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MOLECULAR DYNAMICS SIMULATION OF THERMAL CONDUCTIVITY AND VISCOSITY OF A NANOFLUID: EFFECT OF NANOPARTICLE AGGREGATION

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ABSTRACT

Effect of nanoparticle aggregation on the thermal conductivity and viscosity of nanofluids is studied by molecular dynamics simulation in this work. Thermal conductivity and viscosity of the nanofluid are calculated using Green-Kubo method and results show that the nanoparticle aggregation induces a significant enhancement of thermal conductivity in nanofluid, while the increase of viscosity is moderate. The results also indicate that different configurations of the nanoparticle cluster result in different enhancements of thermal conductivity and increase of viscosity in the nanofluid. The differences between equilibrium molecular dynamics (EMD) approach and non-equilibrium molecular dynamics (NEMD) approach in obtaining the thermophysical properties of nanofluids are also discussed.

INTRODUCTION

Nanofluids are a new class of nanotechnology-based heat transfer fluids that are devised by stably suspending a small amount (1 vol % or less) of nanoparticles, nanofibers, or nanotubes with length on the order of 1-50 nm in the traditional heat transfer fluids [1]. Researches have shown that the nanofluids exhibited very high thermal conductivity even for low concentrations of suspended nanoparticles [2, 3]. Moreover, some researchers have demonstrated that, by experimental method, the enhancement of thermal conductivity for nanofluids will increase as temperature increases [4, 5] and this makes nanofluids even more attractive as cooling fluid for devices with high energy density.

The anomalous thermal properties of nanofluids mentioned above attracted attentions from many researchers and prompted them to reveal the mechanism of heat transfer in nanofluids. Keblinski et al. [6] suggested four possible mechanisms that might explain the anomalous thermal conductivity enhancement in nanofluids. One of these mechanisms, whose importance is being recognized by some researchers in the resent years, is the aggregation effect of nanoparticles. Xuan et al. [7] and Murshed et al. [8] observed the nanoparticle aggregation using transmission electron microscope (TEM) in their experiments. Also by carrying out experiment, Philip et al. [9] suggested that nanofluids containing well-dispersed nanoparticles, i.e., without aggregates, did not exhibit significant enhancement of thermal conductivity; while the maximum enhancement was observed when chain-like aggregates are uniformly dispersed without clumping. Keblinski et al. [10] summarized the published experiment data and found that they all laid between the well-known Hashin and Shtrikman (H-S) effective medium bounds which takes the nanoparticle aggregation effect into account. However, some researchers do not agree with this explanation for the enhancement of thermal conductivity in nanofluids. Rather, they believed that the nanoparticle aggregation and the formation of aggregates reduced the efficiency of the energy transport enhancement of the suspended nanoparticles, either by theoretical analysis [7] or experiment [11]. The role of nanoparticle aggregation on the enhancement of thermal conductivity in nanofluids is still under debate and is not conclusive.

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Viscosity is another important property that should be taken into account in choosing a heat transfer fluid. Although the nanofluid has a thermal conductivity higher than the traditional heat transfer fluids, as a solid-liquid mixture, its viscosity is also higher than the base fluids. The increase of viscosity may diminish the potential benefits of nanofluids. Prasher et al. [12] suggested that the increase in the nanofluid viscosity is higher than the enhancement in the thermal conductivity. If the viscosity has a increase of more than a factor of 4 relative to the increased thermal conductivity, it will make the nanofluid worse than the base fluid. Grag et al. [13] also mentioned that the nanofluid would not be beneficial as a coolant in heat exchangers without changing the tube diameter. Therefore, it is imperative to conduct more comprehensive studies on the viscosity of nanofluids.

In this paper, a molecular dynamics (MD) simulation is performed to study the effect of nanoparticle aggregation on the enhancement of thermal conductivity and increase of viscosity in nanofluids. Unlike many other MD simulations on nanofluid which have only one nanoparticle in the simulation box with periodic boundary condition, in this work multiple nanoparticles are placed in the simulation box which makes it possible to simulate the aggregation of the nanoparticles.

