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Enhancing Heat Transfer in Internal Combustion Engine by Applying Nanofluids

Wenzheng Cui, Zhaojie Shen, Jianguo Yang and Shaohua Wu

Abstract

Nanofluids exhibit novel properties including significant heat transfer properties that make them potentially useful in internal combustion engine cooling. However, although there is a substantial number of mechanisms proposed, modeling works related to their enhanced thermal conductivity, systematic mechanisms, or models that are suitable for nanofluids are still lacked. With molecular dynamics simulations, thermal conductivities of nanofluids with various nanoparticles have been calculated. Influence rule of various factors for thermal conductivity of nanofluids has been studied. Through defining the ratio of thermal conductivity enhancement by nanoparticle volume fraction, K, the impacts of nanoparticle properties for thermal conductivity are further evaluated. Furthermore, the ratio of energetic atoms in nanoparticles, E, is proposed to be an effective criterion for judging the impact of nanoparticles for the thermal conductivity of nanofluids. Mechanisms of heat conduction enhancement are investigated by MD simulations. Altered microstructure and movements of nanoparticles in the base fluid are proposed to be the main reasons for thermal conductivity enhancement in nanofluids. Both the static and dynamic mechanisms for heat conduction enhancement in nanofluids have been considered to establish a prediction model for thermal conductivity. The prediction results of the present model are in good agreement with experimental results.

Keywords: nanofluids, internal combustion engine, heat transfer, mechanism

1. Introduction

In recent years, nanofluids (NFs) have received much attention due to their strengthening heat transfer properties, which possess important application in heat transfer. The concept of nanofluids was first proposed by Choi in 1995, which indicates the fluids containing nanometer-sized particles, called nanoparticles (NPs) [1]. These fluids are engineered colloidal suspensions of nanoparticles in a base fluid. Numerous experimental studies discovered that nanofluids exhibit thermal properties superior to those of base fluid or conventional solid-liquid suspensions. Most of the thermal properties of nanofluids measured greatly exceed the values predicted by classical macroscopic theories and models. Nanofluids possess significantly increased thermal conductivity and improved convective heat transfer coefficient. Therefore, they are potentially useful in many enhanced heat transfer application, including engine cooling, vehicle thermal management, and power battery. Researchers are working to explain the significant high thermal properties of nanofluids [2–4]. However, although there is a substantial number of mechanisms proposed, and modeling works related to their enhanced thermal conductivity, systematic mechanisms, or models that are suitable for nanofluids are still lacked.

Regarding the excellent thermal properties of nanofluids, researchers are interested in the application of nanofluids in internal combustion engine, and began the study of applying nanofluids in internal combustion engine. In 1999, Wambsganss in Argonne national laboratory proposed the idea of applying nanofluids in car engine to improve the vehicle thermal management performance [5]. Choi indicates in a report that in Argonne national laboratory a research program of enhanced heat transfer by nanofluids is launched aiming at the cooling and heat transfer problems in the heavy-duty engine [6]. The results show that due to the excellent heat transfer performance of nanofluids, the size and weight of the engine can be reduced by 10%. Choi pointed out that the application of nanofluids in engine is one of the best methods of improving heat transfer performance of the cooling system. Saripella et al. studied the heat transfer performance of nanocoolant (nanofluids) in Volvo truck engine, and the results indicate that with nanofluids the temperatures of combustion chamber components and coolant are lowered [7]. Lockwood et al. in Valvoline Company reported the application of nanofluids in the cooling for internal combustion engine [8]. The experiments found that adding 1% vol. carbon nanotube in engine oil could increase the thermal conductivity by 150%. Wallner et al. in Delphi Company found that applying nanofluids can efficiently improve the efficiency of internal combustion engine and decrease the size and weight of the cooling system [9]. Huminic et al. studied the performance of nanofluids in a car radiator with a numerical method and found that the convective heat transfer performance is distinctly better than that of single-phase fluids [10]. Furthermore, the heat transfer properties of nanofluids are influenced by many factors, including the volume concentrations, temperatures, and fluid velocities. Vajjha et al. reported their research on the flow and heat transfer properties of Al_2O_3 and CuO nanofluids when applying them in the car radiator [11]. Their results reveal that nanofluids possess improved convective heat transfer properties and the increase rate is increased by increased volume concentrations. Leong et al. found that the heat transfer coefficient and heat transfer rate in the cooling system of internal combustion engine are improved by using nanofluids [12]. Peyghambarzadeh et al. experimentally verified that the

application of nanofluids improves heat transfer efficiency of the car radiator by 45% when using Al_2O_3-H_2O nanofluids [13].

The authors have focused on the application of nanofluids in internal combustion engine (ICE) for heat transfer enhancement. In order to apply nanofluids in ICE, the mechanisms of heat transfer enhancement and the rules of enhanced heat transfer by nanofluids should be clarified first. The original cause of heat transfer enhancement is due to the adding of nanoscale particles. Therefore, we have attempted to use molecular dynamics (MD) simulations to study these microscopic mechanisms [14]. By using MD simulation, we have calculated thermal conductivity of nanofluids via the Green-Kubo equation and proposed an effective criterion for predicting the enhancement of apparent thermal conductivity. Furthermore, possible mechanisms of heat conduction increase in nanofluids are studied by MD simulation, including: (1) the micromotions of nanoparticles, (2) changed microstructure of base fluid by adding nanoparticles, and (3) the influence of absorption layer of base fluid at the surface of nanoparticles. On the basis of the microscopic mechanisms found by MD simulations, we have also proposed a revised thermal conductivity model, which considered both the static and dynamic mechanisms. The revised model is verified by experimental data, which has been proved to be quite accurate for predicting thermal conductivity of common types of nanofluids.

2. Influence rule and criterion for nanofluids' thermal conductivity

2.1. Simulation results of thermal conductivity

MD simulation is used to calculate thermal conductivity of nanofluids via the Green-Kubo equation [14]. A series of influencing factors for the thermal conductivity of nanofluids have been considered, including: nanoparticles' volume concentrations, sizes, materials, and shapes [15]. In this work, inert liquid Ar is chosen as the base fluid because of the mature and credible potential function. The NP materials include Cu, Ag, Fe, and Au. We have chosen these types of nanoparticles because they are commonly reported in the literatures on nanofluids. The MD simulation results reveal that the thermal conductivity of nanofluids can be obviously increased by adding nanoparticles, as shown in **Table 1**. However, the contributions of several influencing factors for thermal conductivity of nanofluids are different.

