Mechanisms of Thermal Motion in n-Octadecane by Copper and Copper Oxide Nanoparticles: Insights from Equilibrium Molecular Dynamics Simulations

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Abstract: *In this study, equilibrium molecular dynamics (EMD) simulations were employed to investigate the thermal motion of n-octadecane upon incorporation of copper (Cu) and copper oxide (CuO) nanoparticles. The results demonstrate a notable increase in diffusion coefficients of nanoparticle based system compared to pure n-octadecane system. The Cu nanoparticle system exhibited a more pronounced enhancement in diffusivity than the CuO counterpart. Radial distribution function (RDF) analysis revealed strengthened intermolecular interactions and higher atomic packing density in nanoparticle-integrated systems, attributed to the compact molecular arrangement induced by nanoparticle inclusion.*

Keywords: *n-Octadecane; Copper nanoparticles; Copper oxide nanoparticles; Phase transition; Molecular dynamics simulations.*

1. Introduction

Energy constitutes the fundamental basis for both societal progress and economic development. With the accelerated advancement of industrialization, global energy demand has experienced exponential growth. Contemporary energy systems remain predominantly reliant on fossil fuels, whose combustion processes generate substantial greenhouse gas emissions. This has precipitated a critical surge in carbon output, exacerbating climate crises and accelerating the depletion of non-renewable resources. Confronted with the ecological degradation stemming from energy-related challenges, there exists an urgent imperative to transition towards renewable energy systems through the development and utilization of sustainable alternatives[1]. Currently, predominant renewable energy sources, including solar and wind power, present inherent limitations due to their environmental and temporal dependencies. Specifically, photovoltaic and wind turbine systems exhibit significant intermittency and instability in power generation, characteristics that undermine grid reliability and energy supply consistency. Consequently, the implementation of high-efficiency energy storage technologies has emerged as a crucial pathway to mitigate supply-demand imbalances and facilitate the integration of renewable energy into existing power infrastructures. While conventional energy storage technologies have partially addressed energy storage requirements, most exhibit limited energy density per unit volume or mass. These constraints significantly hinder their capacity to meet rapid regulation demands for highly volatile renewable energy sources such as solar and photovoltaic power. Consequently, the development of novel energy storage materials combining high efficiency, environmental compatibility, and economic viability has emerged as a critical research priority across academic and industrial sectors.

Phase change materials (PCMs) represent one of the most promising thermal energy storage solutions to achieve these objectives[2]. PCMs technology not only enables efficient renewable energy storage but also optimizes energy utilization through stable and high-capacity thermal management. Practically, PCMs demonstrate extensive application potential across multiple domains, including building energy conservation and green construction materials[3-5], solar thermal utilization systems[6-8], thermal management for electronic devices and power batteries[9], industrial waste heat recovery[10], and food preservation and transportation systems[11].

Paraffin wax, as a typical PCMs, demonstrates significant advantages including high latent heat capacity, low cost, excellent chemical stability, and minimal temperature variation during solid-liquid phase transitions. However, its low thermal conductivity has limited their large-scale applications in thermal energy storage. To enhance the thermal conductivity of these materials while improving their thermophysical properties, researchers have achieved this by incorporating nanoparcitles to form nanocomposite phase change materials[12]. Therefore, paraffin-based nanofluids have become a research focus in this field in the past and have been extensively studied. Xie et al.[13] prepared copper nanoparticle-containing liquid paraffin-based nanofluids using a two-step method and studied their thermal conductivity. The study found that the thermal conductivity of the nanofluids significantly increased, and there was an approximately linear relationship between the thermal conductivity enhancement ratio and the volume fraction of copper nanoparticles. Wu et al.[14] examined the thermal properties of Al_2O_3 nanoparticle-enhanced paraffin-based nanofluids under varying volume concentrations and temporal conditions. Their findings revealed that, compared to pure paraffin, the specific heat of paraffin-based Al_2O_3 nanofluids slightly decreased with increasing time and volume concentration. A similar trend was observed in volumetric heat capacity, which also exhibited a marginal reduction over time. This phenomenon highlights the importance of temporal stability in nanofluid applications. Samara et al.[15] investigated the thermal characteristics of paraffin-based nanofluids incorporating Al_2O_3 nanoparticles at varying volume fractions. Experimental results revealed a nonlinear enhancement in thermal conductivity with increasing nanoparticle concentration. Concurrently, a progressive reduction in latent heat capacity was observed as the Al_2O_3 volume fraction increased, demonstrating a critical trade-off between thermal transport properties and energy storage density in nanoparticle-enhanced phase change materials.

