

THE FUNCTION OF NANOLAYER IN ENHANCING THE THERMAL CONDUCTIVITY OF TiO₂-WATER NANOFUIDS

by

Xiaoyan HUANG^{a,b}, Xiaohui ZHANG^{a,b*}, and Shan QING^{a,b}

^a Faculty of Metallurgical and Energy Engineering,

Kunming University of Science and Technology, Kunming, China

^b National Local Joint Engineering Research Center of Energy Saving and Environmental Protection Technology in Metallurgy and Chemical Engineering Industry, Kunming University of Science and Technology, Kunming, China

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Nanoparticles have the capability to effectively improve the thermal conductivity of base fluids, thus improving the heat transfer coefficient of heat transfer systems. In this study, a non-equilibrium molecular dynamics method based on the Fourier law is employed to study the thermal conductivity of TiO₂ (r-TiO₂)-water nanofluids with temperatures ranging between 303 K and 333 K and volume fractions in the range of 1%-2%. The ordered layer structure as a shell is analyzed and its influence is surveyed by calculating the number density and radial distribution function. The results revealed that a clear, solid-like nanolayer of about 0.5 nm can be observed around the nanoparticle. In this regard, the thickness of the nanolayer is less affected by variations in volume fraction and temperature. The $g(r)$ values and the number density decreased with the increase in temperature. Additionally, the $g(r)$ values and the number density at the level of the nanolayer were much higher compared to those at other parts. This indicates the existence of more water molecules in the nanolayer, thereby reducing contact thermal resistance and improving thermal conductivity. Macroscopically, the thermal conductivity increases with the increase in volume fraction. It was found that the increase in the volume fraction from 1%-2% at 303 K resulted in an increase in the effective thermal conductivity from 1.027 and 1.042, respectively. In other words, the thermal conductivity of the nanofluid was 2.7% and 4.2% higher than that of the base liquid under the same conditions.

Key words: *nanofluids, thermal conductivity, microscopic parameters, interfacial layer, nanolayer thickness*

Introduction

Nanofluids are generally characterized as suspensions with nanoparticles dispersed in heat transfer fluids. Due to their excellent thermophysical properties, they have been widely used in various engineering applications, including electronic device cooling systems [1, 2], grinding [3], solar heating, and other heat transfer processes [4]. They exhibited rapid development, providing a new approach to enhancing the heat transfer coefficient of conventional liquids [5, 6]. Thus, nanofluids can be considered the next generation of heat transfer fluids [7]. The rapid growth in research dealing with nanofluids, including the application areas and different nanofluid types [8, 9], has seen a dramatic increase, especially in the past decade [10-12].

* Corresponding author, e-mail: xiaohui.zhang@kust.edu.cn

Thermal conductivity is considered a key factor during the heat transfer process in nanofluid applications. Since the thermal conductivity of nanofluids is a direct reflection of the thermal properties of this new generation of heat transfer mediums, they are a hot research topic [13] and have been studied on a wide scale [14]. The major parameters contributing to the enhancement of nanofluids' thermal conductivity are the particle volume fraction, the size and shape of the nanoparticles, and the aspect ratio. In addition, the thermal conductivity of a nanofluid increases with the increase in the nanoparticle's thermal conductivity (considering different types of nanoparticles), particle volume fraction [15, 16] solution pH [17], and system temperature [18].

Based on the previous review and discussion [15-20], it is noted that the effects of volume fraction or temperature on the thermal conductivity of TiO₂ nanofluids have been dealt with from a macroscopic perspective. In this regard, corresponding results can be obtained through experiments. However, heat conduction is a microscopic process that cannot be observed or fully characterized by experiments. Some studies have shown that one of the major mechanisms exhibited in relation the abnormally enhanced thermal conductivity of nanofluids is the ordered arrangement of liquid molecules on the surface of nanoparticles [21-24]. This ordered layer structure as a shell at nanoparticles surfaces is commonly known as the interfacial layer, which was first reported and characterized by Choi *et al.* [25]. It was shown that the thickness of the interfacial layer plays an intriguing role in heat transmission from nanoparticles to the base liquid [21]. However, the interface layer is still very difficult to characterize by experiments because of its extremely small size. To address this, some researchers tried to use molecular dynamics (MD) simulations to investigate and evaluate the interfacial layer's effect on the abnormal thermal conductivity.

