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Anomalous enhancement in thermal conductivity of nanofluid induced by solid walls in a nanochannel

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ABSTRACT

Thermal conductivity of Ar–Cu nanofluid confined between two parallel walls (in a nanochannel) is calculated by equilibrium-molecular-dynamics (EMD) simulation through Green-Kubo formula. The results show that the vibration of nanoparticle in the channel height direction (*z*-direction) is inhibited due to the presence of solid boundaries and accordingly the thermal conductivity of the confined nanofluid is obviously anisotropic. Anomalous enhancement in the thermal conductivity perpendicular to the *z*-direction (λ^*) appears as a result of the strong coupling interactions between the fluid atoms, especially the nanoparticle atoms, and the wall atoms. The thermal conductivity λ^* of the nanofluid confined in the channel of width $h = 5.148$ nm increases with the increase of the nanoparticle diameter for the strengthened couplings. The nanoparticle volume fraction effect on the thermal conductivity of the confined nanofluid is more obvious than that in macroscale. In addition, the thermal conductivity λ^* of the nanofluid with diameter of nanoparticle $d = 1.370$ nm decreases with the channel width increasing owing to the weakened couplings resulted by a longer interacting distance.

1. Introduction

Nanofluid [1,2] containing nanometer sized particles or fibers suspended in the base fluid has attracted considerable attention, for its better heat transport performance [3,4] than the ordinary fluid. Besides, nanofluid is more stable and has acceptable viscosity and better wetting, spreading and adhesion behaviors on solid surface [5,6]. Hence, nanofluid becomes a potential heat transfer fluid in a wide range of industrial applications such as thermal engineering, chemistry industry and microelectronics.

Much effort has been devoted to the investigations on the enhanced thermal property of nanofluid and its enhancement mechanisms. Garg et al. [7] measured the thermal conductivity of ethylene glycol based nanofluid and found that the increase in the thermal conductivity was twice the value predicted by the Maxwell effective medium theory. Sankar [8] estimated the thermal conductivity of water-platinum nanofluid based on the molecular dynamics simulation model and compared his results with the existing experimental results that indicated great enhancement in the thermal conductivity. Keblinski et al. [9] suggested four possible explanations for the anomalous enhancement in the thermal conductivity of nanofluid and concluded that the key factor in the thermal property of nanofluid is ballistic, rather than diffusive. In contrast, some studies concluded that the increase in the thermal conductivity of nanofluid was not anomalous but consistent with the classical effective medium theory. Buongiorno et al. [10] measured the thermal conductivity of various nanofluids using a variety of experimental approaches and concluded that no anomalous increase of thermal conductivity was observed and the experimental data were good agreement with the effective medium theory developed for dispersed particles. Vladkov et al. [11] simulated the thermal conductivity of nanofluid by molecular dynamics simulation and showed that in the absence of collective effects, the thermal conductivity of the nanofluid was well described by the classical Maxwell–Garnet equation mode.

However, presently the investigations on the thermal property of nanofluid are focused on macroscale. When it comes to nanoscale, small scale effect works and interesting phenomenon appears. Nanofluidics [12] is the study of the behavior, manipulation, and control of fluid that is confined to structures of nanometer (typically 1–100 nm) characteristic dimensions. The study has been drawing interest of researchers from the fields of physics, chemistry, biology, medicine and thermal engineering. It finds

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Nomenclature

r_{ij}	distance between atom i and atom j
r_{cut}	cutoff distance
N	total number of system atoms
V	system volume
T	system temperature
k_B	Boltzman constant
J_q	heat current vector
t	time
$\triangle t$	time step length
$\overrightarrow{1}$	unit tensor
v	velocity of atom
h_α	mean enthalpy
h	channel width
R	central position of nanoparticle
d	nanoparticle diameter
m	mass of an atom
N_{step}	total time step in the simulation
M	time step needed for the calculation of thermal conductivity
L_{wx}, L_{wy}, L_{wz}	dimensions of solid walls
L_{fx}, L_{fy}	dimensions of fluidic zone
Vol%	volume fraction of nanoparticle

Greek symbols

ϕ	LJ potential
ε	energy parameter
σ	length parameter
τ	nondimensional time
λ	thermal conductivity
λ^*	thermal conductivity perpendicular to z-direction
ρ^*	nondimensional liquid number density

Superscripts and subscripts

l	liquid base fluid
s	solid nanoparticle
j,k	number of atoms
α,β	kind of atoms
m,n	time step
x	x component of variables
y	y component of variables
z	z component of variables
K	kinetic part of heat current
P	potential part of heat current
C	collision part of heat current

applications in areas such as Micro-Electro-Mechanical-Systems (MEMS), lab-on-chip, micro-reaction devices, material sciences, biotechnology, separation technology and process engineering. Fluid confined in these structures exhibits physical behaviors not observed in larger structures, e.g. vastly increased viscosity near the pore wall, changes in thermodynamic properties and chemical reactivityof species at the fluid–solid interface.