PCMs exhibit non-uniform dispersion and instability during flow processes, particularly in micro-scale nanoencapsulated and nanoparticle-enhanced PCM systems. Accurately obtaining thermal properties of PCMs proves critical for efficient applications. Therefore, integrating advanced analytical techniques to investigate the thermal performance of nanofluid/nanocomposite materials has become essential. Among these, molecular dynamics (MD) simulations have emerged as a pivotal approach for understanding microscopic material behaviors[16-19]. Analyzing and predicting the thermal characteristics of PCMs at molecular/atomic scales using MD methodologies proves both meaningful and necessary. Li et al.[20] employed equilibrium and non-equilibrium molecular dynamics simulation methods to systematically study the thermal properties of a copper-based nanoparticle-enhanced n-octadecane composite phase change system. They constructed molecular models of four different ratio systems. The study indicated that the addition of copper nanoparticles enhanced the thermophysical properties of the n-octadecane system, with the system's melting point, specific heat capacity, and thermal conductivity all increasing proportionally to the mass fraction of copper nanoparticles. Wang et al.[21] performed MD simulations on nanoparticle-eicosane hybrid systems. The incorporation of nanoparticles was found to restrict variations in the self-diffusion coefficient of eicosane while increasing the molecular packing density around nanoparticles, resulting in a more compact system configuration. These findings underscore the critical role of nanoparticle dispersion states in regulating molecular dynamics during phase transitions. Rao et al.[22, 23] investigated the heat transfer and energy storage mechanisms of nanoparticle-enhanced phase change materials through molecular dynamics simulations, as well as the self-diffusion and heat capacity characteristics of n-alkane-based phase change materials. They verified the effectiveness of MD simulations in studying the thermal performance of nanofluid/nanocomposite phase change materials at the nanoscale.

With the development of paraffin-based thermal energy storage technology, various paraffin with nanoparticles are proposed. A systematic study of the interactions between Cu nanoparticles, CuO nanoparticles, and paraffin contributes to understanding the thermal transport enhancement mechanisms of nanoparticles and designing high-performance phase change materials. This study analyzed the thermal motion mechanisms of n-octadecane incorporated with copper nanoparticles and copper oxide nanoparticles, respectively, based on MD simulations.

2. Model and Calculation Methods

MD is a computational simulation technique that derives atomic or molecular trajectories by numerically solving Newton's equations of motion. The potential energy of the system is calculated based on the molecular positions, from which the forces and accelerations of the atoms in the system are subsequently derived. Within a very short time step, the positions and velocities of each molecule can be determined. Through iterative calculations, the positions and velocities of each atom can be predicted after a certain period, the formulation can be expressed as Eq. (1):

$$\vec{F}_i(t) = m_i \vec{a}_i(t) = m_i \frac{\partial \vec{v}_i}{\partial t} = -\frac{\partial U_{\text{total}}}{\partial \vec{r}_i} \tag{1}$$

where $\vec{F}_i(t)$ is the force acting on the particle, m_i is the mass of the particle, $\vec{a}_i(t)$ is the acceleration of the particle, $\vec{v}_i$ is the velocity vector, U_{total} is a potential energy function.

