 K and then cooling to 100 K at a rate of 0.05 K/ps. Thermal behavior was investigated under the NVT ensemble; heating was performed in 100 K temperature steps from 100 K to 1800 K. This step was reduced to 10 K to obtain more precise

results in the melting region. At each temperature, the system was simulated for a total of 100,000 MD steps, including 50,000 MD steps of stabilization followed by 50,000 MD steps of generation. Atomic motions were calculated using the Leapfrog Verlet algorithm with a time step of 1 fs; temperature and pressure control were provided by a Nose-Hoover thermostat [22] and a Berendsen barostat [23], respectively.

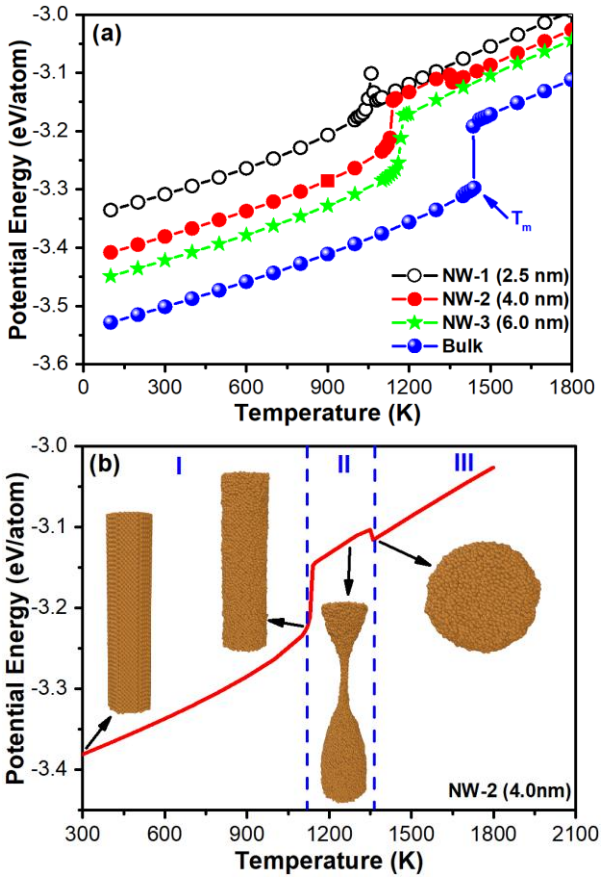


Fig. 1. *(a) Temperature dependence of the potential energy of NW-1, NW-2, NW-3, and the bulk system; (b) temperature dependence of the potential energy of NW-2.*

Examining the energy change exhibited by the system during the thermal process is one of the commonly used methods for determining the temperature at which a first-order phase transition occurs. The temperature-dependent potential energy changes of Cu NWs are presented in Figure 1a in comparison with bulk Cu. The potential energy values of all NWs are higher than that of bulk Cu and increase with increasing wire diameter. While the potential energy increases approximately linearly with temperature in the solid-phase region, a sudden change is observed upon reaching the critical temperature. This behavior characterizes the transition from the crystalline structure to the liquid phase and, consequently, determines the melting temperature (T_m). Following melting, the sudden drop in energy observed at 1070 K for NW-1 and 1360 K for NW-2 is succeeded by a linear increase, whereas for NW-3, the energy continues to rise linearly. To explain the sudden decrease in the potential energy of the NWs observed at temperatures above the melting point, the potential energy curve of NW-2 in Figure 1b is divided into three regions based on its characteristic behavior: the 300–1170 K range is defined as Region I, the 1170–1360 K range as Region II, and the 1360–1800 K range as Region III. Snapshots of the wire in each region are presented in the inset of the figure. In Region I, the potential energy increases approximately linearly with temperature, and this behavior continues up to 1170 K. The sudden change observed in the energy curve at this temperature corresponds to the T_m, where the solid and liquid phases of the nanowire coexist (T_m = 1170 K for NW-2). While the system is in the solid phase in Region I, it transitions to the liquid phase in Region II following melting. In Region II, the potential energy also increases approximately linearly with temperature up to 1360 K. However, a distinct drop in the energy curve is observed at 1360 K. The snapshots provided in the figure show that, at this temperature, the nanowire transforms into a nanoparticle (NP) form, which is a more stable structure. Consequently, this structural transformation constitutes the primary cause of the sudden decrease in potential energy. In Region III, the potential energy of the NP in the liquid phase exhibits an approximately linear increase with temperature. The T_m and heat of fusion (ΔH_m) values obtained from MD simulations for the NWs and the bulk system are presented in Table 1. ΔH_m was calculated

from the energy difference between the solid and liquid phases on the total energy curve. The T_m and ΔH_m values for all NWs are lower than those of the bulk system, and both parameters are observed to increase with increasing wire diameter. The T_m and ΔH_m values determined by MD simulations for the bulk system appear to be in good agreement with experimentally reported values.