Understanding of the flow and heat transfer behaviors of the nanofluid confined in a nanochannel is of significant importance for fundamental researches and engineering applications. Ben-Abdallah [13] investigated the dynamic structure and the formation of clusters of nanoparticle in the nanofluid confined between two parallel walls under the action of an external force field by extensive Brownian-dynamics simulation and demonstrated that an external force was able to reduce the nanoparticles' mobility and to significantly enhance the lifetime of natural phonons. Recently, Lv et al. [14] simulated the flow behaviors of Ar–Cu nanofluid between flat plates, between which the distance was 20.67 nm, under shear flow condition and found that none of the atoms of the nanoparticle dispersed and the nanoparticle vibrated and rotated besides the main flow. Little research was done on the thermal property of nanofluid that confined in a nanochannel except that by Ben-Abdallah et al. [15], as far as our knowledge. They simulated the thermal conductivity of confined nanofluid by Brownian-dynamics method beyond nanometer confinement for numerical stability reason and found orders of magnitude enhancement in longitudinal lattice thermal conductivity by a linear extrapolation at the level of nanometers confinement. However, the nanoscale effect and the enhancement mechanism are still not clear.

Molecular dynamics (MD) simulation is a computational method that solves Newton's equation of motion for a system of particles (atoms or molecules) interacting with a given potential. MD simulation only assumes the form of interparticle potentials of a system, and it directly and accurately calculates the movement of particles at the atomic level. Hence, MD simulation can more accurately predict atomic level transport phenomenon compared with any classical model based on continuum mechanics. Therefore, the present work is dedicated to the investigation of the nanoscale effect on the thermal conductivity of nanofluid by MD simulation.

In Sec.2, MD simulation mode details are illustrated, including the interatomic interaction potential and the Green-Kubo formula for the calculation of thermal conductivity. Sec.3 starts by a brief analysis of the tracks of the nanoparticle atoms. Then, thermal conductivity of confined nanofluid is calculated and influences of nanoparticle diameter and channel width on the thermal conductivity are investigated. Finally, Sec.4 provides a summary of the obtained results.

2. Molecular dynamics simulation model

The simulation is carried out with the system where argon (Ar) based nanofluid suspending copper (Cu) nanoparticle is confined between two parallel infinite walls. The geometric model of the simulation system is shown in Fig. 1. The two physically infinite walls are considered by limited computational lengths through periodic boundary conditions in the x- and y-direction. The two walls are made of the same material as the nanoparticle to reduce the difficulty in the calculation since less potential function is needed to be considered. The walls consist of two layers of Cu atoms in the z-direction such that the interactions between any atoms of the fluid and the wall atoms out of consideration are negligible.

The atoms in the system are originally arranged in regular faced-centred cubic (FCC) lattices. The two walls are consisted of 784 Cu atoms, each wall contains $7 \times 7 \times 2$ lattices and 392 Cu atoms. The FCC lattices for Ar atoms and Cu atom are different according to the densities of their own. The spherical nanoparticle is developed by replacing the same volume fraction of Ar atoms with Cu atoms in another FCC lattices. For convenience and brevity only a single solid nanoparticle is installed in the center of the fluidic zone, which is often done in the MD simulation of nanofluids [8,16]. The original system configuration of the nanofluid with the diameter of nanoparticle $d = 1.0$ nm (38 Cu atoms) in the channel of width $h = 5.148$ nm is shown in Fig. 2. The distance between the two walls