In their work, Li *et al.* [22, 26] investigated an argon thin layer of about 0.5 nm around copper nanoparticles using MD. Based on the evaluation conducted, they reported the effect of the interfacial layer on the thermal conductivity of the nanofluid. This thin interfacial layer will move with the Brownian motion of the copper nanoparticles and water molecules. The investigations also found that the number density is proportional to the diameter of the nanoparticles, which therefore, leads to a significant enhancement of the Cu-Ar nanofluid's thermal conductivity. In connected studies, Wang and Jing [27] investigated the thickness and thermal conductivity of the interfacial layer around the nanoparticle in Cu-Ar nanofluids employing equilibrium molecular dynamics (EMD) simulations. They found that the nanoscale thin interfacial layer is characterized by a more ordered structure and a higher thermal conductivity, compared to the base fluids. In their study, Jin *et al.* [28, 29], examined the thermal conductivity of different metal-water nanofluids using MD methods. The results indicated that the Au-water nanofluid has a higher thermal conductivity and a thicker nanolayer due to the stronger interaction between gold and water molecules ($\epsilon = 1.256$ kcal/mol, $\sigma = 2.895$ Å). The authors also studied the effects of different surface materials and core-shell ratios on the thermal conductivity of nanofluids. It was shown that, the thermal conductivity of core-shell nanofluids can be significantly enhanced compared to that of heat transfer fluids. The studies reviewed here demonstrate that, MD methods serve as a very effective approach to studying and examining nanolayer structures.

Moreover, most researchers have studied the corresponding properties of Cu/Ar nanofluids using MD methods, yet Ar is still not commonly used in industry and practical engineering applications. In this work, rutile-TiO₂ (r-TiO₂)-water nanofluids are selected as the research object. Using non-equilibrium molecular dynamics (NEMD) [30] approach based on the Fourier law, the thermal conductivity of TiO₂ (r-TiO₂)-water nanofluids is studied considering differ-

ent volume fractions. The ordered layer structure as a shell is examined, and then its influence is surveyed by calculating the nanofluid number density and radial distribution function (RDF). Overall, comparison the EMD approach, NEMD considers the influence of heat flux and avoids the generation of temperature gradients. This leads to more stable simulation system [31].

Modelling and simulation

In general, the solid particle size utilized in this study to make nanofluids is between 10 nm and 100 nm. However, it is difficult and unrealistic to simulate the actual size of nanofluids with MD [32], as the actual system is large and complex. Nevertheless, the MD method is a practical numerical simulation approach, that is based on Newtonian mechanics to simulate the motion of molecular systems. The method can evaluate the motion state of atoms in the model system through numerical simulations. In this regard, the mass and velocity of the atoms are calculated in the simulation system [33]:

$$m_i \frac{dv_i}{dt} = F_{ij} = \nabla \phi_{ij} \quad (1)$$

where m_i and v_i are the mass and velocity of the atom, respectively, F_{ij} – the vector sum of all the interaction forces between atoms i and j , and $\nabla \phi_{ij}$ – the gradient of the potential function.

In addition, the thermal conductivities of TiO₂-water nanofluids were calculated using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package, which is an open-source MD code. The MD simulation calculation provides microscopic information about the simulated system. Then, the utilized ensemble converts the related parameters calculated from MD in the microscopic state into macroscopic properties through statistical physics [34]. In this work, all simulations were carried out in canonical (NVT) and microcanonical (NVE) ensembles. A simulation box with 60 Å × 60 Å × 60 Å dimensions was used to release water molecules. A TiO₂ nanocluster from materials studio was placed in the middle of the simulation box and was surrounded by water molecules. The visualization OVITO was used to aid in the visualization and analysis of the atomistic simulation data obtained from the LAMMPS calculations [35].

