Microfluid Nanofluid (2011) 10:475–480
DOI 10.1007/s10404-010-0684-2

SHORT COMMUNICATION

Molecular dynamics simulation on flow behavior of nanofluids between flat plates under shear flow condition

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Received: 14 June 2010 / Accepted: 16 August 2010 / Published online: 1 September 2010

Abstract Molecular dynamic model of nanofluid between flat plates under shear flow conditions was built. The nanofluid model consisted of 12 spherical copper nanoparticles with each particle diameter of 4 nm and argon atoms as base liquid. The Lennard–Jones (LJ) potential function was adopted to deal with the interactions between atoms. Thus, the motion states of nanoparticles during the process of flowing were obtained and the flow behaviors of nanofluid between flat plates at different moments could be analyzed. The simulation results showed that an absorption layer of argon atoms existed surrounding each nanoparticle and would accompany with the particle to move. The absorption layer contributed little to the flow of nanoparticles but much to the heat transferring in nanofluids. Another phenomenon observed during shear flowing process was that the nanoparticles would vibrate and rotate besides main flowing with liquid argon and these micro-motions could strengthen partial flowing in nanofluids.

Keywords Nanofluids · Molecular dynamics method · Shear flow · Absorption layer · Micro-motions

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1 Introduction

Nanofluids are new types of heat transfer fluids engineered by suspending nanoparticles with high thermal conductivity in traditional heat transferring fluids such as water, alcohol, or engine oil, etc. Numerous experimental and theoretical studies on the heat transfer and flow behaviors of nanofluids (Eastman et al. 2001; Xie et al. 2002; Gherasim et al. 2009) have been conducted since they were first proposed by Choi from Argonne National Laboratory in 1995 (Choi 1995) and the results show that nanofluids have significantly increased heat transfer capabilities with low flow resistance increase. Due to the small-scale effect of nanoparticles, problems such as precipitation, blocking, or equipment attrition that large particles suspensions suffer from do not exist in nanofluids. However, presently there still lacks a sufficient explanation to the flowing mechanism of nanofluids.

Traditional theories of heat transfer and fluid flow in macroscale are based on continuous medium hypothesis. When it comes to nanoscale, however, small-scale effect appears and surface forces tend to predominate in the motion of fluid. Intermolecular impact effect should also be considered and the nanoparticles in nanofluid damage the continuity of fluid flowing as well. So the traditional hypothesis is no more appropriate for nanofluids. The basic principle of molecular dynamics method (MD) is solving molecular (or atomic) Newton equations of motion regarding effects of interaction potential between molecules (or atoms) and external restriction. By this method, time-evolving microscopic process of system is simulated; and equilibrium parameters and transport properties could be statistical computed. So using molecular dynamics method would be an effective way to study flowing behaviors of nanofluids between parallel plates under shear flow conditions.

Previous researchers have studied the mechanisms of heat transfer and fluid flow by molecular dynamics method and made a few achievements. Vergeles et al. (1995, 1996) studied the motor behavior of fluid containing nanoparticles in semi-infinite space and kinetic behavior when particles approaching the wall boundary by molecular dynamics method, and the study demonstrated molecular dynamics method was effective to describe the motions of nanoparticles. Nagayama and Cheng (2004) studied the effect of interface wettability on the pressure driven flow of L–J fluid in nanochannel by MD method and the results showed the hydrodynamic boundary condition at the solid–liquid interface depended on both the interface wettability and the magnitude of the driving force. Xue et al. (2004) studied how the ordering of the liquid at the liquid–solid interface affected the interfacial thermal resistance using non-equilibrium molecular dynamics simulations in which a temperature gradient was imposed. Kamali and Kharazmi (2010) developed a molecular based scheme for simulating of surface roughness effects on nano- and micro-scale flows. The simulation results suggested that both the wall–fluid interaction and surface roughness were important and should be considered simultaneously in determining the nanostructures and profiles of monatomic fluid flow in a nanochannel. In addition, the simulation results showed that the roughness and cavitations of the same dimensions induced different local density pattern while the overall average might be the same. Ahadian et al. (2009) performed molecular dynamics simulations to evaluate the penetration of two different fluids (i.e., a Lennard–Jones fluid and a polymer) through a designed nanochannel. It was revealed that the wall–fluid interaction plays a significant role in such transport phenomena, namely, fluid flow in nanochannels. Maroo and Chung (2010) numerically simulated heating/cooling of fluid atoms by wall atoms and compared molecular dynamics simulation results to the analytical solution of 1-D heat equation. The results were found to match well with the analytical solution. Additional simulations were done where liquid argon atoms were heated by both the walls for two different channel heights and it was shown that in such cases, heat transfer occurred at a faster rate than predicted by heat equation with decreasing channel heights.