METHODOLOGY

The nanofluid system studied in this work is formed by disperse copper nanoparticles in the liquid argon. Initially, the simulation box is created with a face centered cubic (FCC) lattice structure using the lattice constant of argon that is determined by the desired density. Then, spherical regions in the simulation box are carved out and new FCC structures are created in these spherical regions using the lattice constant of copper. Finally, different types of atoms, i.e., argon atoms and copper atoms, were displaced in the corresponding regions respectively and a copper-argon nanofluid system is then established.

For a MD simulation, the most important step is to choose an interatomic potential that describes the interaction between atoms. In this work, two different potentials are used. One is the well-known Lennard-Jones (L-J) potential which matched the experimental data reasonably well for the property of liquid argon and this is also why the liquid argon was chosen as the base fluid in this simulation. The other is the embedded atom method (EAM) potential which takes the metallic boding into account and is more accurate in describing the interatomic interaction between metal or alloy atoms.

The interatomic interaction between argon-argon and argon-copper atoms are described by the well-known L-J potential:

$$\Phi\left(r_{ij}\right)=4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12}-\left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

where the L-J potential parameters for copper-argon and argon-argon are $\varepsilon_{Ar\text{-}Ar}$ =1.67 × 10^{-21} J, $\sigma_{Ar\text{-}Ar}$ = 0.3405 nm, $\varepsilon_{copper\text{-}Ar}$ = 10.4153 × 10^{-21} J, $\sigma_{copper\text{-}Ar}$ = 0.2872 nm [14]. For the interaction of copper-copper atoms, the EAM potential is used. The total potential energy E_i (for pure metal) of the atom i is given by [15]:

$$E_i=F_i\left(\sum_{j\neq i}\rho_i\left(r_{ij}\right)\right)+\frac{1}{2}\sum_{j\neq i}\varphi_{ij}\left(r_{ij}\right) \tag{2}$$

where F_i is the embedding energy of atom i and it is a function of the atomic electron density ρ; φ is a short-range pair potential interaction between the atoms i and j.

An equilibrium molecular dynamics (EMD) method, i.e., the Green-Kubo (G-K) method, is used to calculate the thermal conductivity and shear viscosity of the nanofluid. The G-K approach uses flux fluctuations to compute the thermal conductivity and shear viscosity via the fluctuation-dissipation theorem [16]. No driving force is imposed in the simulation system and as a result it will always in the linear response regime. This makes it one of the most important advantages in using G-K approach compared with the non-equilibrium molecular dynamics (NEMD) method. The thermal conductivity using G-K method is obtained from [17]:

$$k=\frac{1}{3k_BVT^2}\int_0^\infty\left\langle\mathbf{J}(0)\cdot\mathbf{J}(\tau)\right\rangle d\tau \tag{3}$$

If the system is homogeneous, Eq. (3) can be reduced to:

$$k=\frac{1}{k_BVT^2}\int_0^\infty\left\langle J_x(0)J_x(\tau)\right\rangle d\tau \tag{4}$$

where k_B is the Boltzmann constant; V is the volume of the system; T is the temperature; J_x is an arbitrary component of $\boldsymbol{J}$, the instantaneous microscopic heat flux vector, and the thermal conductivity k can be determined by averaging over the entire three components. The form of $<J_x(0)J_x(\tau)>$ gives the time correlation function of the heat flux and the angular bracket here denotes the time origin average of the time correlation function. Since the simulations are performed for discrete MD steps of length Δt, Eq. (4) for calculating thermal conductivity can be rewritten as:

$$k\left(t_M\right)=\frac{\Delta t}{k_BVT^2}\sum_{m=0}^{M}\frac{1}{N-m}\sum_{n=1}^{N-m}J_x\left(m+n\right)J_x\left(n\right) \tag{5}$$

where t_M is given by M times Δt and $J_x(m+n)$ is the heat flux in the x direction at time step m+n, which means m time steps delayed with respect to $J_x(n)$. The instantaneous microscopic heat flux for a binary system in the x-direction is calculated as [18]:

$$J_x=\sum_i^N v_{ix}e_i+\frac{1}{2}\sum_i^N\sum_{j\neq i}^N(x_{ij}\cdot f_{ijx})v_{ix}-\sum_i^N v_{ix}h_\alpha \tag{6}$$