Figure 1 shows the MD simulation results of thermal conductivities for nanofluids containing spherical nanoparticles. In this case, the nanoparticle volume fractions, nanoparticle diameter, and thermal conductivity of nanoparticles are considered. For the influencing factors that have been considered in this work, the influencing rules are regular. The thermal conductivity of nanofluids is increased with increased volume fraction of NPs, decreased NP sizes, and higher thermal conductivity of NPs. For instance, the ratios of thermal conductivity enhancement for Ag, Cu, Fe, and Au nanofluids are 1.41, 1.15, 1.11, and 1.08 sequentially when the other conditions are the same.

Diameters (nm)	Volume fractions (%)	Cu	Ag	Au	Fe
2	0.5	1.112	1.326	1.062	1.036
	1	1.149	1.405	1.112	1.059
	2	1.359	1.498	1.205	1.079
	3	1.414	1.570	1.322	1.096
4	0.5	1.095	1.287	1.055	1.041
	1	1.134	1.325	1.096	1.065
	2	1.303	1.396	1.175	1.085
	3	1.376	1.462	1.202	1.112
6	0.5	1.065	1.244	1.049	1.045
	1	1.097	1.265	1.086	1.079
	2	1.266	1.326	1.152	1.098
	3	1.336	1.369	1.256	1.132

Table 1. Ratios of nanofluids' thermal conductivity enhancement with different influence factors.
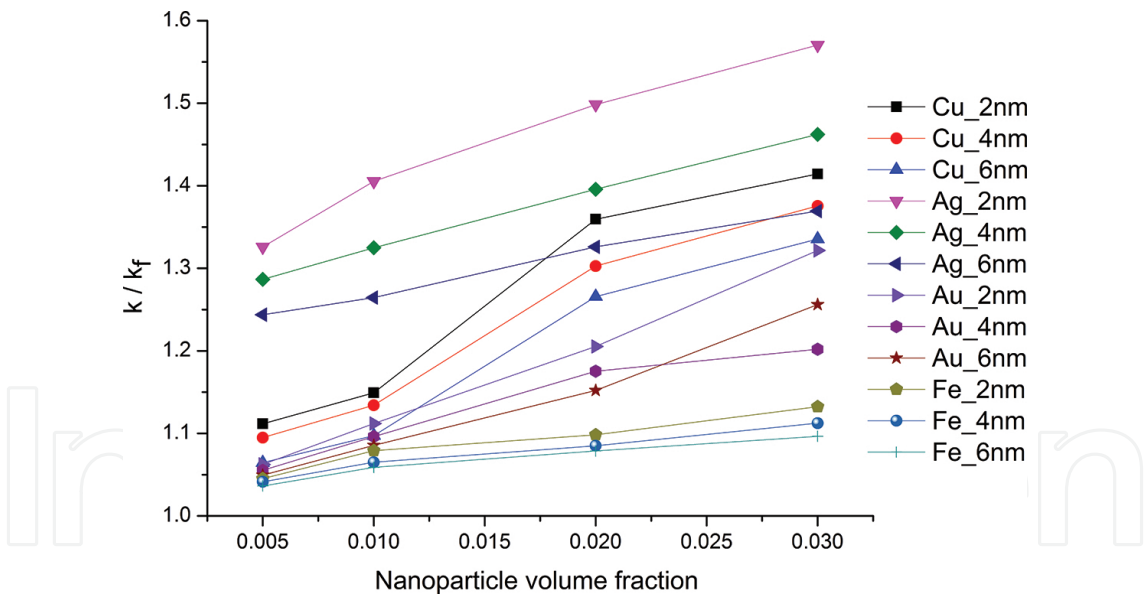

Figure 1. MD simulation results for thermal conductivity of nanofluids.

To examine the influencing rules for thermal conductivity of nanofluids in depth, the ratio of thermal conductivity enhancement by nanoparticle volume fraction, *K*, is defined:

$$K = \frac{k/k_f - 1}{V_{np}/V},$$ (1)

where V_{np} and V are the volume of nanoparticles and nanofluids, respectively; k and k_f represent the thermal conductivities of nanofluids and base fluid, respectively.

The physical significance of K is to evaluate the ratio of thermal conductivity increase and nanoparticle volume fraction. In other words, K could be used to evaluate the impact of nanoparticle properties for thermal conductivity. With K, the contributions from volume fraction and thermal conductivity of nanoparticles could be compared, as shown in **Figures 2** and **3**. From the figures i,t could be easily found that the contributions of nanoparticle materials are in the order of Ag, Cu, Au, and Fe. Furthermore, through comparing K values, it is also found that the influence of nanoparticle materials is weakened when the volume fraction or nanoparticle size is increased. With the help of K value the other influencing factors could be further evaluated, please refer to reference [15].
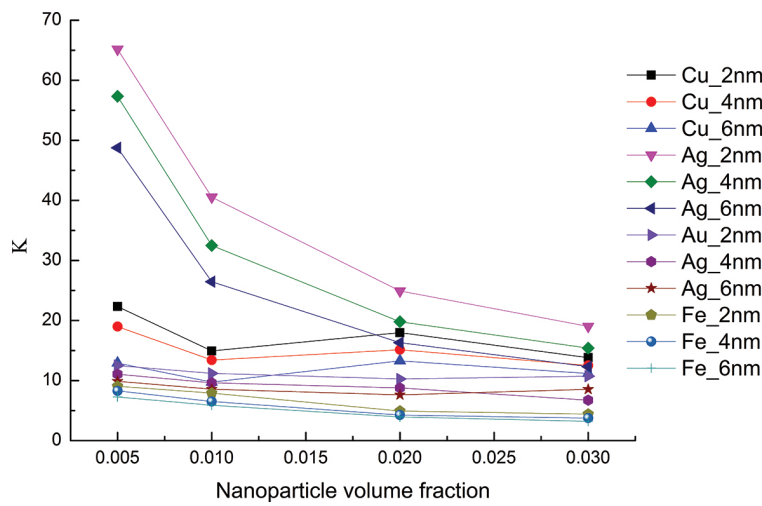