For systems containing a large number of particles, Newton's equations of motion cannot be solved analytically. Therefore, the leap-frog algorithm was employed here to perform numerical integration. This algorithm propagates the system through time by alternately updating atomic velocities and positions within discretized time steps. Atomic trajectories were generated by iterating this integration scheme over millions of steps, thereby enabling the prediction of dynamical behavior and the calculation of ensemble-averaged thermodynamic and structural properties.[21]

2.1. Model Construction

As a predominant component of paraffin wax, n-octadecane comprises an 18-carbon alkane chain in its molecular structure (CH_3-$(CH_2)_{16}$-CH_3). In this study, Cu nanoparticles were modeled as a 2×2×2 unit cell configuration, while CuO nanoparticles were constructed from a 2×2×2 unit cell. It should be noted that, in this 2×2×2 model, surface cleavage was not performed. Instead, a supercell structure was directly generated from the 1×1×1 configuration through 2×2×2 expansion, and the resulting system was subsequently subjected to non-periodic treatment, and the specific crystallographic plane (100) define the exposed surfaces in the 2×2×2 supercell model. Given the complex intermolecular interactions among alkanes, the COMPASS force field[24]—a parameterized molecular mechanics model optimized for condensed-phase systems—was employed to describe the interactions between n-octadecane, Cu atoms, and CuO molecules.

To investigate the effects of Cu and CuO nanoparticles on the thermal motion of n-octadecane, three simulation systems were constructed: (a) A pure n-octadecane system containing 256 molecules (4,608 carbon atoms and 9,728 hydrogen atoms) in a 51.3 × 51.3 × 51.3 Å^3 simulation box; (b) A hybrid system comprising one Cu nanoparticle and 256 n-octadecane molecules (4,608 carbon atoms and 9,728 hydrogen atoms) in a 52.4 × 52.4 × 52.4 Å^3 simulation box; (c) A composite system integrating one CuO nanoparticle with 256 n-octadecane molecules (4,608 carbon atoms and 9,768 hydrogen atoms) in a 52.2 × 52.2 × 52.2 Å^3 simulation box. The initial configurations of these systems, as illustrated in Fig. 1, were generated using the Amorphous Cell module in Materials Studio software. All systems were initialized with a uniform density of 0.8 g/cm³ and equilibrated at 320 K to ensure thermodynamic consistency prior to phase transition analysis.

