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A Theoretical Study on Thermal Conductivity of Zn-Nanofluid

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ABSTRACT

A coupled molecular dynamics (MD)-stochastic model has been developed for predicting the thermal conductivity of a hypothetical water based Zn-nanofluid taking into account the heat transfer during and after collision of the nanoparticles with the heat source. The model has predicted a somewhat lower enhancement in thermal conductivity of water based Zn-nanofluid compared to water based Cu-nanofluid under identical conditions. The theoretical predictions need experimental verification. The model establishes the role of thermal as well as mechanical properties of the nanoparticles in enhancing the thermal conductivity of nanofluids.

Key words: **Molecular dynamics, Nanofluid, Thermal conductivity**

1. Introduction

Nanofluids, i.e. colloidal suspensions of nanoparticles dispersed in liquids, are likely to be the future heat transfer media in advanced heat transfer applications since they have significantly enhanced thermal conductivity compared to that of conventional heat transfer fluids [1-3]. Designing nanofluids for a given practical application requires an accurate theoretical knowledge of the thermal conductivity of nanofluids. However, at present we don't have adequate theoretical understanding on the thermal conductivity of nanofluids [4]. Although some attempts have been made to theorize the thermal conductivity of nanofluids [5-8] it still remains as a subject of hot debate [9]. A generally accepted model which has the capability to explain the thermal conductivity of diverse types of nanofluids is still lacking [10].

The present work aims to theoretically estimate the thermal conductivity of a hypothetical water based Zn-nanofluid. The Zn-nanoparticles suspended in water medium will inevitably undergo Brownian motion, in course of which they will repeatedly collide with the heat source. During the collision rapid conductive heat transfer will take place due to solid-solid contact. Subsequent to the collision, when the nanoparticle undergoes Brownian motion through the bulk fluid it releases the excess heat to the fluid. Therefore, some amount of heat is transferred by conduction mode due to the collision of the suspended nanoparticles with the heat source, in addition to the normal conductive heat transfer through the base fluid itself. The extent of this heat transfer has been estimated with the help of molecular dynamics (MD) simulation in combination with stochastic simulation to compute the enhancement in thermal conductivity of the water based Zn-nanofluid as a function of volume fraction loading of nanoparticles. The scheme of simulation has been presented here. More detailed account of the simulation has been given elsewhere [11]. The thermal conductivity estimated on the basis of the present model for water based Cu-nanofluid has reasonable agreement with the experimental data [11]. However, the predicted thermal conductivity for water based Zn-nanofluid needs to be tested against experimental data. It has been explained with the help of present theoretical model why mechanical properties of nanoparticles are more important than their thermal properties in enhancing the thermal conductivities of nanofluids.

2. Simulation Procedure

In order to theoretically estimate the thermal conductivity of a hypothetical water based Zn-nanofluid first a block shaped Zn-heat source has been generated. A Zn-nanoparticle with diameter 4 nm has also been generated. The Zn-heat source has been equilibrated at 370 K and the Zn-nanoparticle has been equilibrated at temperatures ranging

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from 298 K to 358 K using isokinetic thermostat. After equilibration at the predetermined temperatures the Zn-nanoparticle has been directed towards the Zn-heat source with a velocity equal to the collision velocity. The average collision velocity for a Zn-nanoparticle of 4 nm diameter is 4.640 m/s, as estimated from the preliminary stochastic simulation. During collision of the Zn-nanoparticle with the Zn-heat source the temperatures of both the nanoparticle and heat source has been estimated from the average kinetic energy of the atoms containing them. In the MD simulation Lennard-Jones pair potential [12] has been assumed for all interatomic interactions. The time modulation of phase space of atoms of both the nanoparticle and heat source has been generated by velocity-verlet algorithm [12] using a time step size of 10^{-14} s. The period of collision estimated from impact dynamics [13] is 12.91 ps. MD simulations of the collision have been carried out for different initial temperature of the nanoparticle (298-358 K) in order to estimate the temperature rise of nanoparticle due to collision with the heat source.