Moreover, TiO₂ nanoclusters were set as spheres with radii of 8 Å and 10.1 Å. The SPC water molecular model was applied in the simulations. The number density of water molecules was calculated using eq. (2) [14] and found to be 33.3 nm⁻³, considering a density of 1000 kg/m³:

$$n = \frac{N}{V} \quad (2)$$

where N and V are the number of water molecules and volume of the calculated region, respectively, and n – the indicates the quantity of water molecules in the studied region. Table 1 presents the detailed characteristics of TiO₂ nanoparticles. The SPC water model and the TiO₂ nanocluster model are shown in fig. 1. Figure 2(a) shows the structure of TiO₂ nanoparticles and water molecules, as well as the initial position of TiO₂ nanocluster, which was set into the simulated box, considering volume fractions of 1.0 vol.% and 2.0 vol.%. Additionally, fig. 2(b) depicts a schematic of the simulation box of TiO₂ nanofluids using NEMD.

Table 1. Detailed characteristics of TiO₂ nanoparticles

Nanoparticles	Density [gcm ⁻³]	Specific heat [kJkg ⁻¹ K ⁻¹]	Thermal conductivity [Wm ⁻¹ K ⁻¹]
TiO ₂	4.22	0.71	8.48

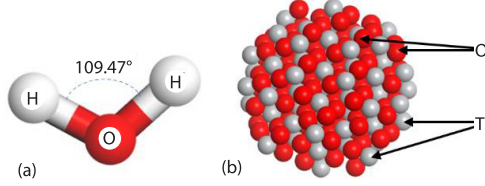


Figure 1. Illustration of models;
(a) SPC water molecular and
(b) TiO₂ nanocluster

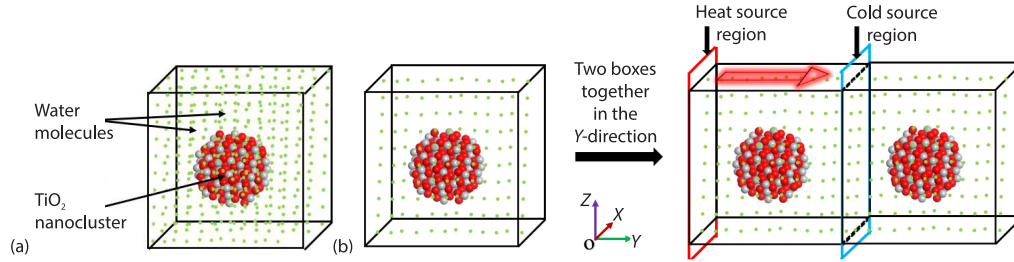


Figure 2. Schematic of the simulation using NEMD;
(a) initial position of TiO₂ nanocluster and (b) simulation box

The interatomic potentials between Ti-O, Ti-Ti, O-O, and Ti-O_w were modeled using the Matsui-Akaogi (MA) potential [36]:

$$U(r_{ij}) = A_{ij} \exp\left(-\frac{r_{ij}}{\rho_{ij}}\right) - \frac{C_{ij}}{r_{ij}^6} + \frac{q_i q_j}{r_{ij}} \quad (3)$$

where $U(r_{ij})$ is the interatomic potential and r_{ij} – the distance between atoms i and j . The atomic charges of the oxygen and titanium are $-1.098e$ and $+2.196e$, respectively. The other parameters A_{ij} , ρ_{ij} , and C_{ij} used by the MA potential function are shown in tab. 2.