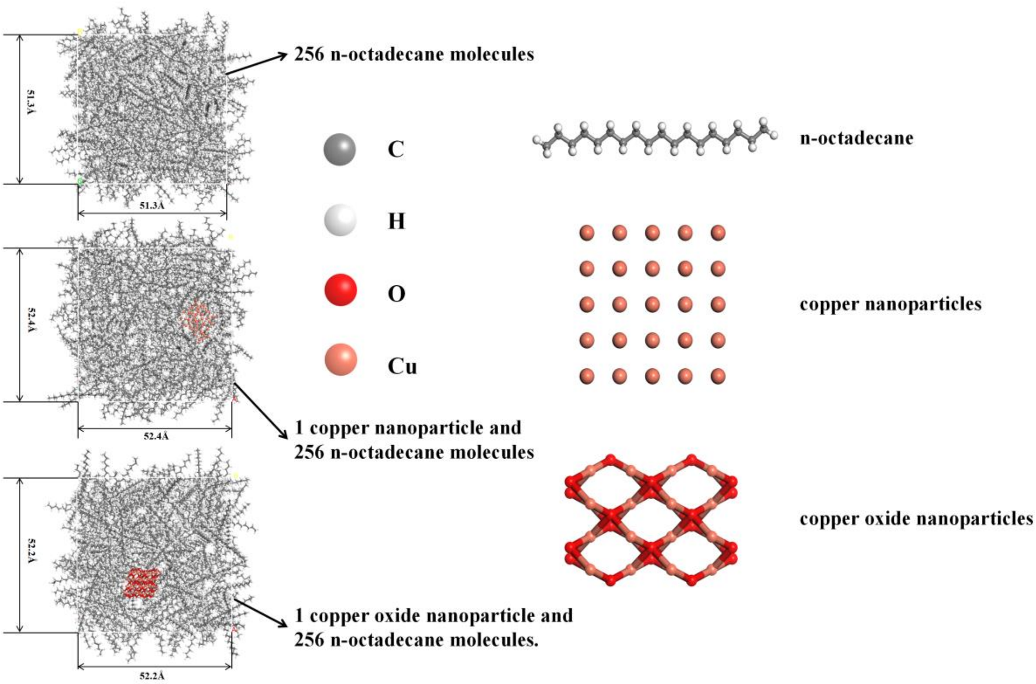

Fig. 1. Initial configuration of the system

2.2. Calculation methods

The simulations were conducted using Materials Studio software with periodic boundary conditions applied in all three spatial dimensions (X, Y, Z). A time step of 1 fs and total simulation duration of 100 ps were implemented. To investigate the thermal behavior of n-octadecane-nanoparticle hybrid systems during phase transitions, NVT ensemble simulations were performed at six temperature points (285 K, 295 K, 300 K, 305 K, 325 K, 345 K) using the Forcite module. These temperatures were strategically selected to encompass the melting point of pure n-octadecane (~301 K), enabling detailed analysis of thermal properties near phase transition regions. Throughout the simulations, both Cu and CuO nanoparticles remained as cohesive clusters, thus providing a reliable basis for subsequent analysis. Subsequently, temperature-dependent analyses, MSD, and RDF characterizations were systematically conducted for the three systems. Finally the results of the given data are summarized and discussed.

2.3. Model Validation

To validate the accuracy of the simulation methodology employed in this study, the density of n-octadecane at 0.1 MPa over the temperature range of 303.15–341.15 K was compared with experimental data reported in the literature[25], showed in Fig. 2. Analysis indicates that the maximum absolute density deviation does not exceed 0.3%, demonstrating that the force field and molecular dynamics approach used in this work are capable of reliably simulating alkane molecules and their hybrid systems with nanoparticles, and that the resulting data are scientifically robust.

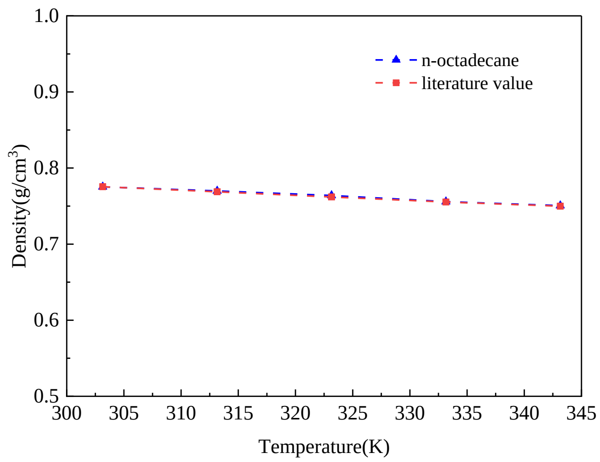

Fig. 2. Comparison between Simulated and Experimental Density Values of n-Octadecane

3. Results and discussion

3.1. Temperature profile

In the simulation experiments, six temperature points (285 K, 295 K, 300 K, 305 K, 325 K, and 345 K) were established to investigate the thermal performance evolution of the three systems under varying thermal conditions. The temperature profiles of the three systems during the simulation are illustrated in Fig. 3**Error! Reference source not found.**, Fig. 4 and Fig. 5. From the temperature trajectories, it is evident that the systems experienced an initial thermal equilibration period before stabilizing at their respective target temperatures. This stabilization behavior confirms the robustness of the thermostat implementation and the attainment of steady-state conditions essential for reliable thermodynamic property analysis.