After the collision the nanoparticle moves through the base fluid by Brownian motion. In the present simulation the Brownian phase space of the particle with progress of time has been evaluated by stochastic simulation [14]. During Brownian motion subsequent to the collision the nanoparticle releases the excess heat to the surrounding fluid as per the rule of flow past a spherical nanoparticle [6]. Based on the characteristic thermal history of the nanoparticles which have been released from different initial distances from the heat source the enhancement in thermal conductivity of the nanofluid for a given volume fraction loading of nanoparticles has been estimated [11].

3. Results and Discussion

Figure 1 shows the temperature variations of the heat source which has been equilibrated at 370 K (Fig. 1(a)) and the nanoparticle which has been equilibrated at 298 K (Fig. 1(b)). It is apparent that at the end of 10000 time steps of 1 fs both the objects get equilibrated at the desired temperatures.

Figure 2 displays the configuration of the nanoparticle and heat source prior to the collision. It is apparent that there is negligible distortion of the objects after equilibration.

The MD simulation of collision of a Zn-nanoparticle (4 nm dia.) with a Zn-heat source has yielded the temperature variations of the nanoparticle and heat source as shown in Fig. 3. Here the initial temperature of the nanoparticle is 298 K and that of the heat source is 370 K, and starting velocity for collision of the nanoparticle with the heat source is 4.640 m/s which is the average collision velocity as estimated from preliminary stochastic simulation for a Zn-nanoparticle of 4 nm diameter undergoing Brownian motion in water. Rapid rise in temperature of the nanoparticle has also been observed here as in the case of Cu-nanoparticle colliding with a Cu-heat source [11]. However, within the collision period of 12.91 ps the Zn-nanoparticle which was initially at a temperature of 298 K did not attain the temperature of the Zn-heat source. Hence, pulse-like heat transfer during the collision is partially effective in this case.

Figure 4 depicts the collision induced temperature rise of the nanoparticle as a function of the initial temperature of the nanoparticle. Here, in all the cases the nanoparticle has been directed towards the heat source with a starting velocity equal to the average collision velocity (4.640 m/s) estimated from preliminary stochastic simulation. It is apparent that the collision induced thermal pick up by the nanoparticle decreases with increasing the pre-collision temperature of the nanoparticle. This is because of the fact that the magnitude of heat flux to the nanoparticle during the collision decreases with decrease in the temperature difference between the heat source and nanoparticle.

The trajectory of a Zn-nanoparticle of 4 nm diameter undergoing Brownian motion in water medium within a time frame of 1 s has been shown in Fig. 5 which is characteristic of Brownian motion of any particle of very small size suspended in a fluid medium. Here the particle has been initially released from a distance of 1 mm from the heat source with zero velocity. It is apparent that during the Brownian motion the nanoparticle repeatedly collides with the heat source. Here the YZ-plane which is passing through origin is the surface of the heat source in contact with the nanofluid.

The characteristic thermal history of a Zn-nanoparticle of 4 nm diameter suspended in a water based nanofluid has been displayed in Fig. 6. This has been evaluated by MD simulation coupled with stochastic simulation. It is apparent that the Zn-nanoparticle (4 nm dia.) which acquires heat from the heat source within ~12 ps during the collision releases the excess heat to the surrounding water medium within 2-3 ms subsequent to the collision.

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The enhancement in thermal conductivity as predicted by MD simulation coupled with stochastic simulation for the hypothetical water based Zn-nanofluid has been shown in Fig. 7. The predicted enhancement in thermal conductivity for water based Cu-nanofluid as a function of volume fraction of nanoparticles [11] has also been superimposed in Fig. 7. It shows that at low volume fraction loading of nanoparticles (<0.3 vol.%) the predicted enhancement in thermal conductivity of water based Zn-nanofluid as well as water based-Cu nanofluid varies linearly with volume% loading of nanoparticles. It is also apparent that for a given volume fraction loading the water based Zn- (4 nm dia.) nanofluid shows ~23% lower enhancement in thermal conductivity compared to that of the water based Cu- (4 nm dia.) nanofluid. This is due to much lower thermal conductivity of Zn (113 W m^{-1} K^{-1}) compared to Cu (401 W m^{-1} K^{-1}) [15]. Thus, the present model predicts lower potential of Zn-nanofluid in enhancing the thermal conductivity compared to that of the Cu-nanofluid. These predictions for water based Zn-nanofluids need to be tested against experimental data.