where e_i denotes the internal energy, i.e., the summation of kinetic energy and potential energy, v_{ix} is the velocity of atom i in the x-direction; f_{ijx} is the force in the x-direction on atom i due to its neighbor j from the potential, and h_α is the mean partial enthalpy that is calculated as the sum of the average kinetic energy, potential energy and virial item energy for atom type α [19]. It is necessary to note that in multi-component systems, like nanofluids, one may obtain a non-physical result if this

partial enthalpy item is not taken into account. In this work, the instantaneous heat flux vector is calculated in every time step and all the time steps were used as time origins of the time correlation function. Also note that the unit of the heat flux vector in Eq. (6) is not W/m^2, rather, it is in the unit of W·m. The real heat flux unit of the system is obtained when it is divided by the volume of the total system.

The determination of shear viscosity using G-K method is similar to the thermal conductivity calculation. The formula is given by [17]:

$$\mu_{xy} = \frac{1}{Vk_BT}\int_0^\infty \left\langle J_P^{xy}(0) J_P^{xy}(\tau)\right\rangle d\tau \tag{7}$$

where k_B, V and T have the same meaning as in Eq. (4); J_P^{xy} is the arbitrary component of the non-diagonal element of the stress tensor which has the form of [18]:

$$J_P^{xy} = \sum_{i=1}^{N} m_i v_{ix} v_{iy} + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j} x_{ij} f_{ijy} \tag{8}$$

where m is the mass of atom i; v_{ix} and v_{iy} are the velocity of atom i in x direction and y direction respectively; f_{ijy} is the force in the y-direction on atom i due to its neighbor j from the potential. Due to the symmetrical property of the stress tensor, only three non-diagonal element of the stress tensor are needed for the calculation of the shear viscosity. For stationary, homogeneous and uniform fluids, like the nanofluid studied in this paper, an average of these three terms can be obtained to determine the shear viscosity of the entire fluid. The calculation procedure of the shear viscosity is exactly the same as the calculation of the thermal conductivity which is described by Eq. (5) and it will not be repeated again. Note that the unit of the stress tensor in Eq. (8) is not N/m^2, rather, it is in the unit of N·m. The real stress tensor unit of the system is obtained when it is divided by the volume of the total system.

RESULT AND DISCUSSIONS

The time step used in this simulation is 4 fs and an NVE ensemble was used throughout the simulation. The cutoff radius in the L-J potential was set to be 2.6 σ_{Ar}, which is in the range of 1.6~3.6 σ_{Ar} proposed by Vogelsang et al. [20]. In this range, the thermal conductivity is independent of the cutoff radius. To obtain an equilibrium state, an initial 20,000 time steps were used with atom velocities rescaled in order to make the system equilibrate at the desired temperature. Additional 80,000 time steps were used to collect the data that were needed to calculate the thermal conductivity and the shear viscosity.

To validate the simulation method, we calculated the thermal conductivity of the liquid argon at T=86 K and ρ=1418 kg/m^3. Sarkar et al. [21] studied the influence of the atom number on the simulation result. They suggested that the results were in good agreement with the experimental value for pure argon when the number of atom is greater than 500. To be on the safe side, we choose 4000 atoms in the simulation domain to compute the thermal conductivity of liquid argon. In other words, the simulation box has a size of 10 lattices along three directions. A parallel computing was performed using 8 CPUs.