In this article, we performed a molecular dynamics simulation of the flowing behaviors of nanofluid constituted with liquid argon and copper nanoparticles between flat plates under shear flow conditions with different shearing velocities. Through the simulation, movements of nanoparticles were observed and their strengthening mechanism to nanofluid flow was analyzed.

2 Simulation methods

The geometric model of the simulation cell has the size of $5.74 \times 32.2 \times 22.1$ nm^3 and the distance between two plates is 20.67 nm which is shown in Fig. 1. The nanofluid is composed of argon atoms and three rows of 4-nm spherical copper nanoparticles. Liquid argon is chosen to be the base liquid for its stability, so the simulation avoids unnecessary complex interaction. The nanoparticles are prepared by carving from copper cubic with initial arrangement of FCC lattice. Then they are put into the liquid argon cuboid which is also arranged as a FCC lattice and the overlapped argon atoms are properly deleted. The purpose of the arrangement of nanoparticles is to observe their movements at different positions in main flow region and their possible interactions during the simulation. Both plates are composed of four-story copper atoms and the atoms are arranged as a face-centered cubic lattice (FCC). The reason of the usage of same materials of plates and nanoparticles is to reduce the difficulty of calculation since less potential functions are needed to be considered. The whole built molecular simulation model is shown in Fig. 2 and the total amount of atoms in it is 127632. The temperature of simulation system is fixed to be 86 K to make the low-boiling liquid argon to remain liquid. For that, in the simulation NTV ensemble is chosen to keep the temperature a constant. The lower plate is fixed and the upper plate is given different translational velocities on y-axis. And the model is simulated twice in order to compare nanofluid flowing behaviors under different shearing velocities.

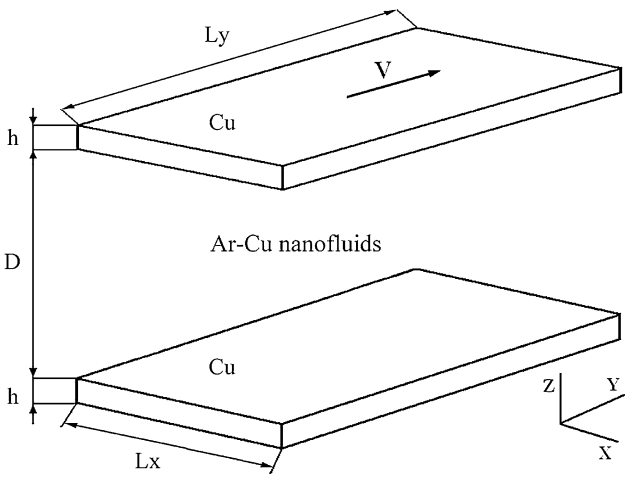

Fig. 1 Geometric model of flat plates with the sizes of $D =$ 20.669 nm, $h = 0.7216$ nm, Lx = 5.7415 nm and Ly = 32.1521 nm. Both plates consist of copper atoms and nanofluid constituted of liquid argon and copper nanoparticles flows between the plates

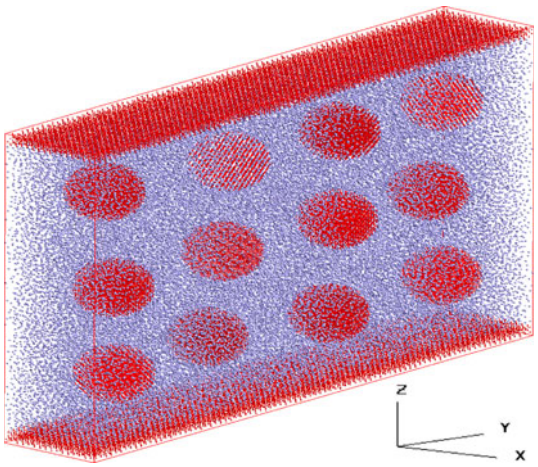

Fig. 2 The whole molecular dynamics model with plate at each side consisted of four layers of copper atoms on z-axis. In the nanofluid, liquid argon is adopted as base liquid and the diameter of each copper nanoparticle is 4 nm. All atoms are arranged as a FCC lattice originally