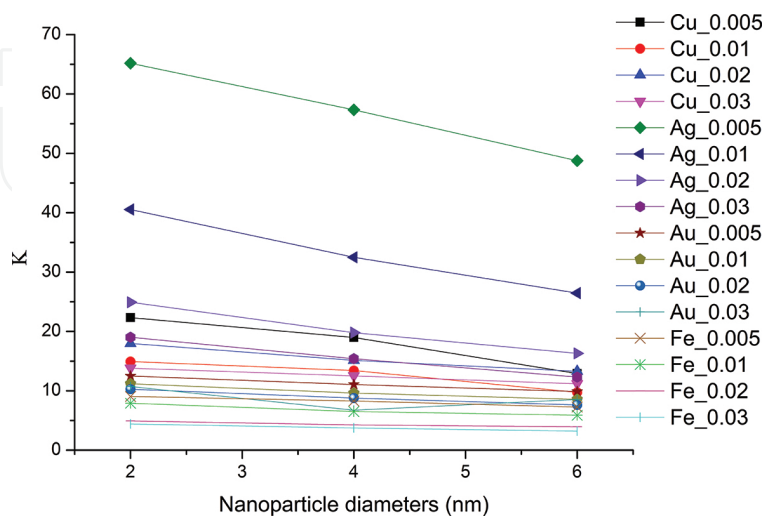**Figure 2.** Comparison of K values against nanoparticle volume fraction for various nanofluids.

Figure 3. Comparison of K values against nanoparticle size for various nanofluids.

2.2. Criterion for the increased thermal conductivity

It is found that the nanoparticles containing higher atomic potential energy (energetic atoms) are better for thermal conductivity enhancement of nanofluids [15]. The ratio of energetic atoms in a nanoparticle E is proposed as a criterion for enhanced thermal conductivity of nanofluids, which is written as:

$$E = \frac{N_E}{N},$$

(2)

where N and N_E are the quantity of atoms and energetic atoms in a nanoparticle, respectively.

If we set a standard for delimiting the energetic atoms in a nanoparticle, E can be calculated according to Eq. (2). **Figure 4** illustrates E of different types of nanoparticles. The ratio of energetic atoms in an Ag nanoparticle is the largest, and that of Fe nanoparticle is the lowest. The larger E value in a nanoparticle is better for thermal conductivity enhancement in nanofluids. **Figure 5** shows the influence of nanoparticle shapes (surface area to volume ratio S/V) for the E value. It is found that nanoparticle with larger S/V value possesses larger E value. **Figure 6** illustrates that the E value of spherical Ag nanoparticle is larger than that of Cu nanoparticle with larger S/V value. Therefore, the thermal conductivity of nanofluids with spherical Ag nanoparticles is higher than that of nanofluids with nonspherical Cu nanoparticles.
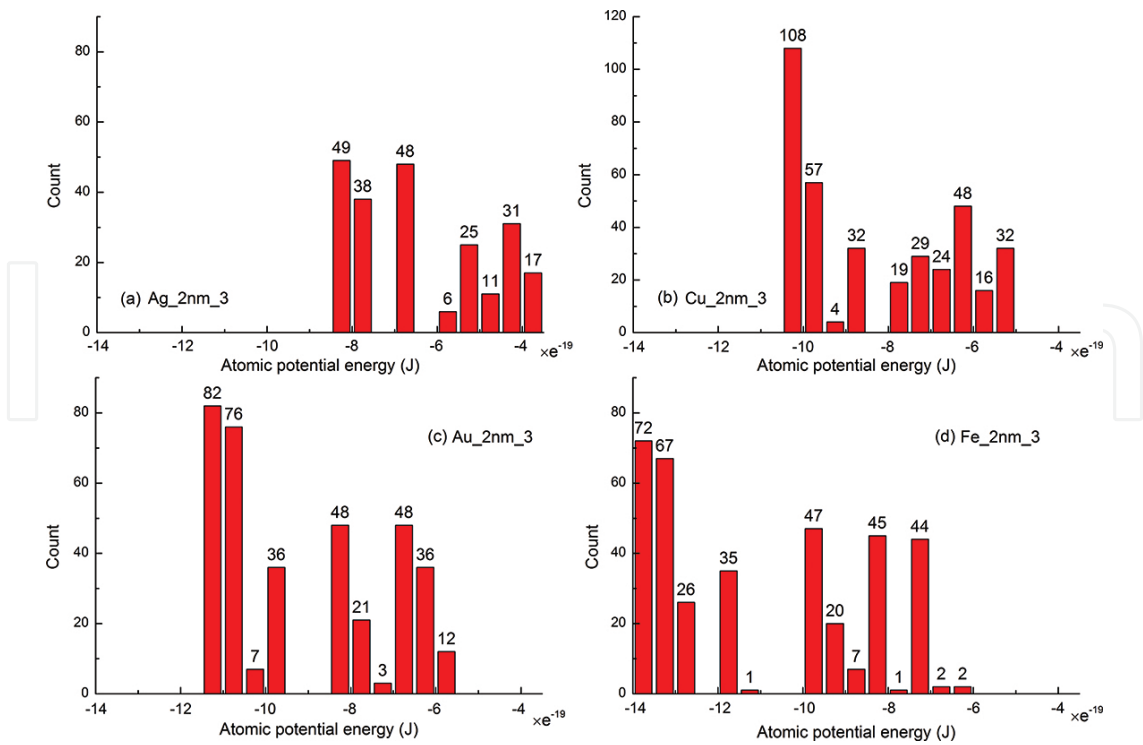