Table 1. *T_m and ΔH_m for Cu NWs and bulk.*

Symbol	T_m(K)	ΔH_m (kJ/mol)
NW-1 (2.5 nm)	1050	9.15
NW-2 (4.0 nm)	1130	10.71
NW-3 (6.0 nm)	1170	12.27
Bulk	1440 (1358)[a]	13.90 (13.20)[b]

[a]Ref [24], [b]Ref [25]

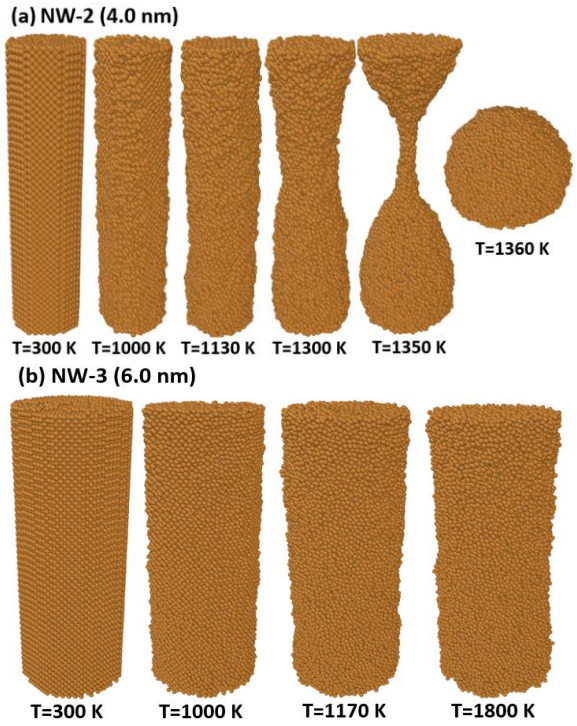


Fig. 2. *Snapshots of Cu (a) NW-2 and (b) NW-3 at different temperatures.*

Figure 2 shows snapshots of atomic coordinates obtained from MD simulations performed at different temperatures for NW-2 and NW-3. While both nanowires maintain their fcc crystal structure at 300 K, at 1000 K, it is observed that the atoms, especially in the surface regions of the wires, begin to deviate from the regular crystal structure. This structural disorder observed in the surface atoms indicates the onset of pre-melting behavior in NWs. Above the melting temperature, a distinct neck formation occurs in the central region of NW-2, and this neck becomes increasingly prominent with increasing temperature. At 1360 K, the nanowire breaks off from the neck region, splitting into two separate pieces and transforming into a nanoparticle-like structure. This indicates that a significant structural transformation occurs in NW-2 due to the increase in temperature. In contrast, NW-3 largely maintains its general wire geometry above the melting temperature and does not exhibit a significant morphological change despite the increase in temperature.

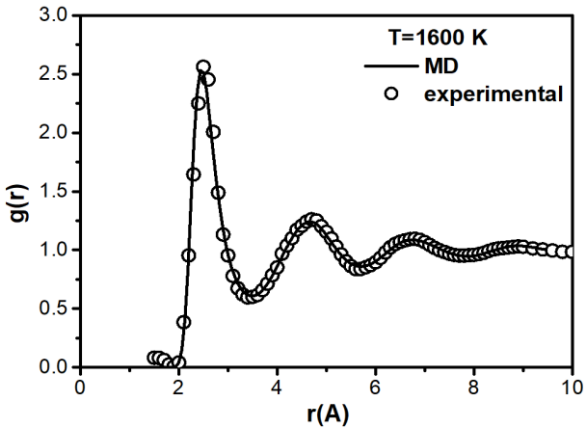


Fig. 3. *The PDFs of liquid bulk Cu.*

Atomic structural changes in bulk systems and NWs during heating processes were evaluated via the pair distribution function (PDF) which characterizes the temperature-dependent distribution of distances between atoms. The PDF, $g(r)$, is expressed as follows [26]:

$$g(r) = \frac{V}{N^2}\langle(\sum_{i=1}^{N} n_i(r))/4\pi r^2 \Delta r\rangle, \qquad (2)$$

where, V and N parameters represent the unit cell volume and the total number of atoms in the simulation system, respectively. The PDF obtained from the MD simulation at 1600 K for bulk Cu was compared with the experimentally reported result in Figure 3. The PDF obtained from MD simulations shows a very good agreement with

experimental results [27]. This agreement indicates that the EAM potential, used to characterize interatomic interactions in MD simulations, reliably represents Cu–Cu interactions. Figure 4 presents the PDF curves calculated for the Cu NW-2 system at different temperatures. The PDF obtained at 300 K reveals a distinct peak structure characteristic of the ideal fcc crystal-structure. While the amplitude of the peaks decreases with increasing temperature, a significant increase in peak width is observed. At 1130 K, the PDF curve shows that the system has neither a completely crystalline nor a completely liquid structure. Since solid and liquid phases can coexist around the melting temperature, 1130 K, where these two structural characteristics are observed together, is considered the melting point for Cu NW-2. This finding from the PDF analysis supports the T_m value determined using thermal properties. In contrast, at 1140 K, above the melting temperature, the PDF curve exhibits a characteristic distribution specific to the liquid phase.