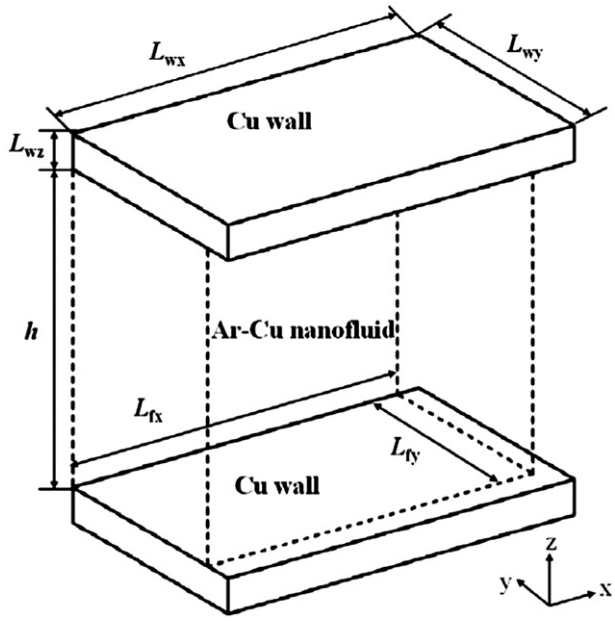

Fig. 1. Geometric model of the simulation system where Ar–Cu nanofluid is confined between two copper parallel walls. The copper wall has the size of $L_{wx} = L_{wy} = 2.529$ nm, $L_{wz} = 0.723$ nm. The lengths of the fluidic zone in the x- and y-direction $L_{fx} = L_{fy} = 2.288$ nm. The channel width h varies in the simulation, which is connected with the number of Ar atoms by constant number density $\rho^* = 0.844$ (in units of σ^{-3}).

(channel width h) is of nanometers during the simulation, which can be widened by increasing the lattice number in the z-direction.

The widely accepted Lennard–Jones (LJ) potential matches experimental data well for pure argon fluid and requires reasonable computation time. Although the most accurate potential for modeling copper atoms is embedded atom method (EAM) potential as it can take care of metallic bonding, the LJ potential also can predict well the qualitative trend of thermal conductivity enhancement [14,16]. In this system, the interatomic interactions between the atoms are modeled by the well-known LJ 12–6 potential [16] which is originally proposed for liquid argon.

$$\phi(r_{ij}) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] & (r_{ij} < r_{cut}) \\ 0 & (r_{ij} \geq r_{cut}) \end{cases} \quad (1)$$

where r_{ij} is the distance between particles i and j, and σ and ε are the energy parameter which governs the strength of the interaction and the length scale, respectively. For argon, the LJ parameters σ and ε are equal to 0.3405 nm and 1.670×10^{-21} J, respectively [16]. For copper, the LJ parameters σ and ε are equal to 0.2338 nm and 65.625×10^{-21} J, respectively [16]. To determine the parameters between argon atoms and copper atoms, the common Berthlot mixing rule [17] is used:

$$\sigma_{sl} = \frac{\sigma_{ss} + \sigma_{ll}}{2} \quad (2a)$$

$$\varepsilon_{sl} = \sqrt{\varepsilon_{ss}\varepsilon_{ll}} \quad (2b)$$

Therefore, σ and ε between argon and copper are 0.2871 nm and 10.469×10^{-21} J, respectively. To improve the computational efficiency, only the neighboring particles within a certain cutoff radius (r_{cut}) are included in the force calculation since the distant particles have a negligible contribution. In this calculation, the cutoff distance r_{cut} is set to be 2.5 σ.

NVT ensemble is used in the simulation, where the total number of system atoms N, system volume V, and system temperature T are constant. To employ the NVT ensemble, the most simple and intuitive velocity rescaling method [18] is used, which changes the velocities of particles at t time by multiplying a factor determined by the instantaneous temperature and the reference temperature. The tracks of the motion of particles are obtained by integrating the motion equation with an effective Velocity-Verlet algorithm [18].

Equilibrium molecular dynamics (EMD) can simulate transport coefficients, such as self-diffusion, thermal conductivity and shear viscosity, based on the linear response theory [19]. Thermal conductivity is obtained by relating the equilibrium heat current autocorrelation function (HCACF) through the Green-Kubo formula [20]

$$\lambda = \frac{1}{Vk_BT^2}\int_0^\infty < J_q^x(t)\cdot J_q^x(0) > dt \quad (3)$$

where λ is the thermal conductivity, V the system volume, T the system temperature, k_B the Boltzman constant, J_q the heat current vector, and the angular brackets denote the ensemble average or the average over time.