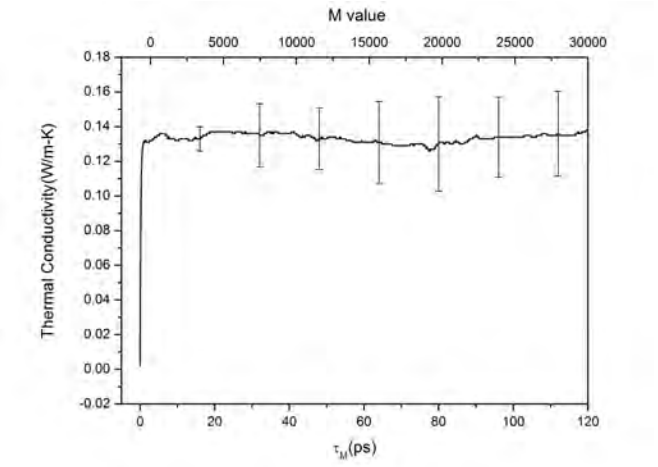


Fig. 1 Thermal conductivity of pure argon using G-K method

Figure 1 shows the result of our simulation for thermal conductivity of the liquid argon. Sixteen independent runs were carried out to get an averaged value. To obtain the thermal conductivity, as described in Eq. (5), a proper M value is needed. This M value should be larger than the time steps that the time correlation function needs to decay to zero and also should be much smaller than the total simulation time steps to ensure a reasonable statistical averaging. In this work, instead of choosing an arbitral M value, we take advantages of M from 4000 all through to 30000 and then get an average [22]. The thermal conductivity of the liquid argon obtained in this simulation is 0.134 W/m-K, which agreed very well with the experiment value of 0.132 W/m-K [23]. The result of the shear viscosity for the liquid argon at the given state point is shown in Fig. 2. Following the same procedure as we did for the thermal conductivity, the value of the shear viscosity is obtained as 0.279×10^{-3} Pa·s, which agreed very well with the value of 0.280 $\times10^{-3}$ Pa·s reported in the literature [24].

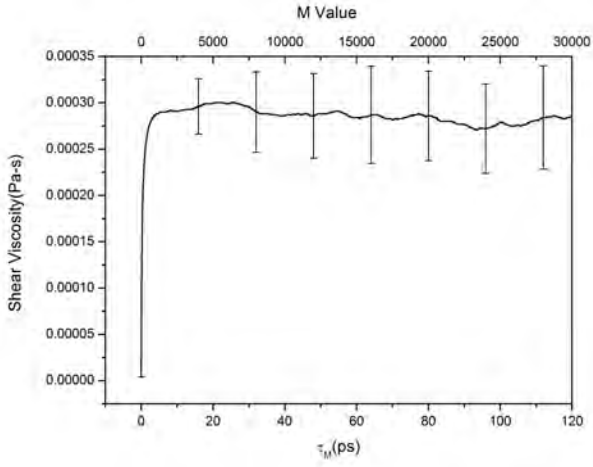
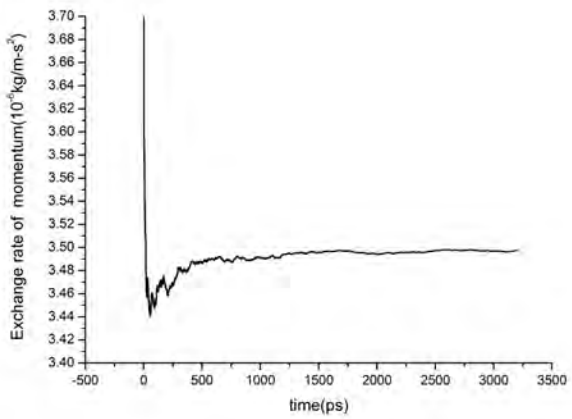
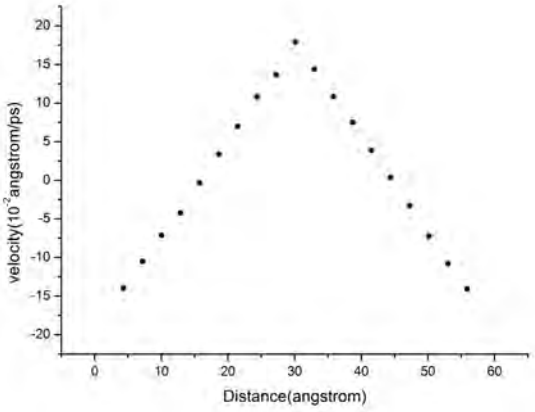


Fig. 2 Shear viscosity of pure argon using G-K method



(a) Exchange rate of momentum



(b) Velocity profile

Fig. 3 Exchange rate of momentum with respect to time and the corresponding velocity profile