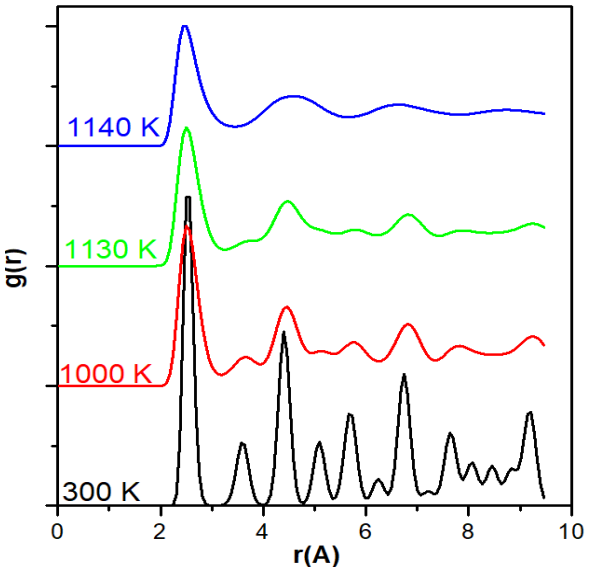


Fig. 4. *PDFs of Cu NW-2 at different temperatures.*

To characterize the atomic mobility and dynamic structural change of NW during the melting process, the self-diffusion coefficient (D) was calculated. D, which quantitatively expresses the time-dependent displacement behavior of atoms, is an important parameter in evaluating the dynamic properties of atomic mobility and thus phase transformation in the system. D was calculated as follows using the Einstein relation related to mean squared displacement (MSD) [28]:

$$D = \lim_{t\to\infty} \frac{MSD}{6t} \quad (3)$$

$$MSD = \frac{1}{N}\sum_{i=1}^{N} |r_i(t + t_o) - r_i(t_o)|^2. \quad (4)$$

Here, $r_i(t_o)$ represents the position vector of the i-th atom at the initial moment, while $r_i(t)$ represents the position vector of the atom at time t.

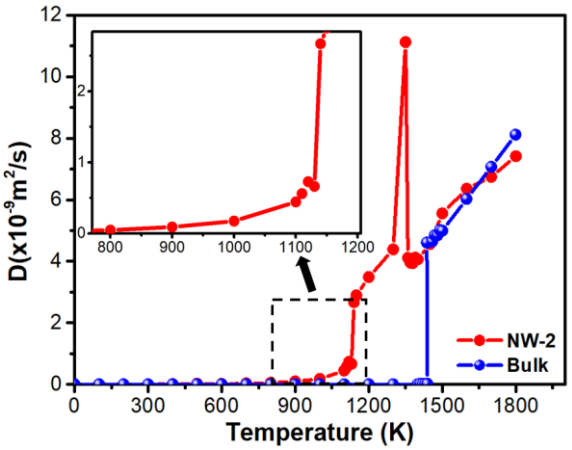


Fig. 5. *Temperature dependent variation of the self-diffusion coefficient for Cu NW-2 and the bulk system.*

Figure 5 compares the temperature-dependent variation of the self-diffusion coefficients obtained from MD simulations for Cu NW-2 and the bulk system. In NW-2, the self-diffusion coefficient remains close to zero until approximately 900 K, but begins to increase above this temperature (see inset of the figure). This is an indication that NW undergoes pre-melting. The abrupt increase observed at the melting point indicates a significant increase in atomic mobility and disruption of the crystal structure. At the transformation temperature of NW to NP (1360 K), an anomalous change in the self-diffusion coefficient occurs. This is due to the structural change observed in NW. In the bulk system, the self-diffusion coefficient remains close to zero until the melting point and shows an abrupt increase at Tm. At high temperatures, the

values obtained for NW-2 and the bulk system are quite close to each other.

CONCLUSION

In this study, the thermal and structural properties of Cu NWs during the melting process were investigated using MD simulations based on EAM potentials. The results indicated that while the T_m and ΔH_m increased with wire diameter, these values remained lower than those of the bulk system. Furthermore, it was determined that the NWs exhibited pre-melting behavior prior to homogeneous melting. Structural analyses revealed the formation of a neck above the melting temperature in wires with diameters of 2.5 and 4.0 nm; as the temperature rose, these wires split into two segments and transformed into NPs. In contrast, no such structural change was observed in the 6.0 nm diameter NW, and the wire maintained its overall geometric integrity throughout the temperature range investigated.

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