For a two-component system, the heat current is expressed as the constitution of the kinetic part, the collision part, and the potential part. An extended form is used to calculate the heat current vector [21,22].

$$J_q^x = \sum_{\alpha=1}^{2}\sum_{j=1}^{N_\alpha}\frac{1}{2}m_\alpha v_{j\alpha}^2 v_{j\alpha}^x - \frac{1}{2}\sum_{\alpha=1}^{2}\sum_{\beta=1}^{2}\sum_{j=1}^{N_\alpha}\sum_{\substack{k=1\\k\neq j}}^{N_\beta}\left[r_{j\alpha k\beta}\frac{\partial\phi\left(r_{j\alpha k\beta}\right)}{\partial r_{j\alpha k\beta}} - \phi\left(r_{j\alpha k\beta}\right)\overrightarrow{I}\right]v_{j\alpha}^x - \sum_{\alpha=1}^{2}h_\alpha\sum_{j=1}^{N_\alpha}v_{j\alpha}^x \quad (4)$$

where subscripts j and k are the number of particles, and α and β denote two different kinds of particles. N_α and N_β are the number

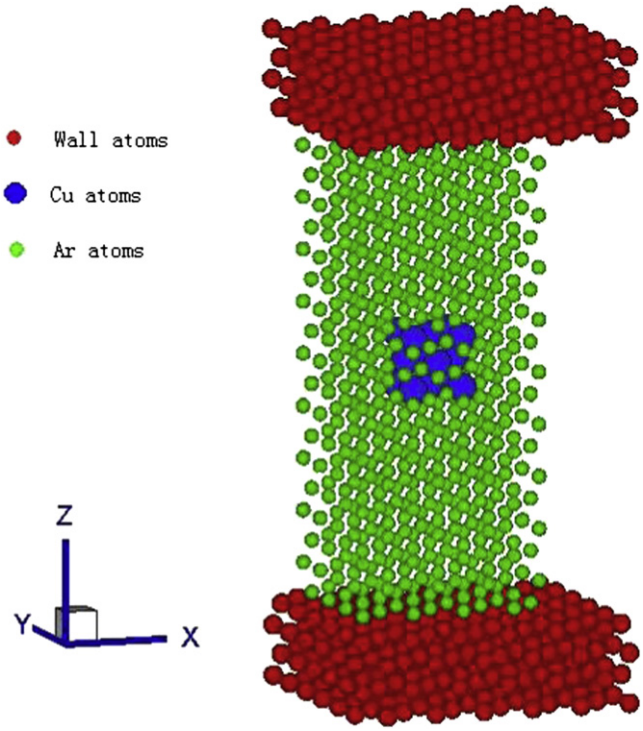

Fig. 2. Original system configuration of nanofluid with $d = 1.0$ nm. The atoms in the system are originally arranged in a regular faced-centred cubic lattice.

of particles of α and β, respectively. m_α is the mass of particles of α, $v_{j\alpha}$ is the velocity of a particle j of α, h_α stands for the mean enthalpy per particle of α, and $\overrightarrow{I}$ is the unit tensor. The mean enthalpy is calculated as the sum of the average kinetic energy, potential energy, and average virial terms per particle of each species [16]. For a single-component system, the last term of Eq. (4) equals zero. The y- and z-component of thermal conductivity can be obtained by corresponding formula.

Since the simulation is performed for discrete time steps, Eq. (3) for the calculation of thermal conductivity is written as

$$\lambda(t_M) = \frac{\Delta t}{Vk_BT^2}\sum_{m=1}^{M}\frac{1}{N_{\text{step}}-m}\sum_{n=1}^{N_{\text{step}}-m}\left(J_q^x(m+n)\cdot J_q^x(n)\right) \quad (5)$$

where t_M is given by $M\Delta t$, $J_q^x(m+n)$ is the heat current vector at MD time step $m+n$, N_{step} is the total time step in the simulation and M is the time step needed for the calculation of thermal conductivity. The average heat current vector over time is known as heat current autocorrelation function (HCACF).

Periodic boundary conditions [18] are imposed in the x- and y-direction of the simulation system (Fig. 1). The thermal wall model [23,24] is applied at the interfaces between the walls and the fluid in the z-direction, which is the height direction of the channel. In this model, when a fluid particle strikes the wall surface, it is assumed to undergo a series of collisions with the surface molecules and rebound at a randomized velocity, which is not correlated with the particle's initial velocity but determined by the wall temperature and chosen by the random sampling from the Maxwell distribution. In a typical simulation, 1,000,000–1,200,000 MD steps are needed. The initial 100,000 time steps are ignored in the calculation of thermal conductivity with the Green-Kubo formula to allow the system to reach the temperature equilibrium.

3. Results and discussion

3.1. Nanoparticle's track

According to the position of every fluid atom at each time step, the movement and position of the atoms are visualized. Fig. 3 shows the positions of nanoparticle atoms at different times in the channel of width $h = 5.148$ nm, where 1 represents the positions at $t_1 = 1000$ ps and 2 the positions at $t_2 = 1100$ ps. In the figure, only the positions of argon atoms at time t_1 are shown to clearly reveal the movement of nanoparticle atoms. It can be seen that the nanoparticle atoms aggregate without dispersed atoms and move together for Brownian motion.