Table 2. Interaction parameters for the MA force field on TiO₂ and water oxygen

$i-j$	A_{ij} [kcalmol ⁻¹]	ρ_{ij} [Å]	C_{ij} [kcalmol ⁻¹ Å ⁶]
Ti-O	391049.1	0.194	290.331
Ti- Ti	717647.4	0.154	121.067
O-O	271716.3	0.234	696.888
Ti-O _w	28593.0	0.265	148.000

O_w: O in water.

In the SPC water molecular model, the interatomic potentials between O_w-O_w, H-H, and O_w-H were modeled using the Lennard-Jones (L-J) potential [31]:

$$U(r_{ij}) = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad r_{ij} < r_c \quad (4)$$

$$U(r_{ij}) = 0 \quad r_{ij} > r_c$$

where r_{ij} is the distance between atoms i and j , σ_{ij} and ε_{ij} are the energy and length scales, respectively, and r_c – the cutoff distance, selected as 1.0 nm in this study for all intermolecular interactions. The interatomic potentials between O-O_w were modeled using the L-J potential [37]. The interaction between hydrogen atoms is neglected because of their very small mass. This means that the interaction between TiO₂ and water molecules is mainly based on the interaction between Ti, O atoms, and water oxygen.

During simulations, the time step was set to 1 fs in the NEMD simulation box, and the long-range Coulomb forces were calculated to reflect the long-range interactions of the molecules. To reduce the effect of the simulated box size, periodic boundary conditions were set in the x -, y -, and z -directions of the considered system. To avoid any impact of the initial state on the simulation results, the model was completely relaxed under canonical ensemble (NVT) and microcanonical ensemble (NVE) for 100000 steps. This allows for achieving stable temperature and energy conditions. Then, the same energy amount was added to the cold source and heat source regions, and the simulation box ran for 70000 steps in NVE to generate a stable temperature gradient and heat flow parallel to the y -axis. Finally, the NEMD simulation box ran for another 100000 steps to calculate the parameters of TiO_2 -water nanofluids in NVE.

Implementing the aforementioned steps, the heat flux rate, Φ , and the temperature gradient values in the y -direction dt/dy can be obtained. Using these, the thermal conductivity, λ , can be calculated using Fourier's thermal conductivity law, combining:

$$q_y = \frac{\Phi}{2(l_x l_z)} \quad (5)$$

$$q_y = -\lambda \frac{dt}{dy} \quad (6)$$

where Φ is the heat flux rate of the added cold or heat source. As, the added energy Φ will flow to both sides of the simulated box, Φ needs to be divided by 2 in eq. (5). The l_x and l_z represent the lengths of the simulation box on the x - and z -axes, respectively. The $l_x l_z$ represents the area perpendicular to the heat flux and q_y is the heat flux density.