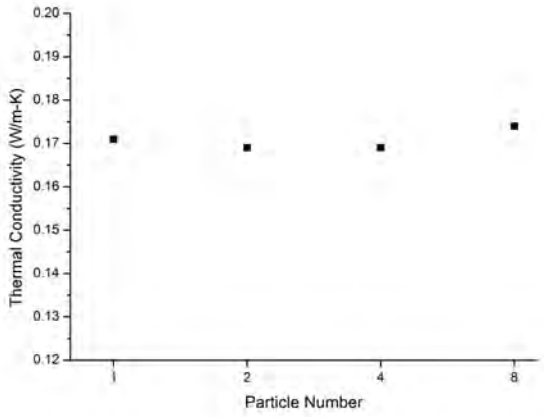
In addition, we also performed a NEMD simulation using the method described in Ref. [25] to further verify the result of the shear viscosity obtained by G-K method. In addition to this simple purpose of verification, we also would like to discuss the advantages and disadvantages in EMD and NEMD methods. The change of the momentum and the corresponding velocity profile are shown in Fig. 3(a) and (b), respectively. It can be seen that after 1500 ps the system becomes stable and the velocity profile is almost linear. The value of the shear viscosity can be obtained as the ratio of the stable change of momentum and the gradient of the velocity. The final result of shear viscosity using this NEMD method is 0.286×10^{-3} Pa·s, which is consistent with that obtained by G-K method and from the literature.

Although the results obtained by EMD and NEMD method are consistent with each other, there are still some differences that need to be pointed out. The calculation time using NEMD method is much less than using EMD method, or exactly, the G-K method. According to our simulation, it will need more than 60% additional calculation time in using the G-K method compared with using the NEMD method. What's more, the NEMD method needs much less storage space on the hard disk. Besides these advantages, the NEMD method also has its drawback that makes it not applicable in some situations. One of the key points in using NEMD method is to get a precise linear property profile, like the temperature profile in the thermal conductivity calculation or the velocity profile in the shear viscosity calculation, corresponding to the external perturbation. However, getting a precise linear property profile is not that easy. A slight external perturbation cannot make the property profile, i.e., the gradient, stand out of the noise and as a result no clear property profile is obtained; while on the other hand, a large external perturbation may lead the system to the non-linear response regime and the corresponding property profile will be non-linear.

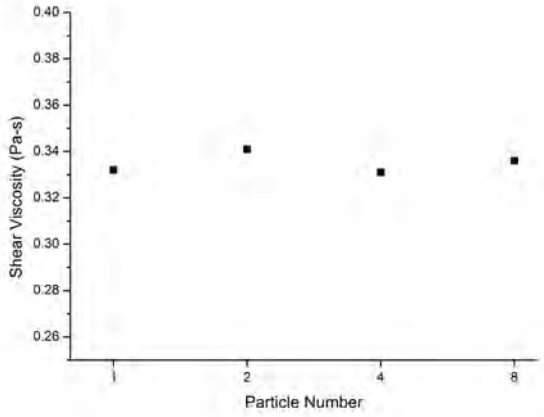
In addition, as there is a temperature difference in the simulation system using the NEMD method to calculate the thermal conductivity, it can not be used in the situation where the material to be simulated is sensitive to the temperature difference like the liquid argon, which has a narrow temperature range between its melting point and boiling point. What's more, the transport coefficient calculated by NEMD method can be obtained only in one direction in each single run, in other words, if the transport coefficient of a homogeneous fluid is studied, three single runs will be needed to get an average for the final result and this diminishes the advantage that the NEMD method needs less computation time. For the reason discussed above, the NEMD method was only used as a verification of the shear viscosity calculation for pure liquid argon using G-K method. In the rest of this paper, all the thermal conductivity and shear viscosity of the nanofluid are calculated using the G-K method.

In some MD simulations on nanofluid done by other researchers (e.g., [21, 26]), only one nanoparticle was placed in the simulation box with periodic boundary conditions. This makes it impossible to simulate the collision or aggregation of the nanoparticles. In other words, in this situation it only simulates the case that nanoparticles are always well-dispersed in the base fluid. As many researchers stated that it is the aggregation of the nanoparticles that makes the nanofluid have a large enhancement of thermal conductivity, it is meaningful to study the cases which have multi-nanoparticles in the simulation box. Based on this motivation, two, four and eight nanoparticles were put in the simulation box with the same particle diameter of 2.692 nm and the same volume fraction of 5.5%. This means that the size of the simulation box will change proportionally to the change of nanoparticle number. Generally speaking, the more nanoparticles are in the simulation box the more likely that they will collide or aggregate, which is why we did not just put two particles in the simulation box. But unfortunately, no such collision or aggregation had been observed in the simulation, even not for the eight-nanoparticle cases, within the time domain of 3.2 ns. The thermal conductivity and shear

viscosity of these cases are shown in Fig. 4(a) and Fig. 4(b). These results are consistent with the values obtained under the one particle case, which is not a surprise.