For a more profound understanding of the motion of the nanoparticle atoms, the central positions of the nanoparticle in three directions during the simulation are further obtained. R_x, R_y and R_z denote the central position of the nanoparticle in the x-, y- and z-direction, respectively. The three values are calculated by averaging the corresponding positions of each nanoparticle atom, respectively. Fig. 4 displays the variations of the central positions in three directions with the simulation time steps. As shown in the figure, R_x, R_y and R_z fluctuate around the center of the fluidic zone in the x-, y- and z-direction, while the fluctuation in the z-direction is obviously weaker than that in the other two directions. Since the fluctuation intensity reflects the intensity of the nanoparticle's vibration, it can be concluded that the vibration of the nanoparticle in the z-direction is limited due to the presence of the solid walls.

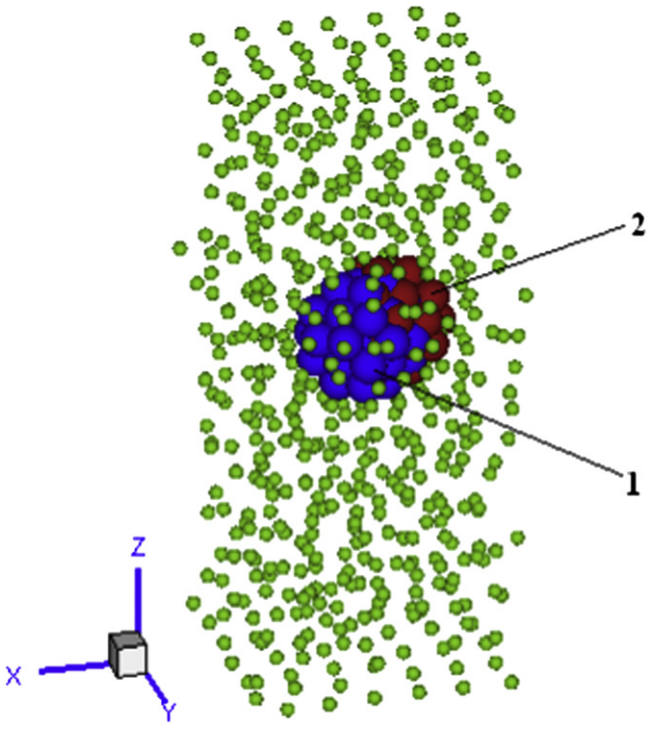

Fig. 3. Positions of nanoparticle atoms at $t_1 = 1000$ ps and $t_2 = 1100$ ps. Wall atoms are not included, while Ar atoms are in green and Cu atoms in blue at time t_1 and in red at time t_2. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.2. Thermal conductivity anisotropy and enhancement

Thermal conductivity of confined Ar–Cu nanofluid in the x-, y- and z-direction is calculated by integrating the corresponding heat current autocorrelation function (HCACF) at time step according to Green-Kubo formula, respectively. Fig. 5a and b show the HCACF diagrams and thermal conductivity integrals with m (in Eq. (5)) in three different directions for the nanofluid with $d = 1.0$ nm and $h = 5.148$ nm. The liquid argon is in its state point system temperature $T = 86$ K and average base fluid density $\rho^* = 0.844$ (in units of σ^{-3}).

As Fig. 5 shows, the thermal conductivity of the confined nanofluid is obviously anisotropic. The HCACF in the z-direction decays to zero more rapidly and sharply, while the HCACF in the x- and

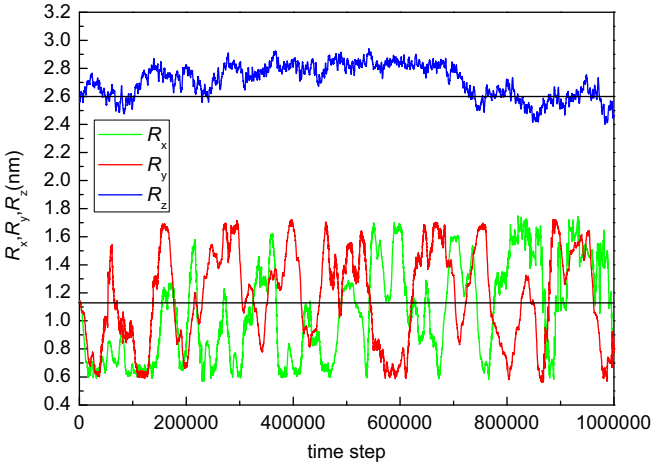

Fig. 4. Central positions of the nanoparticle in three directions during the simulation. Center of fluidic zone in three directions is marked by level lines.