It is to be noted here that the present model considers collision period and thermal conductivity of nanoparticles as important parameters for the enhancement in thermal conductivity of nanofluids. The collision period [13] depends on the density, collision velocity and elastic properties of the nanoparticle. The collision velocity which depends on the Brownian motion parameters has been evaluated based on the preliminary stochastic simulation. The data of thermal conductivity, density, Young's modulus, Poisson's ratio, collision velocity and calculated collision period of Zn, Cu and Ag nanoparticles of 4 nm diameter suspended in respective water based nanofluids have been presented in TABLE 1. It is apparent that Cu and Ag have comparable thermal conductivity (TABLE 1). However, recent studies [16] have revealed 7 times more enhancement in thermal conductivity of water based Ag- (4 nm dia.) nanofluid compared to water based Cu- (4 nm dia.) nanofluid. This is due to ~25% higher collision period [13] of Ag nanoparticle (16.98 ps) compared to the Cu nanoparticle (13.59 ps). On the other hand, the collision period of Zn and Cu are comparable to each other (TABLE 1). However, the thermal conductivity of Zn (113 W m^{-1} K^{-1}) is ~72% less than that of Cu (401 W m^{-1} K^{-1}) [15]. This results in only ~23% lower enhancement in thermal conductivity of water based Zn-nanofluid compared to water based Cu-nanofluid for the same volume fraction loading of nanoparticles. Thus, it appears from the present model that compared to the thermal conductivity of nanoparticles, the collision period which in turn depends on the mechanical properties of the nanoparticles is much more effective in enhancing the thermal conductivity of nanofluids.

4. Conclusions

In conclusion, a model has been developed for predicting the thermal conductivity of water based Zn-nanofluid on the basis of MD simulation coupled with stochastic simulation. In the nanofluid the nanoparticles collide with the heat source repeatedly in course of their Brownian motion through the base fluid. MD simulation has revealed that during the collision rapid heat transfer takes place, although to a less extent compared to Cu-nanofluid. The thermal energy which is acquired by the nanoparticles within ~12 ps during the collision is dissipated to the surrounding water medium within 2-3 ms during subsequent Brownian motion of the nanoparticles through the base fluid. Repeated occurrence of this phenomena results in a significant enhancement in thermal conductivity of the nanofluid. The model predicts a linear variation in the enhancement in thermal conductivity of water based Zn-nanofluid with volume fraction loading of nanoparticles. It is also predicted that for a given volume fraction loading water based Zn-nanofluid would show ~23% lower enhancement in thermal conductivity compared to water based Cu-nanofluid. The theoretical predictions for water based Zn-nanofluids are amenable to experimental verification. The model points out that compared to the thermal properties, the collision period which depends on the mechanical properties of the nanoparticles is a much more effective parameter for the enhancement in thermal conductivity of nanofluids.

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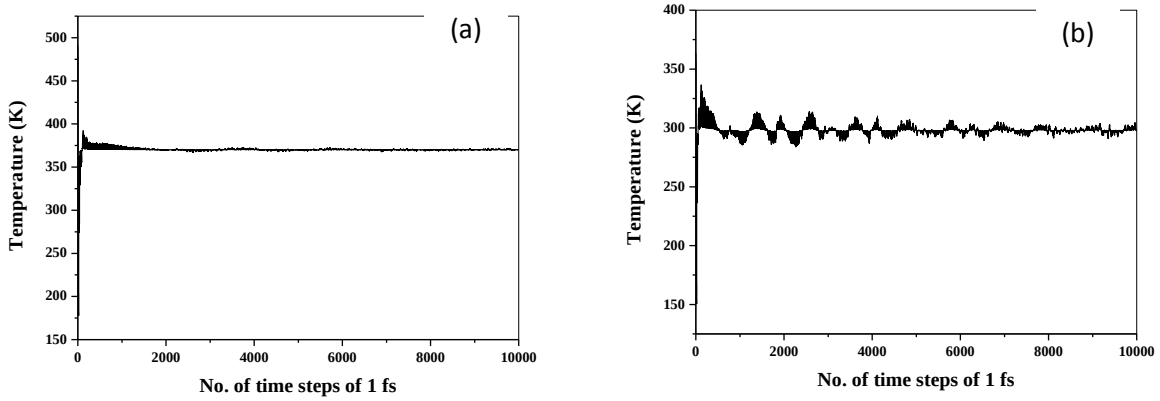

Fig. 1: Temperature variations of a Zn-heat source (a) and a Zn-nanoparticle (b) of 4 nm diameter during equilibration at 370 K and 298 K, respectively.