(a) Thermal conductivity

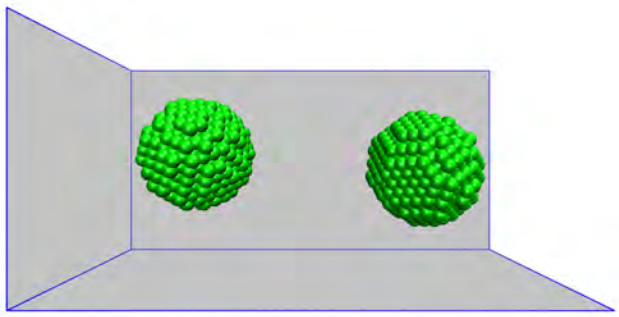


(b) Shear viscosity

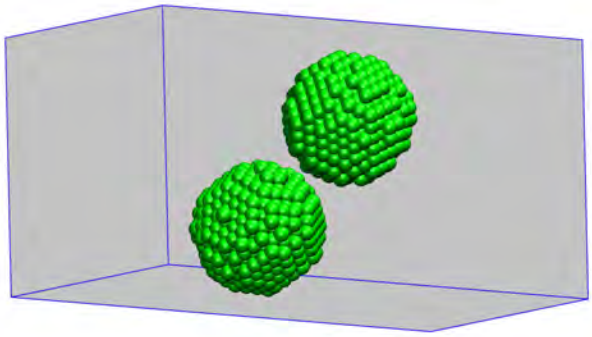
Fig. 4 Comparison of results in thermal conductivity and shear viscosity for different number of nanoparticles

In order to see whether the nanoparticle collision or aggregation would happen in a MD simulation, we enlarged the simulation time domain up to 40 ns, i.e., ten million time steps, but just for the two nanoparticles case because it needed the shortest computation time among these multi-nanoparticle cases. As shown in Fig. 5, the nanoparticle collision and aggregation was observed. It took place at about 36 ns, which is really a long time for a regular MD simulation and this makes it unrealistic to calculate the thermal conductivity and shear viscosity using G-K method that needs multiple runs to get an averaged result.

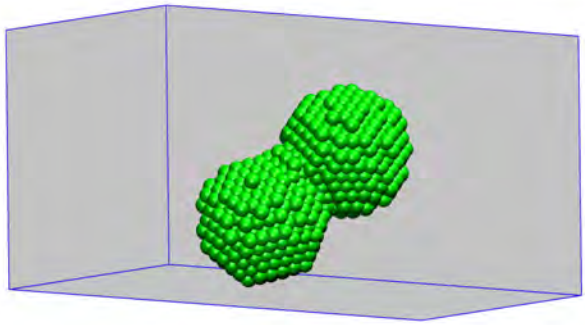
As our purpose is to study the nanoparticle aggregation effect on the enhancement of thermal conductivity of nanofluids, we can initially put the nanoparticles stick together, which makes it more like the situation that the aggregate



(a) Position of nanoparticles at t = 0 ns



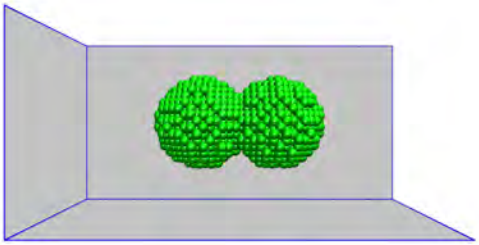
(b) Position of nanoparticles at t = 36 ns



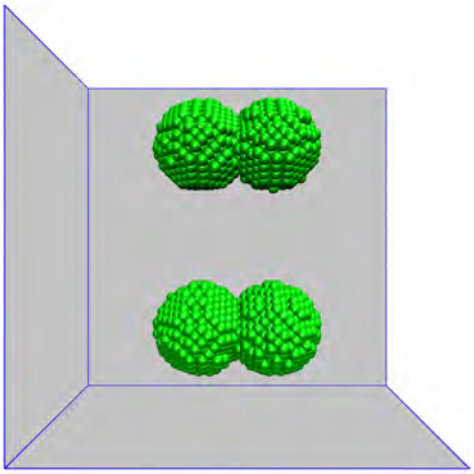
(c) Position of nanoparticles at t = 37 ns