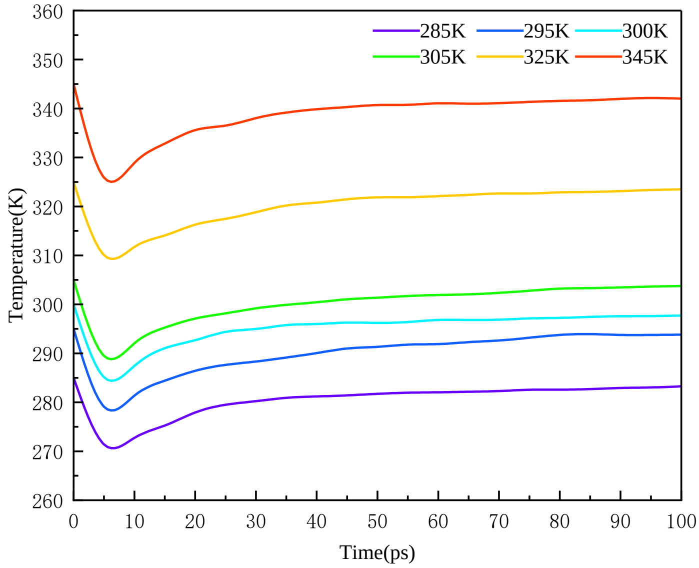

Fig. 3. Temperature profile of 256 n-octadecane molecules

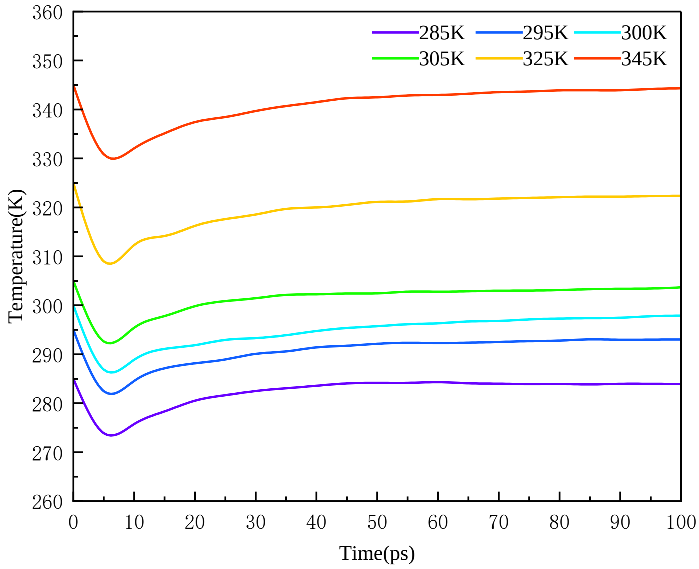

Fig. 4. Temperature profile of 1 Cu nanoparticle and 256 n-octadecane molecules

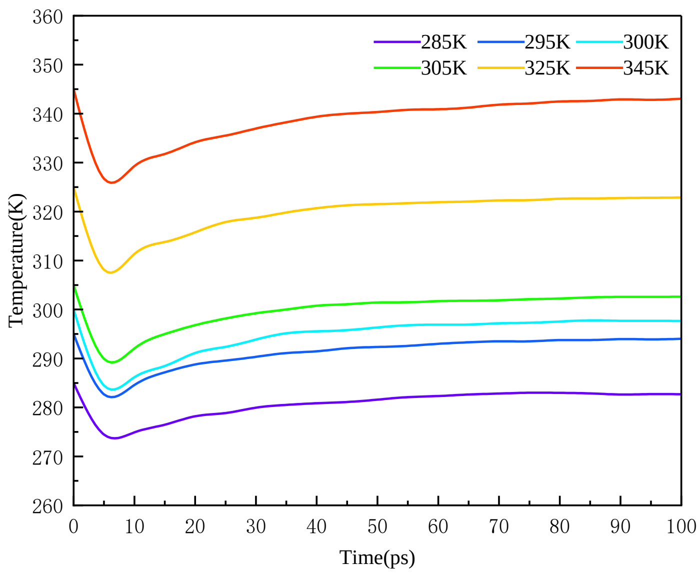

Fig. 5. Temperature profile of 1 CuO nanoparticle and 256 n-octadecane molecules

3.2. Diffusion coefficient

The MSD serves as a fundamental characterization parameter in molecular dynamics simulations, whose value quantitatively represents the average squared displacement of the molecular center of mass within the time domain. This parameter provides quantitative characterization of the molecular displacement rate from initial positions to equilibrium positions over time[26]. The mathematical definition of MSD is expressed by the following equation:

$$MSD = \langle (\vec{r_i}(t) - \vec{r_i}(0))^2 \rangle \tag{2}$$

where $\vec{r_i}(t)$ and $\vec{r_i}(0)$ represent the position vectors of a molecule at time t and the initial reference time (t=0), respectively. The diffusion coefficient (D) is derived from the linear regime of the MSD curve under equilibrium conditions, where D corresponds to one-sixth of the slope of MSD over extended observation times[27, 28]:

$$D = \lim_{t\to\infty} \frac{1}{6t} (|\vec{r}(t) - \vec{r}(0)|^2) \tag{3}$$

In the MD simulations, the variation patterns of the MSD of the system under varying temperature conditions (285K to 345 K) are illustrated in Fig. 6, Fig. 7 and Fig. 8**Error! Reference source not found.**. Analysis reveals that the MSD exhibits an increasing trend over time, and after the simulation duration exceeds a specific threshold (observed as 20 ps in this work, where linear characteristics emerge), the MSD and time display an approximately linear dependence. Based on this, the diffusion coefficient is calculated using Eq. (3) mentioned above, specifically by determining the slope of the MSD-time curve for the time period t>20ps. In addition, the MSD increases with increasing temperature, which is due to the fact that the higher the temperature, the higher the mobility of the atoms[27].

Next, the diffusion coefficients of the studied systems at different temperatures were calculated as shown in Fig. 9. The diffusion coefficient of the material was improved by the enhancement of the collision between atoms after the addition of nanoparticles. Among them, the increase in the diffusion coefficient after the addition of Cu nanoparticles is more significant, followed by CuO nanoparticles particles. This phenomenon can be attributed to the superior thermal conductivity of Cu nanoparticles relative to their CuO counterparts, which facilitates more efficient energy transfer within the composite systems. The enhanced thermal transport intensifies molecular thermal motion, thereby indirectly augmenting diffusion capabilities through enhanced phonon-mediated energy propagation.

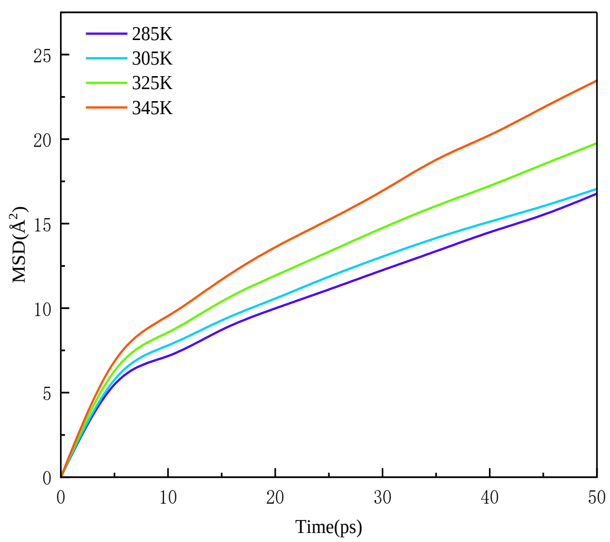

Fig. 6. MSD curves of 256 n-octadecane molecules at different temperatures

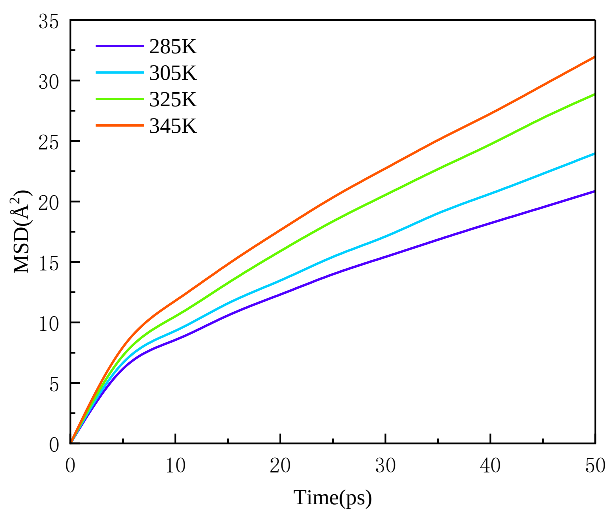

Fig. 7. MSD curves of 1 Cu nanoparticle and 256 n-octadecane molecules at different temperatures