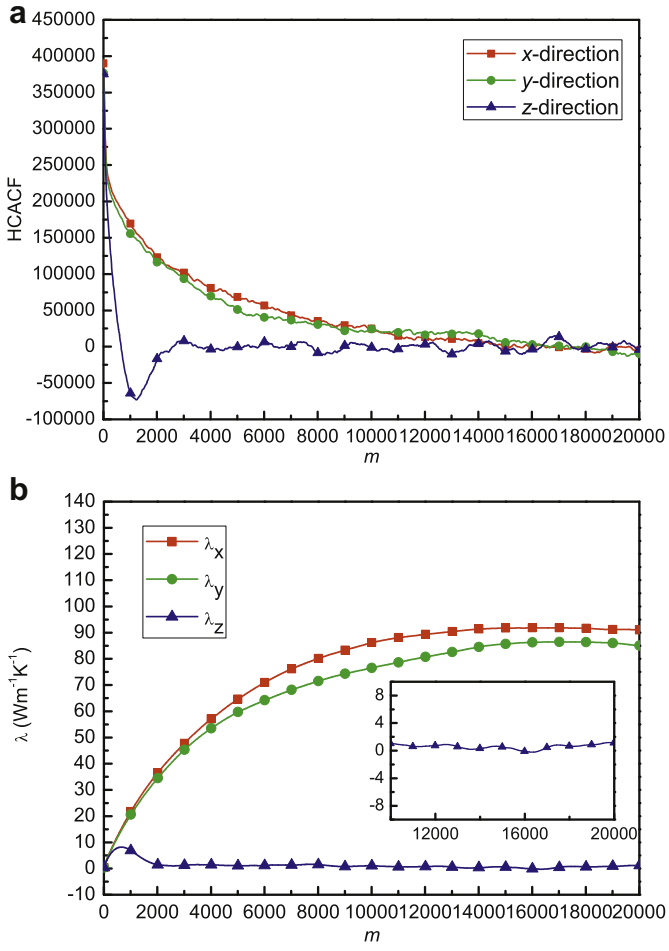

Fig. 5. HCACF (a) and thermal conductivity (b) of nanofluid with $d = 1.0$ nm confined in a nanochannel of width $h = 5.148$ nm in x-, y- and z-direction.

y-direction stay correlated more strongly and for a longer time. The thermal conductivity is related to the integral of the HCACF, and therefore the thermal conductivity in the z-direction is remarkably lower than that in the x- and y-direction. This is caused by the distinct boundary condition applied in the calculation when the fluid atoms come across the walls during the simulation. From the physical point of view, the fluid mobility in the z-direction, especially the vibration of nanoparticle, is small owing to the presence of the solid boundaries, as illustrated in the above section. Accordingly, the thermal transport in the z-direction is inhibited.

Thermal conductivity in the z-direction is greatly limited, and thus will not be discussed below. The average thermal conductivity $\lambda^* = (\lambda_x + \lambda_y)/2$ (thermal conductivity perpendicular to the z-direction) is meaningful in the following discussion, because there is slight difference between thermal conductivity in the x- and y-direction resulted by the limited size of the simulation system. It can be found from Fig. 5(b) that the thermal conductivity λ^* is anomalously enhanced in the nanochannel compared with the results in macroscale (10^{-1} $Wm^{-1}K^{-1}$) by Sarkar and Selvam [16]. Orders of magnitude enhancement in the thermal conductivity of nanofluid confined in nanochannels is also found by Ben-Abdallah et al. [15] through linear extrapolation from their original results obtained in microchannel.

As mentioned earlier, the heat current consists of the kinetic part (K), the potential part (P) and the collision part (C). Hence, the thermal conductivity can be expressed as a sum of nine terms which can be conveniently grouped together into self correlations