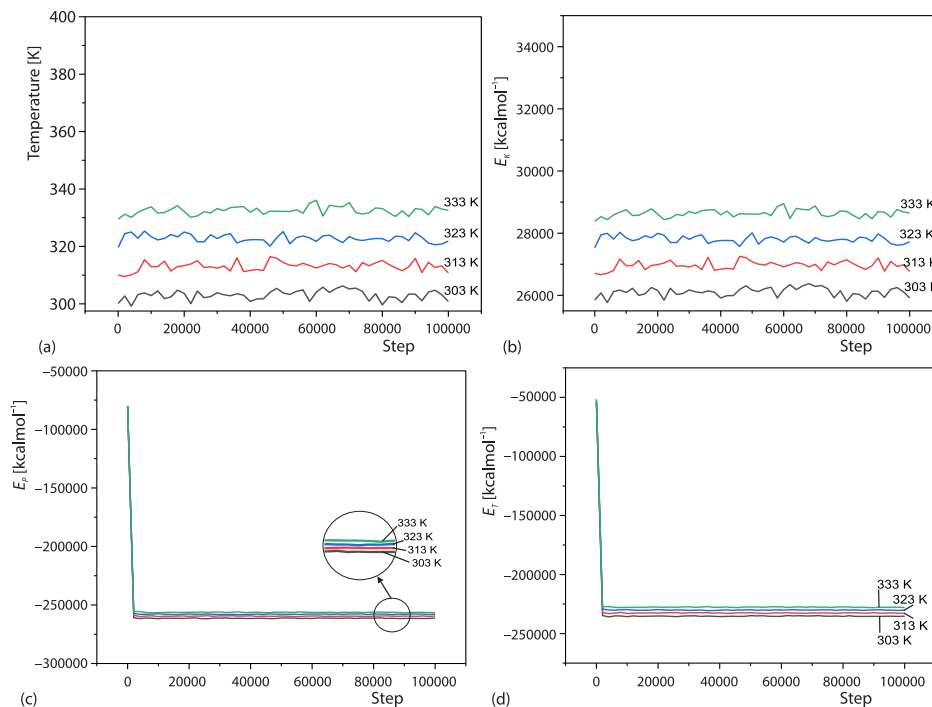


Figure 3. Variations with steps, at volume fractions of 1.0 vol.%; (a) temperature, (b) kinetic energy, (c) potential energy, and (d) total energy

Figure 3 shows the evolution of the temperature, kinetic energy, potential energy, and total energy of the system considering a temperature range of 303-333 K. It is noted that the system is in equilibrium within less than 100000 steps in all the considered cases. Therefore, the system is considered stable before calculating the thermal conductivity by running 100000 steps under the NVT and NVE ensembles.

Results and discussion

Validation of methods

Before calculating the thermal conductivity of the TiO₂-water nanofluid, the accuracy and stability of the simulation system were evaluated, considering a pure water system using the NEMD method. The validation results are presented in fig. 4.

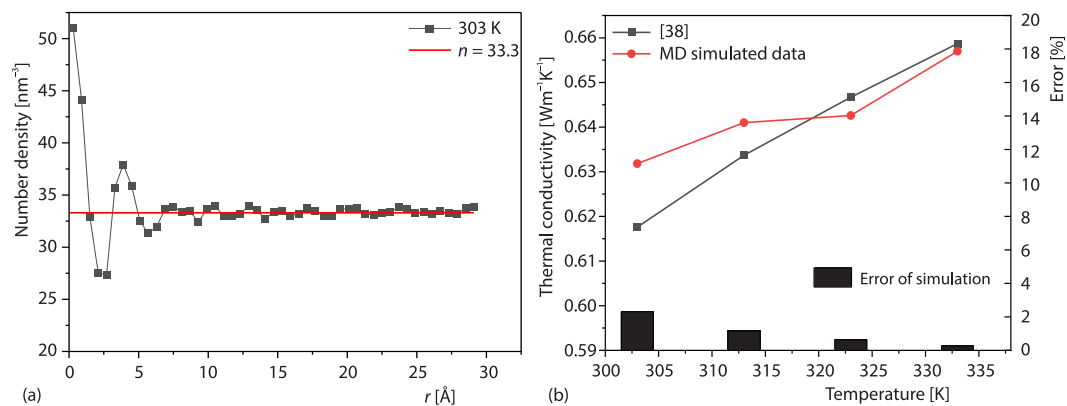


Figure 4. Comparison of the simulation data and standard data from the literature [38]; (a) number density and (b) thermal conductivity

Figure 4 shows the number density at 303 K in NEMD simulations and a comparison of the thermal conductivity data obtained in the present study and that reported in the literature. In the conducted simulations, fig. 4(a), the number density is found to gradually converge to a constant value at 303 K, which is close to the standard value of 33.3 nm³. As shown in fig. 4 (b), the simulated data is found to be very close to the experimental data reported by Yang and Tao [38]. The maximum error between the simulated values and the literature results is about 2.3% in the temperature range of 303-333 K. This finding verifies the reliability of the model established in this work.