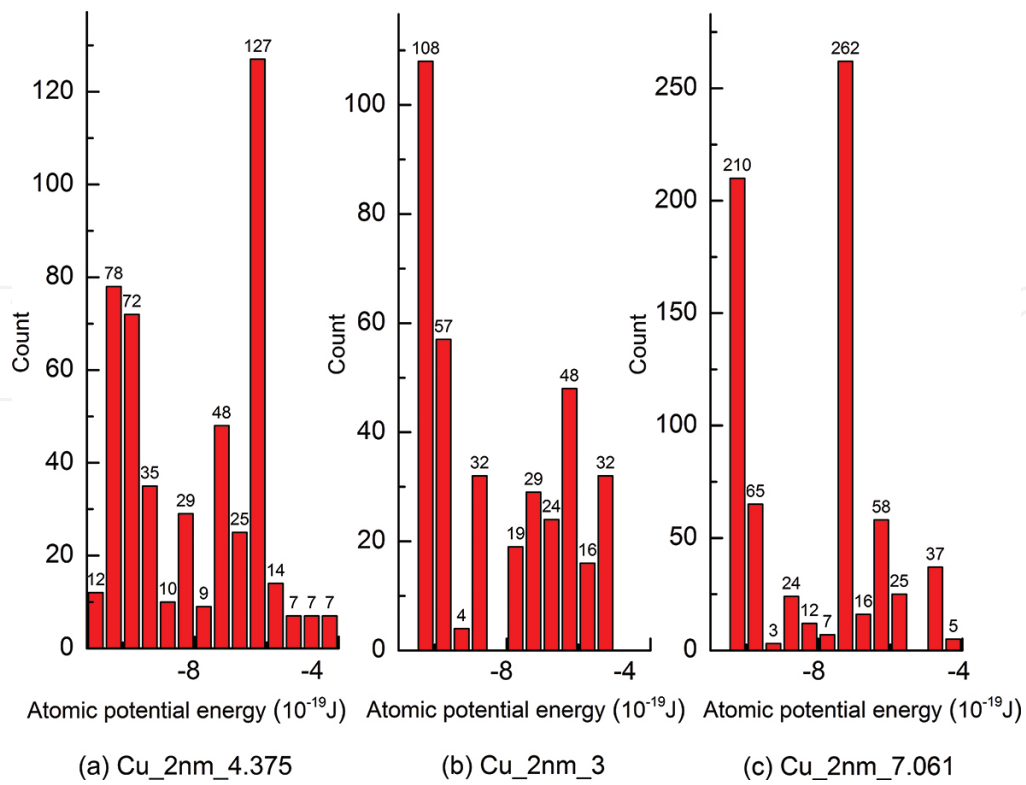**Figure 4.** Atomic potential energy distributions of various nanoparticles.

Figure 5. Comparison of atomic potential energy distributions for nanoparticles with different shapes.
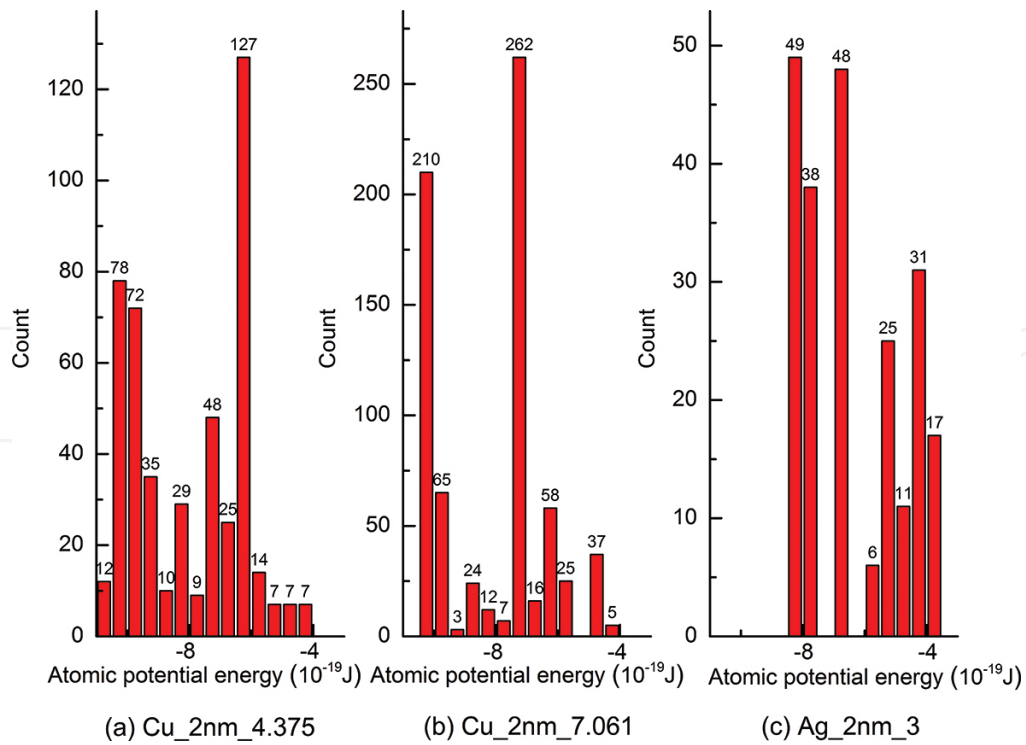

Figure 6. Comparison of atomic potential energy distributions for nanoparticles with different materials.

3. Proposed mechanisms of heat conduction in nanofluids

3.1. Altered microstructure of nanofluids

In order to analyze the microscopic structure characteristics of nanofluids, number density distribution, radial distribution function (RDF), coordination number, and potentials of mean force (PMF) should be considered [16].

Number density distribution represents the distribution of liquid atoms around a centered nanoparticle. **Figure 7** illustrates the number density distributions of base fluid atoms in different types of nanofluids. It is found that at the positions of 0.25 and 0.5 nm all the curves show the first and second peak values. But for different types of nanoparticles, the first peak values of curves are different. The order of first peak values is of the same order of thermal conductivity of bulk materials of nanoparticles.
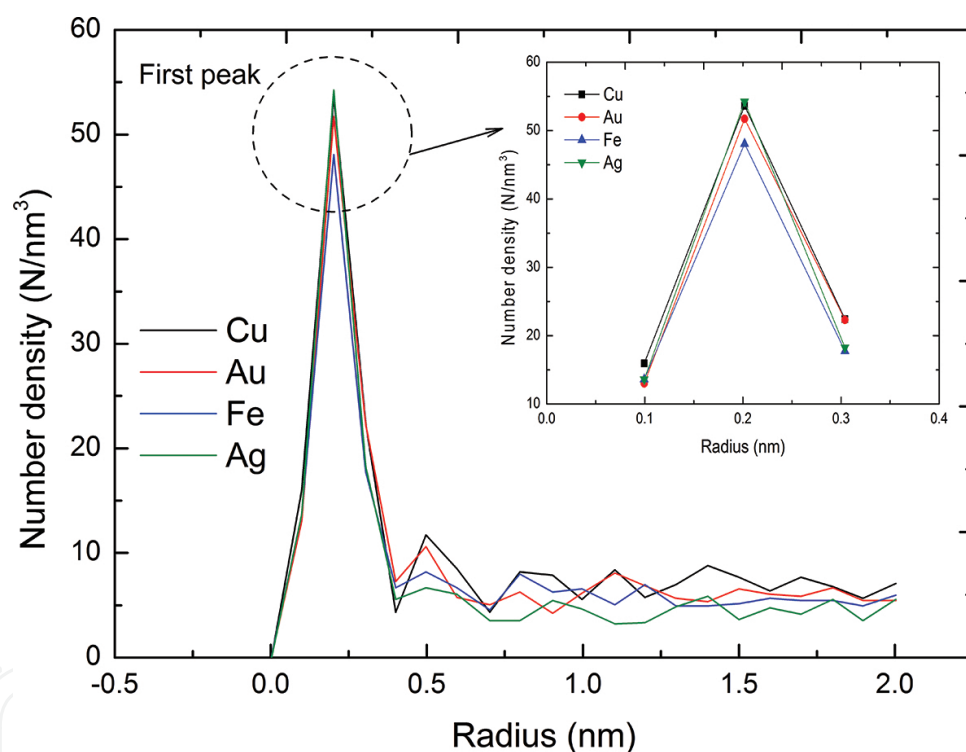