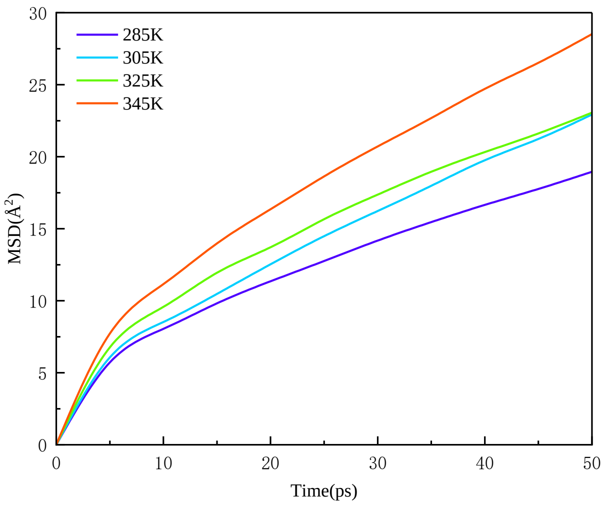

Fig. 8. MSD curves of 1 CuO nanoparticles and 256 n-octadecane molecules at different temperatures

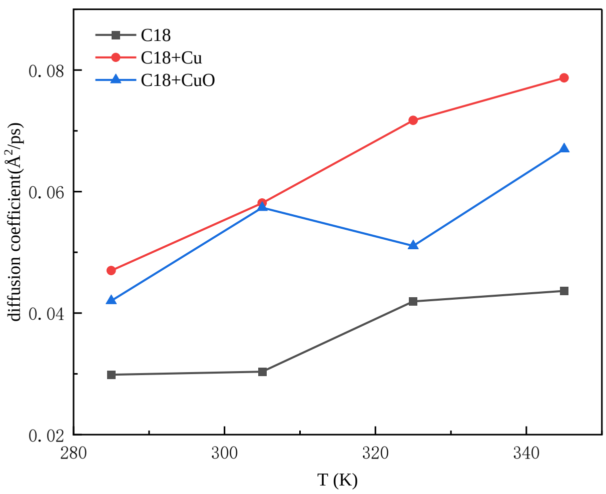

Fig. 9. Diffusion coefficients of the three systems at different temperatures

3.3. RDF curves

The RDF is employed to characterize the normalized probability of particle occurrence at a specific radial distance r around a reference particle within a system. In molecular dynamics simulations, RDF profiles capture variations in morphological configurations and density of material components, and enable the prediction of alterations in other thermodynamic and mechanical properties[26]. g(r) can provide insight into the relative distribution and strength of interactions. It is important to note that the greater the height of the first peak in the RDF curve and the shorter the distance, the stronger the interaction. In this study, for the pure n-octadecane system, RDF were exclusively computed between n-octadecane molecules. In nanoparticle-containing systems, the analysis specifically targeted RDF between nanoparticles and n-octadecane molecules. Additionally, the RDF calculation represents the average RDF over all frames in the time interval from 20 to 100 ps. The following Fig. 10 shows the radial distribution function for the three systems at 285K, 305K, 325K, 345K. It can be seen that at these four temperatures, the first peak in the RDF of the system containing one Cu nanoparticle and 256 n-octadecane molecules exhibits the greater height, followed by that of the system with one CuO nanoparticle and 256 n-octadecane molecules, and the distance of the first peak are nearly identical across all three systems, which indicates the system containing Cu nanoparticles exhibits the strongest interaction[29], meanwhile, the radial distribution function is the density of the other particles separated from the reference particle, which can be interpreted as the ratio of the regional density of the system to the average density, and it can be concluded that the presence of nanoparticles makes the system's molecules more compact and the number of atoms per unit of volume has more number of atoms. In addition, the RDF curves of the different systems show multiple peaks when the radial distance r is small, while the RDF curves of the working medium slowly converge to 1 when r is gradually increased. This indicates that the simulated three working medium are an amorphous structure with both proximally ordered and long-range disorder[26], which is also in perfect agreement with the microstructure of the actual working medium.