Analysis of thermal conductivity

Macroscopically, the thermal conductivity increases with the increase in volume fraction. It was found that the increase in the volume fraction from 1%-2% at 303 K resulted in an increase in the effective thermal conductivity ($\lambda_{\text{eff}} = \lambda_{\text{nf}}/\lambda_{\text{bf}}$) from 1.027 and 1.042, respectively. In other words, the thermal conductivity of the nanofluid was 2.7% and 4.2% higher than that of the base liquid under the same conditions. Figures 5(a) and 5(b) show the nanofluid's thermal conductivity, λ_{nf} , and effective thermal conductivity, λ_{eff} , obtained from simulations at a volume fraction of 1.0 vol.%. It can be observed from fig. 5 that the thermal conductivity of TiO₂-water nanofluids increases with an increase in temperature. The reason for the obvious enhancement in thermal conductivity at higher temperatures is attributed to the increase in the intense Brownian motion and interfacial potential of atoms and molecules [39].

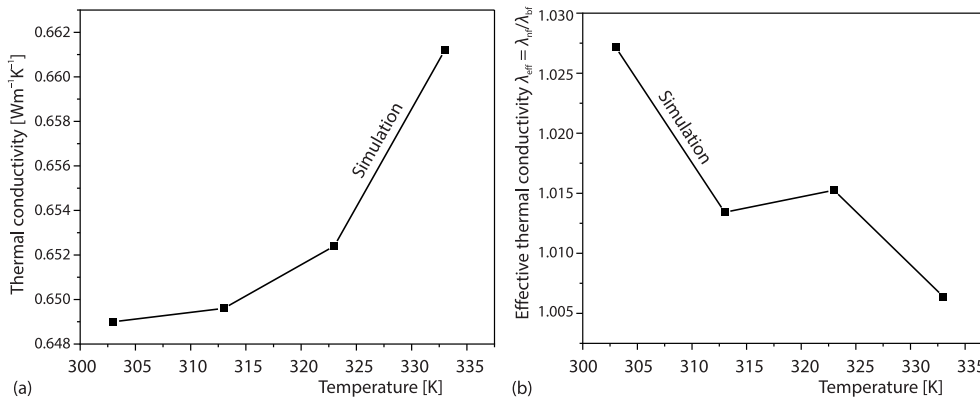


Figure 5. The thermal conductivity obtained from simulations at 1.0 vol.%; (a) thermal conductivity and (b) effective thermal conductivity

The function of the nanolayer in the enhancement of TiO₂-water nanofluid thermal conductivity

The relationship between the nanolayer and heat transport, especially in terms of enhancing thermal conductivity, needs to be clarified. To evaluate whether the nanolayer can improve heat transport, the mechanism of enhancement of the nanofluids' thermal conductivity is examined and discussed with reference to RDF and, microscopic parameters such as nanolayer thickness and number density. The RDF function is a radial distribution function, denoted by $g(r)$. The RDF represents the probability of finding an atom at a given distance away from the central atoms [40], and the number density shown in eq. (2) is defined as the number of particles or substances per unit volume.

Figure 6 shows the variation in the number density and $g(r)$ with the change in the atomic distance, r , considering 1.0 vol.% and 2.0 vol.%. It can be seen from fig. 6 that the number density and RDF function exhibited similar trends at different volume fractions. The number density distribution of water molecules around the TiO₂ central nanosphere is shown in fig. 6(a). As shown in the figure, at the beginning, the number density changes periodically with the atomic distance. Then, with the increase in the distance, r , the number density approaches a fixed value of 33.3 nm⁻³ (the number density of pure water). This indicates that the central nanosphere has a range of effects on the surrounding water molecules of about 0-0.5 nm, as shown in fig. 6(a). The first peak obtained for the number density is the strongest, with about 50 nm⁻³. This is followed by a second peak of about 38 nm⁻³, while the rest of the peaks can be neglected. This result is consistent with the findings reported by Heyhat *et al.* [37]. So, two distinct interfacial layers are formed around the central nanosphere.