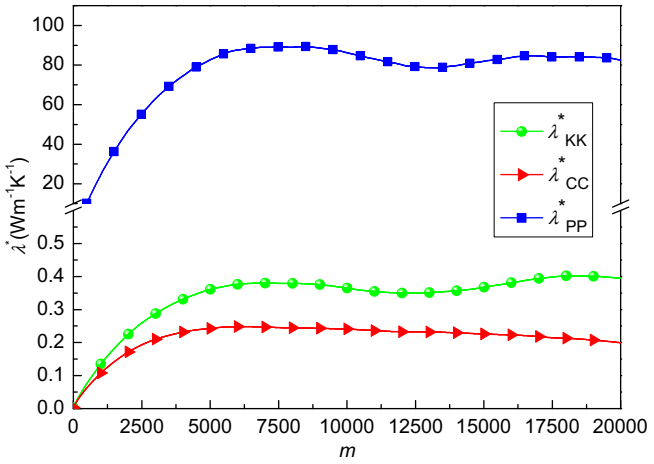

Fig. 6. Contributions of each part to thermal conductivity λ^* of nanofluid with $d = 1.0$ nm (λ^*_{KK} denotes contribution of KK correlation, λ^*_{PP} contribution of PP correlation, and λ^*_{CC} contribution of CC correlation).

(KK, PP and CC) and cross correlations (PC, PK, etc.). According to Eapen et al. [22], the contribution of the KK correlation is negligible. In contrast, the contribution of the PP correlation increases with the increase of the volume fraction of nanoparticle and the contributions of the CC+PC+CP correlations remain constant. For the confined nanofluid, the contributions of the three self correlations to the thermal conductivity λ^* of the nanofluid are displayed in Fig. 6. As shown in the figure, λ^*_{PP} plays a leading role, while λ^*_{KK} and λ^*_{CC} are negligible. Because the KK correlation represents the Brownian motion, the CC correlation the vibrational or phonon modes and the PP correlation the interacting potential [22]. Hence, it can be concluded that the anomalously enhanced thermal conductivity λ^* is a direct consequence of the strong coupling interactions between the fluid atoms, especially the nanoparticle atoms, and the wall atoms. In contrast, the roles of the Brownian motion and the phonon mode to the anomalous enhancement in the thermal conductivity are very small.

3.3. Nanoparticle size effect

Thermal conductivity of the base fluid and the nanofluid containing different size nanoparticle in the channel of width

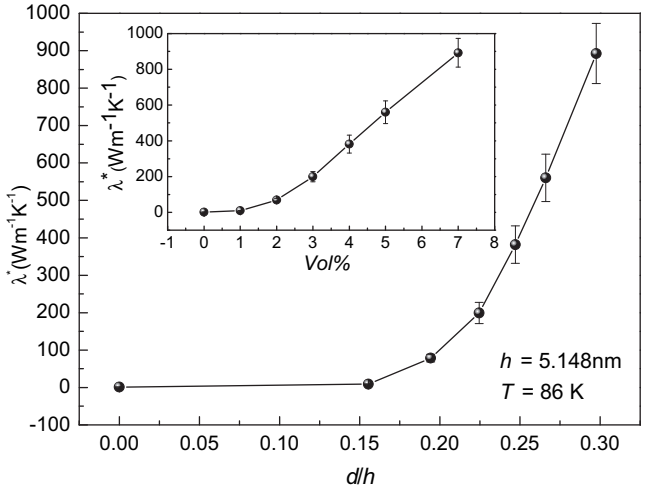

Fig. 7. Thermal conductivity λ^* of nanofluid confined in the nanochannel varies with the ratio of nanoparticle diameter to channel width d/h and the volume fraction of nanoparticle.

Table 1
System dimensions at different channel widths (Channel width is connected with the number of Ar atoms by constant base fluid density $\rho^* = 0.844$ (in units of σ^{-3})).

Case	h (nm)	wall atoms	Ar atoms	Cu atoms
1	5.148	784	538	116
2	8.579	784	922	116
3	12.011	784	1306	116
4	15.443	784	1690	116
5	18.874	784	2074	116

$h = 5.148$ nm is calculated. Fig. 7 shows the thermal conductivity λ^* vs. the ratio of the nanoparticle diameter to the channel width d/h. For $d/h = 0.155$, 0.194, 0.225, 0.247, 0.266 and 0.296, 6, 14, 14, 14, 38 and 38 of argon atoms are replaced by 14, 38, 68, 92, 116 and 156 copper atoms to model the nanofluid, respectively. It can be found from the figure that the thermal conductivity increases sharply as the ratio d/h increases. For the base fluid ($d/h = 0.0$) the thermal conductivity $\lambda^* = 1.13$ $Wm^{-1}K^{-1}$, while for the nanofluid with $d/h = 0.194$ the thermal conductivity $\lambda^* = 78.50$ $Wm^{-1}K^{-1}$ and $d/h = 0.296$ the thermal conductivity $\lambda^* = 892.57$ $Wm^{-1}K^{-1}$. Anomalous increase in the thermal conductivity appears only for a slight increase in the diameter of nanoparticle. This phenomenon is caused by the strengthened couplings between the fluid atoms and the wall atoms with the diameter of the nanoparticle increasing, which is the main reason for the enhancement in the thermal conductivity of the confined nanofluid, as mentioned earlier.