Figure 7. Statistical result of absorption layers around nanoparticles of different materials.

RDF represents the probability of finding an atom of a specified type near the central atom. Through RDF, the microscopic structure of fluid could be examined. **Figure 8** illustrates the RDF of Cu nanofluids with a 2 nm-diameter nanoparticle. In the figure, the RDF curve of "Ar-Ar" represents the chance of finding an Ar atom near the central Ar atom. It could be found that the Ar-Ar RDF shows typical characteristics of the liquid: "short-range order and long-range disorder." In the figure, the "total" RDF represents the chance of finding an atom of any type near the central atom, which represents the microscopic structure of nanofluid. It is found that the first curvilinear peak in the RDF of nanofluids is larger than that of base fluid, which

means the probability of finding an atom is higher than that in a single-phase base fluid. It could also be found that there are several diminutive curvilinear peaks in the RDF of nano-fluids, which is due to the adding of nanoparticles in base fluid. In general, the microscopic structure of nanofluid exerts a mixed up structure characteristics of liquid and solid. Both the liquid characteristic of "short-range order and long-range disorder" and the solid character-istic of "long-range order" have been found in the microscopic structure of nanofluids. Therefore, the microscopic structure of nanofluids is always ordered.
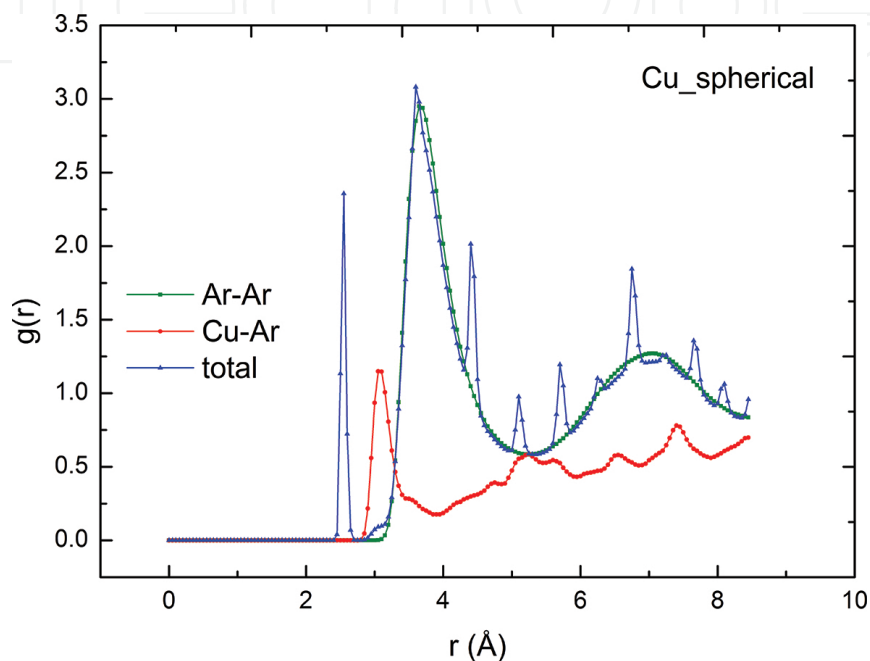

Figure 8. Radial distribution functions of nanofluids with spherical copper nanoparticle.

Coordinate number indicates the average adjacent atomic number for a certain atom within an interval of r. By comparing the coordinate number curve of Cu nanofluids with a 2 nm-diameter spherical nanoparticle, it is found that the coordinate number curves of Cu-Ar and Ar-Ar cross at 0.35 nm, which confirms that the local density of Ar atoms near a Cu atom is larger (**Figure 9**). Therefore, the existence of absorption layer is verified.

PMF reflects the combining capacity between particles in pairs. The value of PMF could be used to investigate the combining capacity between different particle pairs. **Figure 10** shows the PMF curve for Cu-Ar nanofluids. The contact minimum (CM), separated minimum (SM), and the layer barrier (LB) could easily be found in the PMF curve of nanofluids. But the positions and values of CM, SM, and LB are different for disparate atom pairs. The cis-trans direction of energy barrier between molecular layers of liquid Ar is different. When an atom is approaching the central particle, then it needs to conquer the energy barrier between the first and second molecular layers. But the atom is harder to leave the central particle. An atom of base fluid needs to conquer greater energy barrier to reenter the base fluid. The PMF of nanofluids is different from that of base fluid. At 0.3 nm, there is a huge energy barrier in the PMF of nanofluids, which indicates the surrounding atom needs to conquer two energy