Fig. 5 Aggregation of nanoparticles

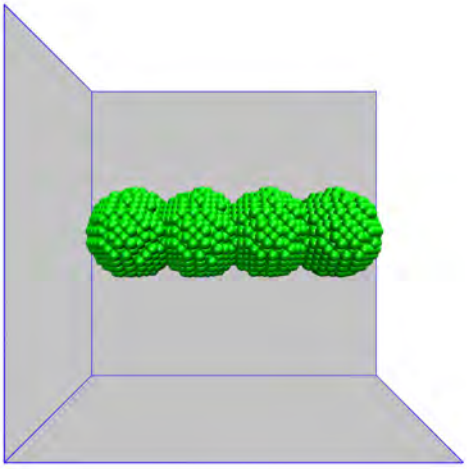
nanoparticles are initially dispersed in the base fluid. The configurations of the nanoparticle clusters suspended in base fluid are shown in Fig. 6. For the two particles case, there is only one possible aggregate configuration and the only parameter that affects this configuration is the distance between the centers of mass of these two nanoparticles. This distance was set to be 0.8 times of the nanoparticle diameter, which was obtained by the results shown in Fig. 5(c). This distance was used throughout the simulations to investigate the nanoparticle aggregation effect. It should be pointed out that this distance is consistent with the result of nanoparticle sintering process at room temperature [27], which is somewhat similar to the



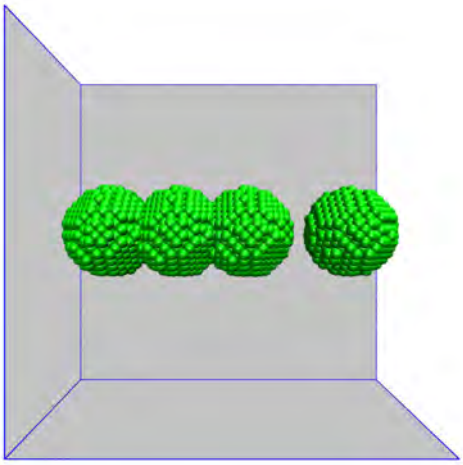
(a) Two nanoparticles case



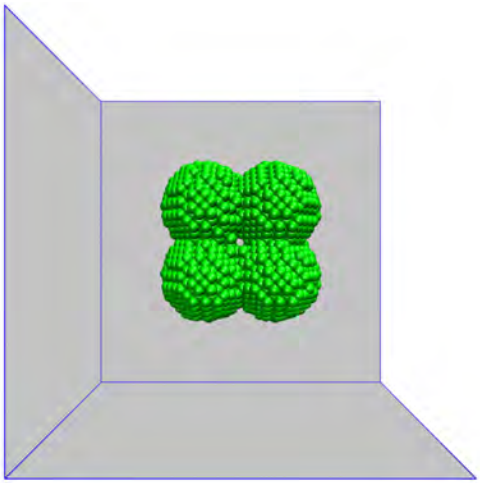
(b) Two nanoparticle pairs



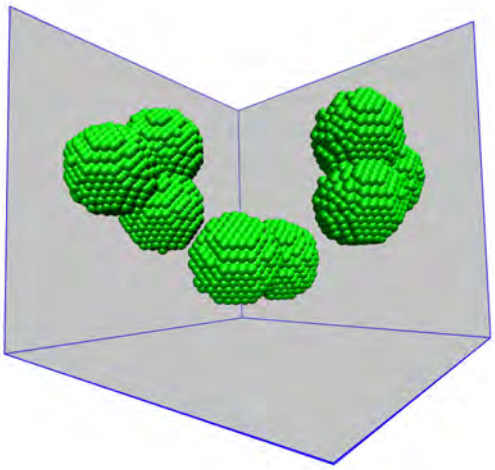
(c) Four nanoparticles clustered as a line