Comparing figs. 6(b) and 6(c), the trend of $g(r)$ is found to be similar at different volume fractions. In the range of 0-0.5 nm away from the TiO₂ central nanosphere surface, two obvious peaks are highlighted. This indicates that the probability of O_w appearing near Ti and O atoms is higher. Moreover, it is evident that the fluctuation of RDF is similar to that of the number density. If the shape is relatively sharp, it indicates that the number density is much higher than the average density within a specific area [41].

In addition, a larger value of the number density, or $g(r)$ denotes a denser distribution of water molecules in the interfacial nanolayer, similar to the solid-like water molecular layer. In connection with this, Keblinski *et al.* [42] reported that the arrangement of liquid mole-

cules is more ordered in such a layer. It is well known that solids possess better heat transfer properties compared to liquids. Thus, liquid layering at the interface of the nanoparticle would be expected to lead to higher thermal conductivity. Figure 7 shows the schematic structure of two typical interfacial nanolayers around the center nanoparticle, obtained using OVITO. It is shown that a high heat conduction channel (center nanoparticle-interfacial nanolayers-random liquid molecules) is formed. Some studies have characterized the heat conduction channel as a thermal bridge [43].

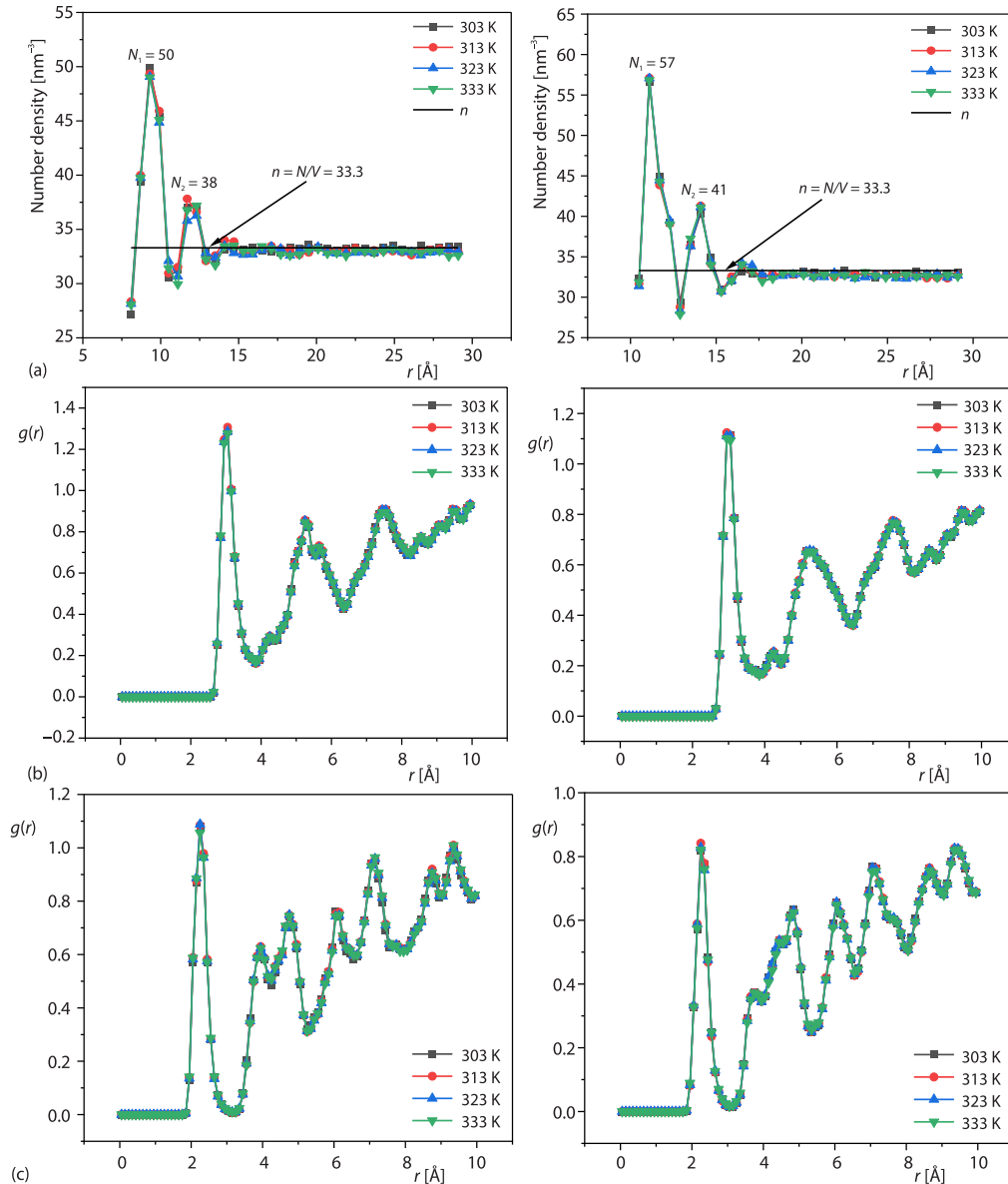


Figure 6. Variations with the change in atomic distance at (left) 1.0 vol.% and (right) 2.0 vol.%; (a) number density, (b) $g(r)$, of $O-O_w$, and (c) $g(r)$, of $Ti-O_w$