According to the dimensions of the fluidic zone and the diameter of the nanoparticle, the volume fraction of the nanoparticle (*Vol%*) can be obtained. Hence, the variation of the thermal conductivity with *Vol%* is also shown in Fig. 7. The volume fraction effect on the thermal conductivity of the nanofluid confined in a nanochannel is more obvious than that in macroscale as investigated by Sarkar and Selvam [16]. A slight increase in the volume fraction of nanoparticle induces obvious increase in the thermal conductivity of the confined nanofluid.

3.4. Channel width effect

For the nanofluid suspending nanoparticle with the same diameter ($d = 1.370$ nm), the thermal conductivity λ^* is calculated at different channel widths h. Table 1 shows the system dimensions at different channel widths and Fig. 8 displays the thermal conductivity λ^* vs. the channel width h. The thermal conductivity integrals with m for $h = 15.443$ nm and $h = 18.874$ nm are inserted in Fig. 8.

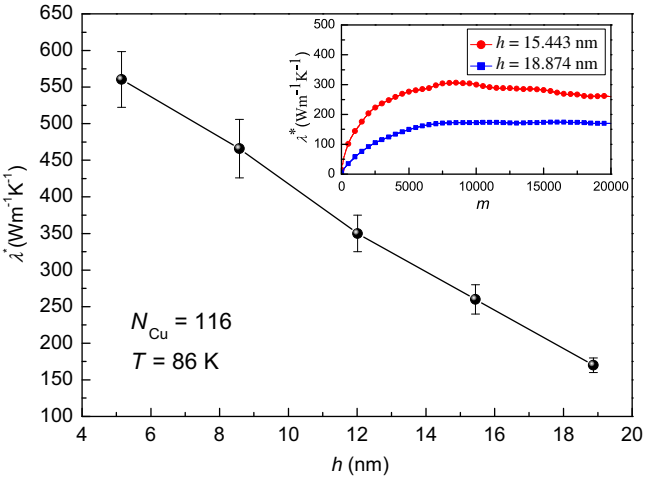

Fig. 8. Thermal conductivity $\lambda^*$of nanofluid suspending nanoparticle with the same diameter varies with channel width h.

Fig. 8 shows that the thermal conductivity λ^* decreases with the increase of the channel width h. As the channel width increases, the couplings between the fluid atoms and the wall atoms are weakened owing to a longer interacting distance. Therefore, the thermal conductivity of the confined nanofluid decreases as the channel width increases. Beyond a critical channel width the thermal conductivity is expected to decrease to its macroscale value. Unfortunately, the critical width can not be found by the simulation due to the limited computing power.

4. Conclusions

In this paper, thermal conductivity of the argon based nanofluid suspending copper nanoparticle confined between two parallel walls is calculated by EMD simulation with Green-Kubo formula. The main conclusions are as follows.

The vibration of nanoparticle in the z-direction is inhibited due to the presence of solid walls and accordingly the thermal conductivity of the confined nanofluid in the z-direction is obviously lower than that in the x- and y-direction. The thermal conductivity perpendicular to the z-direction (λ^*) is anomalously enhanced compared with its macroscale value for the strong couplings between the fluid atoms and the wall atoms which can be deduced from the leading role of the potential part in heat current.

In a nanochannel of width $h = 5.148$ nm, the thermal conductivity λ^* increases sharply with the increase of the nanoparticle diameter, as a result of the strengthened couplings between the fluid atoms and the wall atoms. The nanoparticle volume fraction effect on the thermal conductivity of the nanofluid confined in a nanochannel is more obvious than that in macroscale. Meanwhile, for the nanofluid suspending nanoparticle with the same diameter $d = 1.370$ nm, the thermal conductivity λ^* decreases as the channel width h increases for the weakened couplings due to a longer interacting distance.

Anyway, all the results may be attributed to the nanoscale effect on the thermal conductivity of confined nanofluid, that is, the thermal conductivity deviates distinctly from that in macroscale when the nanofluid is limited to a distance of nanometers. Meanwhile, these results have instructive significance on probing the enhancement mechanisms of the thermal conductivity of nanofluid in macroscale. Additional simulations are under way to get more accurate and extensive results. The results by the numerical calculation are expected to be verified by further experimental studies.

Acknowledgements

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