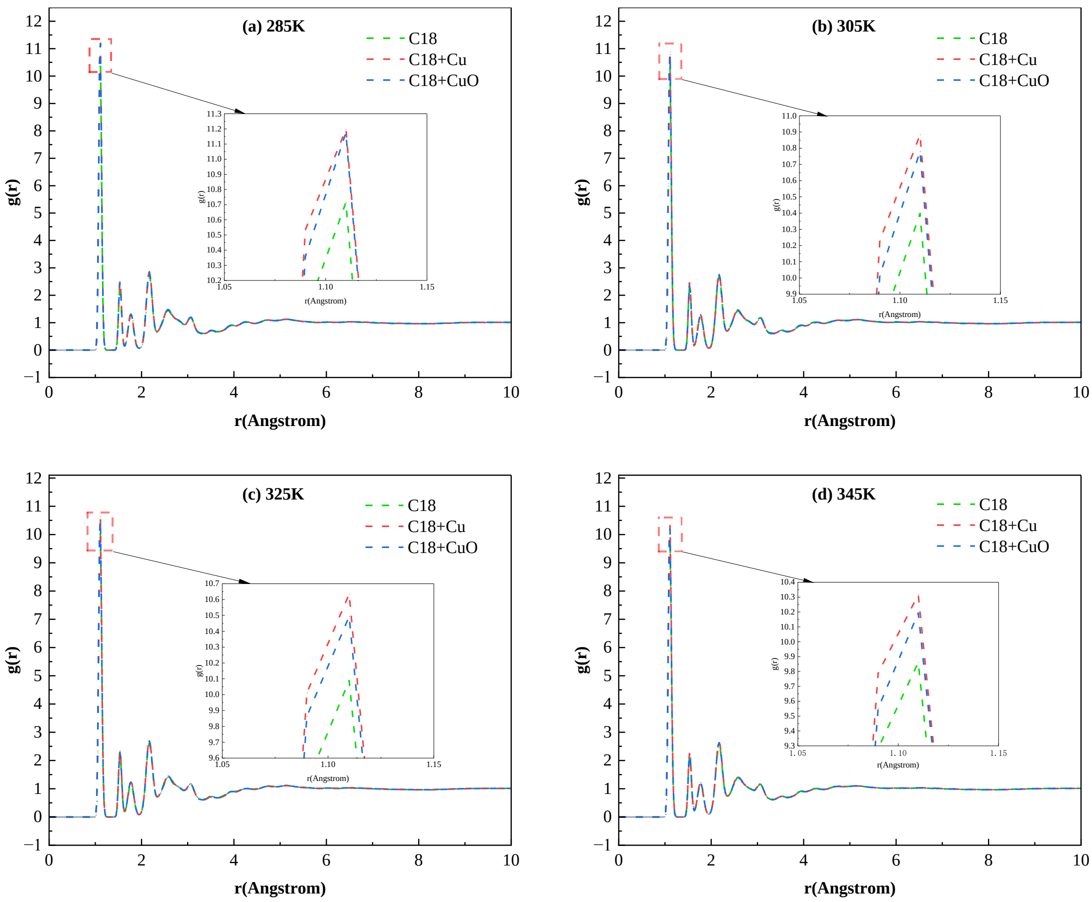

Fig. 10. RDF curves of the three systems at 285 K, 305 K, 325 K, and 345 K

4. Conclusion

This study employed molecular dynamics simulations to investigate the thermodynamic properties of n-octadecane hybridized with nanoparticles during phase transitions. The key findings are summarized as follows:

The incorporation of nanoparticles significantly enhanced the molecular mobility of n-octadecane/nanoparticle system. RDF profiles demonstrated strengthened intermolecular interactions within hybrid systems, while structural analyses indicated increased molecular packing density and higher atomic concentration per unit volume due to nanoparticle integration.

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