As shown in fig. 6(a), the thickness of the first and second interfacial nanolayers is about 0.5 nm for TiO₂-water. According to the numerical density and RDF function, it noted that the density of water molecules is much higher than the density of the base liquid in the range of 0-0.5 nm. At the same temperature of 333 K, compared with pure water, the thermal conductivity of nanofluids has increased, and a clear solid-like nanolayer can be observed around the nanoparticles. Therefore, the nanolayer plays a certain role in increasing the thermal conductivity of nanofluids.

Conclusions

In this study, a simulation model was established to estimate the thermal conductivity of TiO₂-water nanofluids for volume fractions of 1.0% and 2% of TiO₂. The thermal conductivity enhancement in nanofluids was described and evaluated considering the RDF, the number density and nanolayer thickness. Based on the obtained results, the main conclusions that can be drawn from this conclusions are as follows.

- By considering the numerical simulations, it can be seen that the thermal conductivity of TiO₂-water nanofluids increases with an increase in temperature and volume fraction. A clear solid-like nanolayer (about 0.5 nm) can be observed around the nanoparticles.
- The influence of volume fraction and temperature on number density and nanolayer thickness is relatively small.
- In the process of heat transfer from the nanoparticles to the water molecules, the nanolayer acts as a connection. Regarding the increase in thermal conductivity of nanofluids, the nanolayer plays a certain role.

Due to the fact that the number density is less affected by temperature under the same volume fraction, there is still a need to study the interaction between the surface of TiO₂ nanocluster and water molecules.

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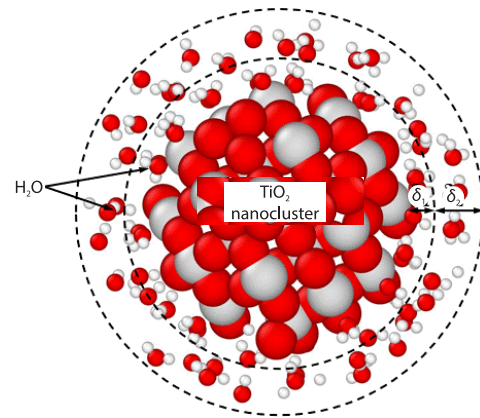


Figure 7. Microscopic structure of the interfacial layer by OVITO

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