barriers to get close to the central atom. The cis-trans direction of the first energy barrier is nearly the same, but the cis-trans direction of the second energy barrier is obviously different. Once a base fluid atom enters the adjacent area of the central atom, then it is very hard to reenter the base fluid because of the large energy barrier.
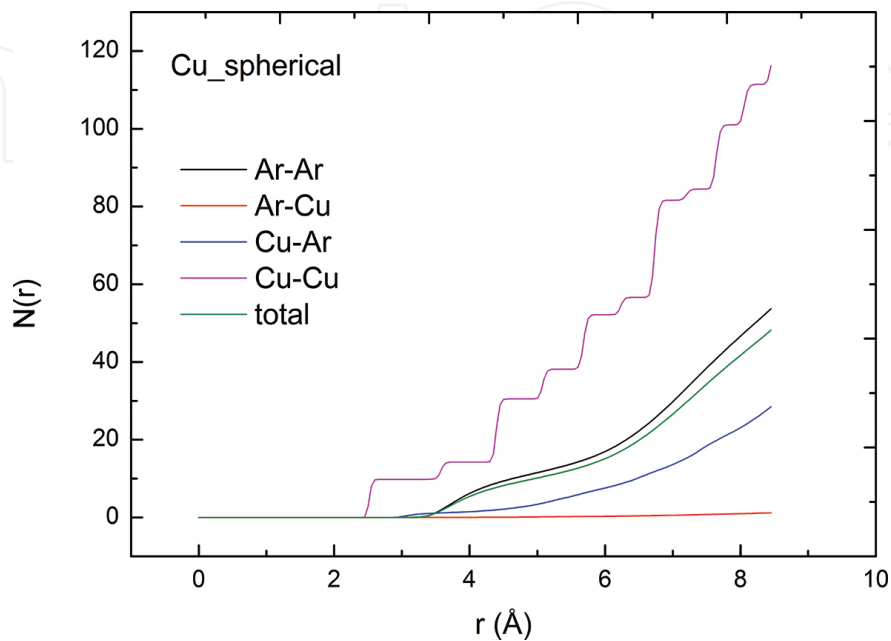

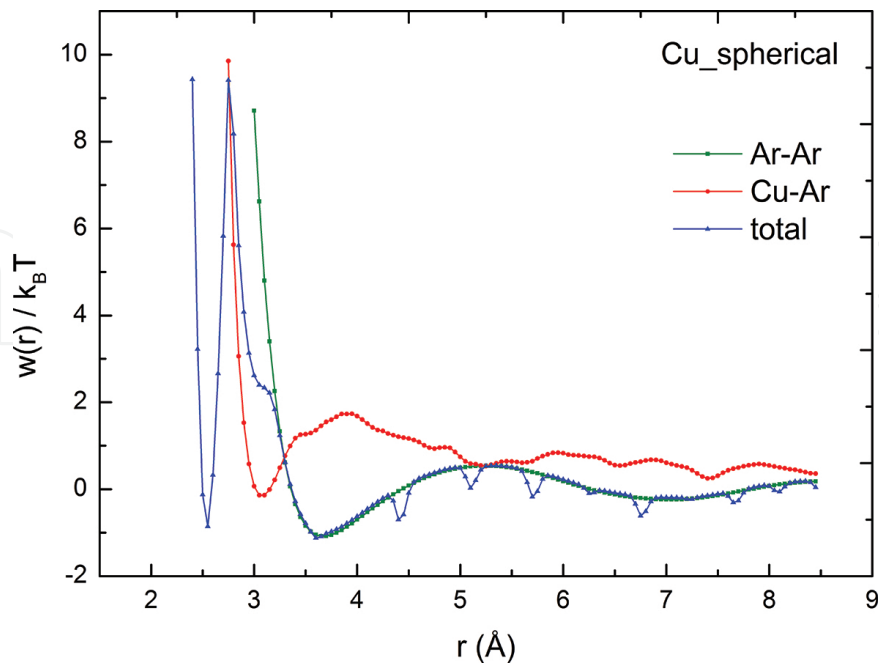**Figure 9.** The coordination number of nanofluids with spherical copper nanoparticle.

Figure 10. PMF of nanofluids with spherical copper nanoparticle.

3.2. Movements of nanoparticles in the base fluid

Through MD simulation, the nanoparticles are observed to move chaotically at high speed in the base fluid. Through MD simulation, the instantaneous velocity and position coordinates of each atom could be obtained [17]. The translational and rotational velocity of nanoparticles could be acquired by defining a group for the Cu atoms within the nanoparticle. With commands provided by LAMMPS the time-averaged translational and rotational velocity of the atom group could be calculated and output derived. For the case of imposed shearing velocity v = 50 m/s on the fluid, the translational velocity components of nanoparticles are statistically analyzed, as shown in **Figure 11**. Along x-directions, the average translational velocity components are -2 m/s~2 m/s, and the instantaneous peak value can reach 5 m/s. The translational velocity components of nanoparticles oscillate sharply, which demonstrate the chaotic movements of nanoparticles are mainly caused by their Brownian motion.
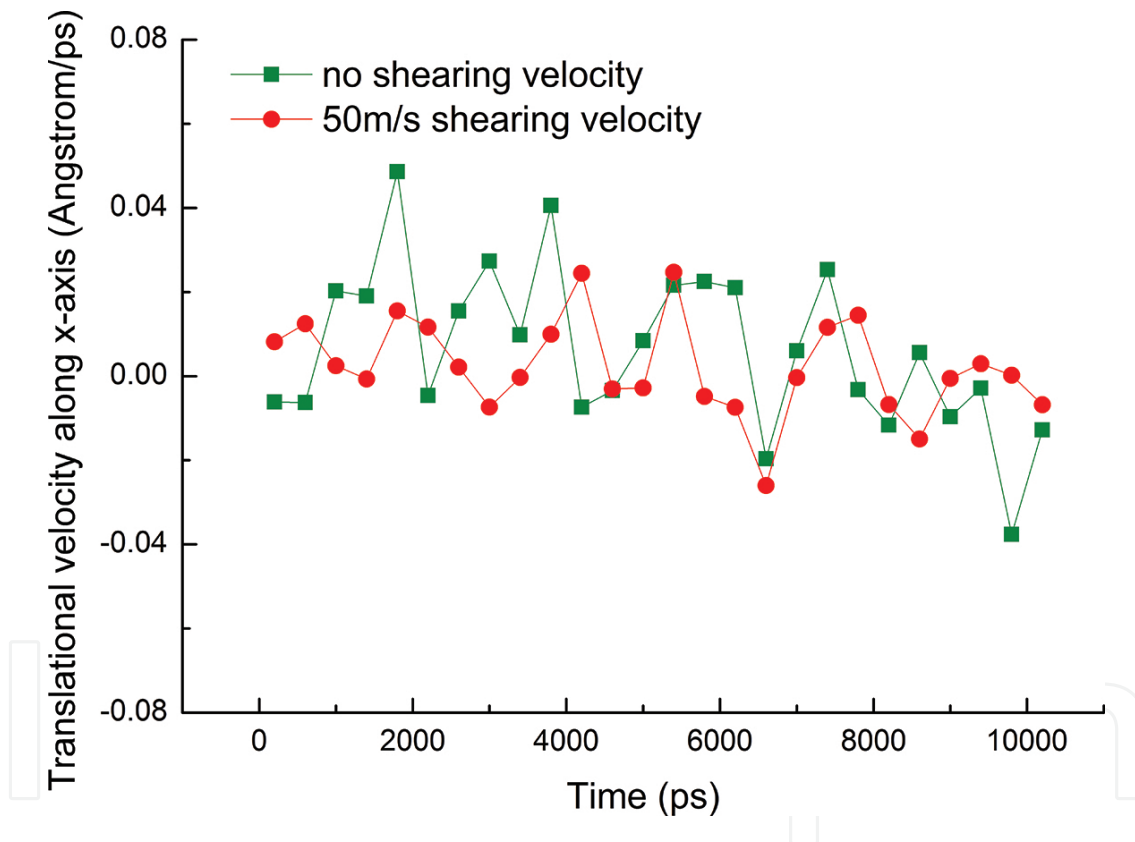