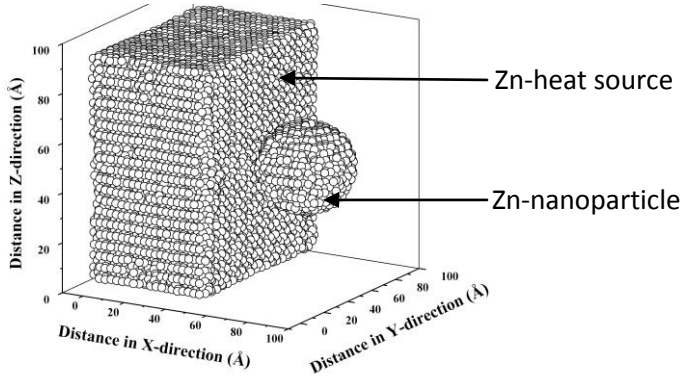

Fig. 2: Configuration of the Zn-nanoparticle (4 nm dia.) and Zn-heat source prior to the collision with each other. The nanoparticle was equilibrated at 298 K and the heat source was equilibrated at 370 K.

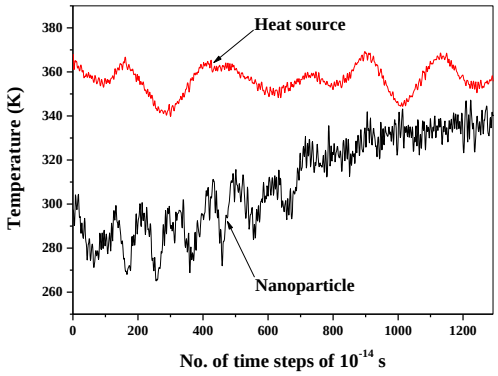

Fig. 3: Temperature variations of a Zn-nanoparticle (4 nm dia.) and a Zn-heat source during collision with each other. The initial temperature of the nanoparticle is 298 K and that of the heat source is 370 K.

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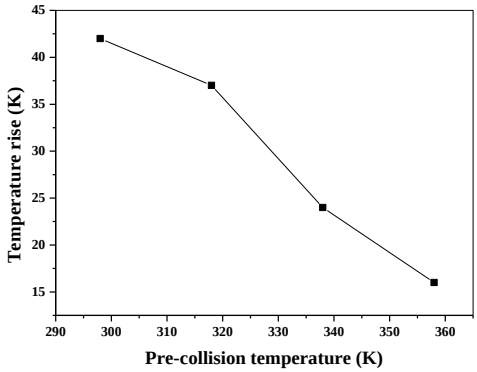

Fig. 4: Temperature rise of a Zn-nanoparticle of 4 nm diameter colliding with a Zn-heat source at a starting velocity of 4.640 m/s, as a function of initial temperature of the nanoparticle.

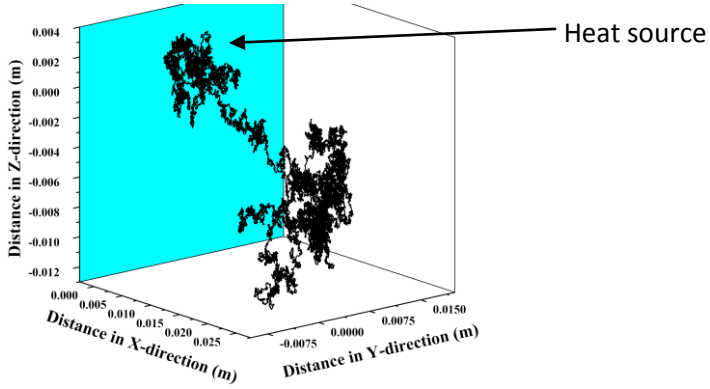

Fig. 5: Trajectory of Brownian motion of a Zn-nanoparticle of 4 nm diameter in water medium within a time frame of 1 s.