(d) Three-nanoparticles line and a single nanoparticle



(e) Four-nanoparticles square



(f) Eight nanoparticles case

Fig. 6 Different configurations of nanoparticle clustering

Table 1 Summary of thermal conductivity and viscosity

		Thermal Conductivity W/m-k	Thermal conductivity Enhancement	Shear Viscosity Pa-s	Increase of Shear Viscosity
Pure fluid		0.133	-	0.279×10^{-3}	-
Two nanoparticles	Without aggregation	0.169	27.1%	0.341×10^{-3}	22.2%
	With aggregation (Fig. 6(a))	0.195	46.6%	0.357×10^{-3}	30.0%
Four nanoparticles	Without aggregation	0.168	26.3%	0.331×10^{-3}	18.6%
	Two nanoparticle-pairs (Fig. 6(b))	0.201	51.1%	0.349×10^{-3}	25.1%
	Four nanoparticles clustered as a line (Fig. 6(c))	0.215	61.7%	0.350×10^{-3}	25.4%
	Three-nanoparticles line and a single nanoparticle (Fig. 6(d))	0.215	61.7%	0.366×10^{-3}	31.2%
	Four-nanoparticles square (Fig. 6(e))	0.227	70.7%	0.351×10^{-3}	25.8%
Eight nanoparticles	Without aggregation	0.173	30.1%	0.336×10^{-3}	20.4%
	With aggregation (Fig. 6(e))	0.200	50.4%	0.374×10^{-3}	34.1%

nanoparticle aggregation process studied in this paper. When two particles aggregate, the size of each particle will slightly increase as there is an overlap region in the aggregated area. When the number of particles increases, the possible configurations of the aggregate particles also increase and this makes it almost impossible to capture all the possible situations. As a result, for the four particles case, four different kinds of particle aggregation configuration were employed to calculate the thermal conductivity and shear viscosity. It should be pointed out that the four configurations for the four-nanoparticle cases are illustrative, rather than inclusive. For the eight particles case, only one situation was simulated due to the consideration of computational cost.

The results of the nanoparticle aggregation cases are all shown in Table 1, along with the pure fluid case and the other multi-nanoparticle cases without aggregation. These results clearly show that the existence of the nanoparticle aggregation causes a significant enhancement of thermal conductivity in nanofluid. It almost doubled the enhancement of thermal conductivity in nanofluid for the case with nanoparticle aggregation compared with the case without nanoparticle aggregation. While on the other hand, the shear viscosity of the nanofluid also increases when the nanoparticle clusters are formed. Compared with the enhancement of the thermal conductivity, however, this shear viscosity increase is gentle. Different configurations of the nanoparticle cluster resulted in different thermal conductivity and shear viscosity enhancements in nanofluid; the effect of configuration on the thermal conductivity is more significant as is shown in the table. When more nanoparticles are placed into the simulation box, it is crucial to determine which nanoparticle aggregate configurations are most likely to form and the simulation results of these most possible configurations can lead to a better prediction for the thermal conductivity in nanofluids. A combination of the experiment and fractal theory may help to deduce these configurations.

CONCLUSION

The thermal conductivity and shear viscosity of the nanofluid were calculated using Green-Kubo method, which represents an equilibrium molecular dynamics (EMD) approach. Although the non-equilibrium molecular dynamics (NEMD) approach has a merit of simple, shorter computation time and less storage space, the dependence of the external force field intensity and the simulating material property makes it not applicable in some situations like the copper-argon nanofluid system studied in this paper. In the simulation process, more than one nanoparticle was put into the simulation box and no aggregation was observed in the time domain of 3.2 ns; and the results of the thermal conductivity and shear viscosity for the multi-nanoparticle case are consistent with the result of the one particle case. A long run which has a time domain of 40 ns was performed for the two nanoparticles case and an aggregation process was observed at about 36 ns. Therefore, it is unrealistic to calculate the thermal conductivity and shear viscosity using G-K method, which needs multiple runs to get an averaged result, in such a long simulation time. In order to simulate the effect of nanoparticle aggregation on the

thermal conductivity and viscosity, nanoparticles that are originally stuck together were dispersed in the base fluid. Results showed that the existence of the nanoparticle aggregation induces a significant enhancement of thermal conductivity in nanofluid, while the increase of shear viscosity is gentle. Different configurations of the nanoparticle cluster will cause different thermal conductivity and shear viscosity enhancements in nanofluid; the effect of configuration on the thermal conductivity is more significant.

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