Figure 11. Translational velocity component of nanoparticle along x-axis in shearing flow.

Rotation of nanoparticles is also statistically analyzed. For the case of imposed shearing velocity 50 m/s, the angular velocity component along the x-axis of nanoparticle is shown in **Figure 12**. The peak angular velocity of nanoparticles can reach 6×10^9 rad/s, meanwhile the rotational directions of nanoparticles change randomly because of their nanoscale size. It is found that imposing shearing velocity affects little for rotation of nanoparticles. Imposed shearing velocity or not, the angular velocity components of nanoparticles are of the order of magnitude of 10^9 rad/s.
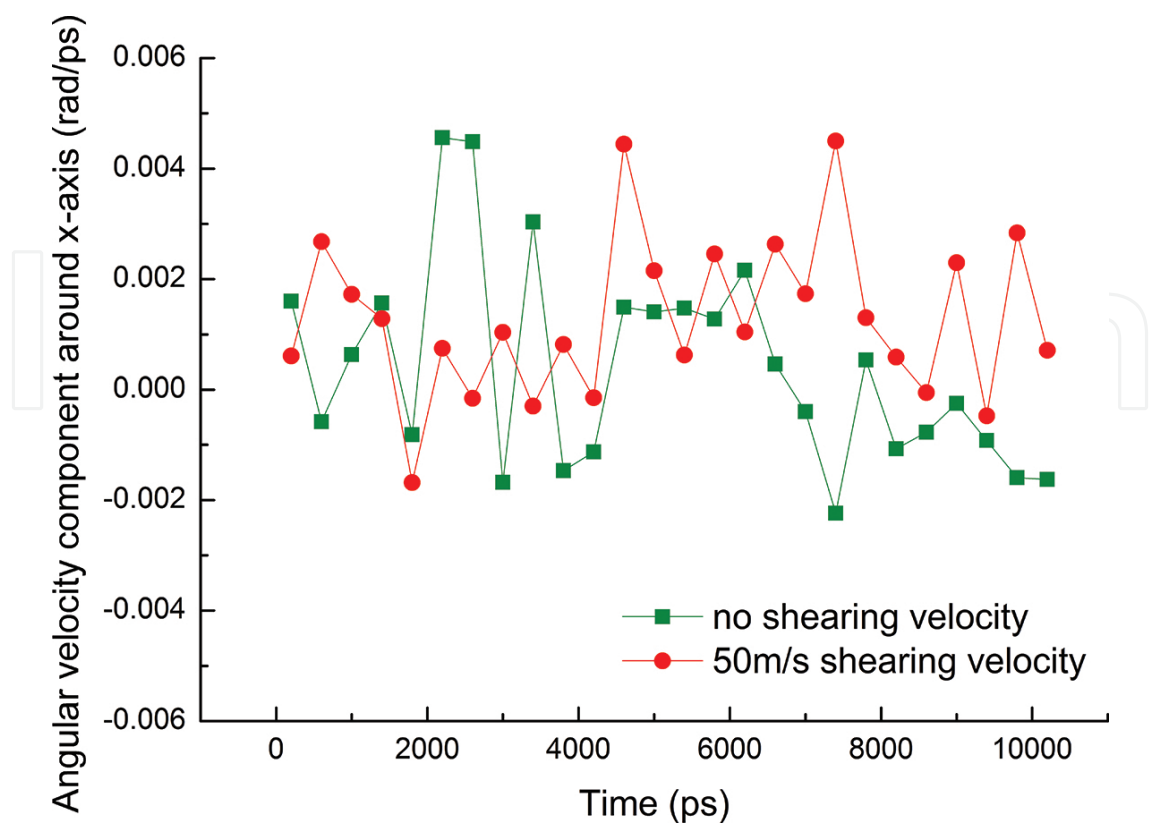
Figure 12. Angular velocity component of nanoparticle around *x*-axis.

4. Modeling thermal conductivity of nanofluids

Jeffrey applied Green's function method and relaxed the requirement of uniform configuration for particles. The formula, which is suitable for predicting suspensions with nonuniformly distributing nanoparticles and relatively large volume concentration, is written as [18],

$$\frac{k}{k_f} = 1 + 3\beta\phi_p + 3\beta(\beta + \Sigma)\phi_p^2,$$

(3)

where Σ is a convergent series, which depends on the specific value of thermal conductivity of nanoparticle and base fluid k_m/k_f. β is a coefficient, which is determined by k_m/k_f:

$$\beta = \frac{\alpha - 1}{\alpha + 2},$$

(4)

where α is the specific value of thermal conductivity of nanoparticle and base fluid k_m/k_f:

$$\alpha = \frac{k_m}{k_f}.$$

(5)

Through considering the above-mentioned mechanisms of thermal conductivity enhancement in nanofluids, a revised model for predicting thermal conductivity of nanofluids that takes into account both the static and dynamic mechanisms is proposed, which is written as[19]:

$$\frac{k_{nf}}{k_f} = \frac{k_S}{k_f} + \frac{k_D}{k_f} = 1 + 3\beta \left(1 + \frac{2t_{ab}}{d_p}\right)^3 \phi_p + c \left(1 + \frac{2t_{ab}}{d_p}\right)^6 \phi_p^2 + \frac{\phi_p (\rho c_p)_p}{2k_f} \sqrt{\frac{k_B T}{3\pi r_{cl} \mu_f}}$$