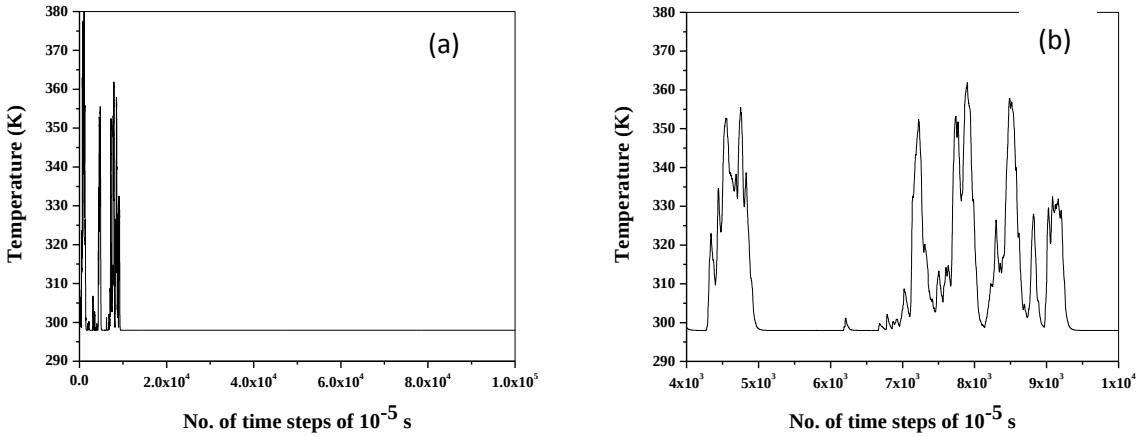

Fig. 6: (a) Simulated thermal profile of a Zn particle of 4 nm diameter moving in water by Brownian motion. Here wider peaks depict multiple collisions with the heat source. (b) A magnified plot of temperature variation of a nanoparticle undergoing multiple collision with heat source in the time interval of 0.04 to 0.10 s in (a).

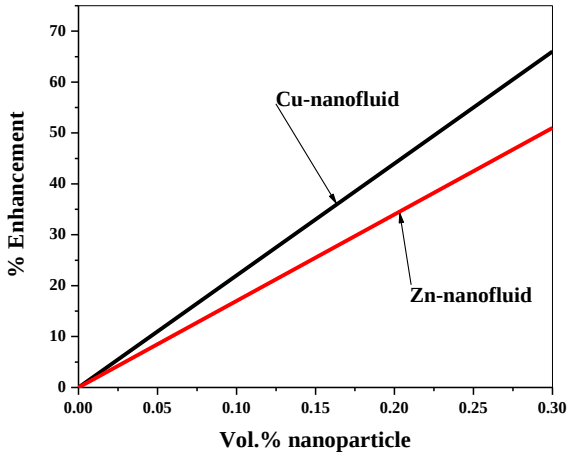

Fig. 7: The enhancement in thermal conductivity of water based Zn- (4 nm dia.) nanofluid, predicted on the basis of MD simulation coupled with stochastic simulation as a function of volume fraction loading of nanoparticles, compared with the predicted enhancement in thermal conductivity of water based Cu- (4 nm dia.) nanofluid.

TABLE 1: Thermal conductivity, density, Young's modulus, Poisson's ratio, collision velocity and collision period of Zn, Cu and Ag nanoparticles of 4 nm diameter.

Nanomaterial	**Thermal conductivity (W/mK)**	**Density (Kg/m^3)**	**Young's modulus (GPa)**	**Poisson's ratio**	**Collision velocity (m/s)**	**Collision period (ps)**
Zn	113	7140	108	0.25	4.640	12.91
Cu	401	8920	120	0.32	4.151	13.59
Ag	429	10500	83	0.37	3.746	16.97