(6)

In the equation, k_{nf} is thermal conductivity of nanofluids; k_f is thermal conductivity of base fluid; k_S is the static part of thermal conductivity model for nanofluids, which takes into account the static mechanisms of heat conduction enhancement; k_D is the static part of thermal conductivity model for nanofluids; $\beta = (\alpha - 1)/(\alpha + 2)$ and $\alpha = \dfrac{k_{cl}}{k_f}$, where k_{cl} is thermal conductivity of nanoparticle cluster; t_{ab} is the thickness of absorption layer formed by absorbed liquid molecules which can be estimated by Langmuir monolayer equation; d_p is the average diameter of nanoparticles; Φ_p is the initial volume concentration of nanoparticles in nanofluids; $c = 3\beta^2 + 3\beta\Sigma$ is a coefficient in Jeffrey Model; ρ is the density of nanoparticle bulk material; c_p is the specific heat of nanoparticle bulk material; k_B is the Boltzmann constant and $k_B = 1.381 \times 10^{-23} J/K$; T is thermodynamic temperature; r_{cl} is the radius of the nanoparticle cluster; and μ_f is the viscosity of base fluid.

Compared with existing prediction models for thermal conductivity of nanofluids, the present model takes into account the static and dynamic mechanisms of strengthened heat conduction in nanofluids simultaneously and possesses more definite physics meaning. In addition, parameters used in the current model are more precise that ensures the veracity of prediction result. For instance, the thermal conductivity of nanoparticles k_p is distinguished with that of bulk material of nanoparticles k_m and used in the prediction model as an independent parameter. And the thermal conductivity of nanoparticles-cluster k_{cl} is introduced as an independent parameter to include the heat conduction of absorption layer, which further improves the prediction accuracy of the present model.

Through comparing the prediction results of the present model and existing experimental data, the present prediction model is proved to be quite effective for predicting thermal conductivity of common nanofluids, as shown in **Table 2**. For various types of nanofluids (with different materials including: metal, metallic oxide, and nonmetallic oxide, different volume fractions, or different nanoparticle diameters), the present model gives good predictions.

References	NF	NP size (nm)	Volume fraction (%)	Thermal conductivity ratio (k_{nf}/k_f)	Present model	Maximum error
Masuda [20]	Al$_2$O$_3$/Water	13	1.3–4.3	1.107–1.318	1.097–1.322	0.9%
Teng et al. [21]	Al$_2$O$_3$/Water	20	0.001–0.005	1.018–1.065	1.010–1.043	2.1%
Chon et al. [22]	Al$_2$O$_3$/Water	13	1	1.081	1.072	0.9%
Xie et al. [23]	Al$_2$O$_3$/EG	25	1.7–5	1.097–1.294	1.103–1.303	0.8%
Vajjha [24]	Al$_2$O$_3$/ (60:40% EG/W)	53	1–4	1.069–1.159	1.048–1.195	3.1%
Wang et al. [25]	Al$_2$O$_3$/EG	28	5–8	1.246–1.404	1.276–1.445	2.9%
Eastman et al. [26]	CuO/EG	35	1–4	1.050–1.227	1.061–1.245	3.7%
Lee et al. [27]	CuO/EG	24	1–4	1.060–1.242	1.047–1.212	3.2%
Xuan and Li [28]	Cu/Water	100	1–5	1.078–1.434	1.090–1.459	3.1%
Li et al. [29]	Cu/Water	20	1–3	1.120–1.289	1.096–1.293	2.1%
Eastman et al. [26]	Cu/EG	10	0.33–0.55	1.041–1.101	1.061–1.122	2%
Hwang et al. [30]	CuO/Water	33	1	1.05	1.08	2.9%
Zhang et al. [31]	SiO$_2$/Water	7	0.5–3	1.016–1.084	1.014–1.088	0.4%
Hwang et al. [30]	SiO$_2$/Water	12	1	1.03	1.03	0

Table 2. Comparison between the prediction results and experimental data.

5. Concluding remarks

Thermal conductivities of nanofluids with various nanoparticles have been calculated through MD simulations. Influence rule of various factors for thermal conductivity of nanofluids has been studied. Through defining the ratio of thermal conductivity enhancement by nanoparticle volume fraction, K, the impacts of nanoparticle properties for thermal conductivity are further evaluated. Furthermore, the ratio of energetic atoms in nanoparticles, E, is proposed to be an effective criterion for judging the impact of nanoparticles for the thermal conductivity of nanofluids.

Mechanisms of heat conduction enhancement are investigated by MD simulations. Altered microstructure and movements of nanoparticles in the base fluid are proposed to be the main reasons for thermal conductivity enhancement in nanofluids. Number density distribution, radial distribution function (RDF), coordination number, and potentials of mean force (PMF) are used to analyze the microscopic structure characteristics of nanofluids. Through MD simulation, the average translational and rotational velocities of nanoparticles are obtained.

Both the static and dynamic mechanisms for heat conduction enhancement in nanofluids have been considered to establish a prediction model for thermal conductivity. The parameters in

the model have definite physical meaning and are more precise. The prediction results of the present model are in good agreement with experimental results.

Acknowledgements

Nomenclature

E	Ratio of energetic atoms in a nanoparticle
K	Ratio of thermal conductivity enhancement by nanoparticle volume fraction
N	Quantity of atoms in a nanoparticle
N_E	Quantity of energetic atoms in a nanoparticle
S/V	Surface area to volume ratio
T	Thermodynamic temperature
V	Volume of nanofluids
V_{np}	Volume of nanoparticles
c_p	Specific heat of nanoparticle bulk material
d_p	Average diameter of nanoparticles
k	Thermal conductivity
kB	Boltzmann constant
k_f	Thermal conductivity of base fluids
k_m	Thermal conductivity of bulk material
k_p	Thermal conductivity of nanoparticles
k_{cl}	Thermal conductivity of nanoparticles' cluster
r_{cl}	Radius of the nanoparticle cluster
t_{ab}	Thickness of absorption layer
α	Specific value of thermal conductivity of nanoparticle and base fluid
μ_f	Viscosity of base fluid
ρ	Density of nanoparticle bulk material
Φ_p	Volume concentration of nanoparticles in nanofluids

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