To choose a suitable potential function is a crucial procedure to make sure the results are accurate and reliable in molecular dynamics simulation. Presently empirical or semi-empirical correlations are adopted in most classic molecular dynamics simulation. Among them, Lennard–Jones (LJ) potential function is the most commonly known one which is frequently used to describe the interactions between atoms or molecules of liquids and gases. LJ potential function (u_{ij}) is given by

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

where r_{ij} is the interatomic spacing between atoms i and $j(r_{ij} = r_j - r_i)$, ε and σ are parameters describing the bonding energy and bonding distance, respectively. The first term in the equation on the right side represents the strong repulsion caused by inner electrons or ion overlap and the second one represents electrostatic interaction between dipoles.

The model of nanofluid presented consists of liquid argon and copper nanoparticles. In order to apply LJ potential to the nanofluid model, the potential parameters should be calculated according to Lorentz–Berthelot mixing rule (Allen and Tildesley 1987) which is given by

$$\sigma_{\mathrm{Cu-Ar}} = (\sigma_{\mathrm{Cu}} + \sigma_{\mathrm{Ar}})/2 \quad (2)$$

$$\varepsilon_{\mathrm{Cu-Ar}} = \sqrt{\varepsilon_{\mathrm{Cu}}\varepsilon_{\mathrm{Ar}}} \quad (3)$$

The LJ potential parameters suitable for argon and copper nanofluid are shown in Table 1 (Sarkar and Selvam 2007).

The nanofluid is simulated by molecular dynamics simulation on a 4 core parallel computer in NTV ensemble

Table 1 LJ potential parameters for simulation

	σ (nm)	ε (J)
Argon	0.3405	16.5402 E−22
Copper	0.2338	65.5815 E−21
Cu–Ar nanofluid	0.2872	10.4153 E−21

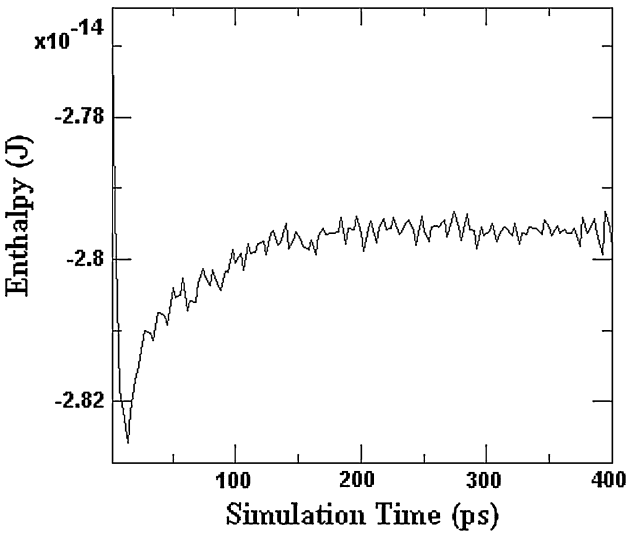

Fig. 3 The enthalpy of system in relaxation process trends to converge and indicates the system reaches the equilibrium state

at constant temperature of 86 K and the cut-off ratio is chosen to be $2.5\sigma_{\mathrm{Ar}}$. The initial simulation system has a man-made atom distribution, so it needs to be relaxed adequately in order to allow the system to adapt itself to a more natural balance condition. In the present study, it is relaxed for 400 ps with each time step length of 2 fs. The computer running time of relaxation takes about 32 h. And the energy distribution in relaxation process is shown in Fig. 3. The enthalpy of system trends to converge which indicates the system reaches the equilibrium state. After the relaxation, the upper plate is given translational velocities of 10 and 50 m/s on y-axis, respectively, and the system is simulated for 1,600 ps with the same length of time step as relaxation, and the computer running time takes about 130 h. So the movements of the nanoparticles in nanofluid at different translational velocities could be observed and compared.

3 Results and discussion

In the whole simulation process, none of the copper atoms in nanoparticle dispersed; all atoms assembled and moved forward. Around each nanoparticle and on the surface of the plates, there existed an absorption layer consisted of argon atoms which had a more even distribution than that

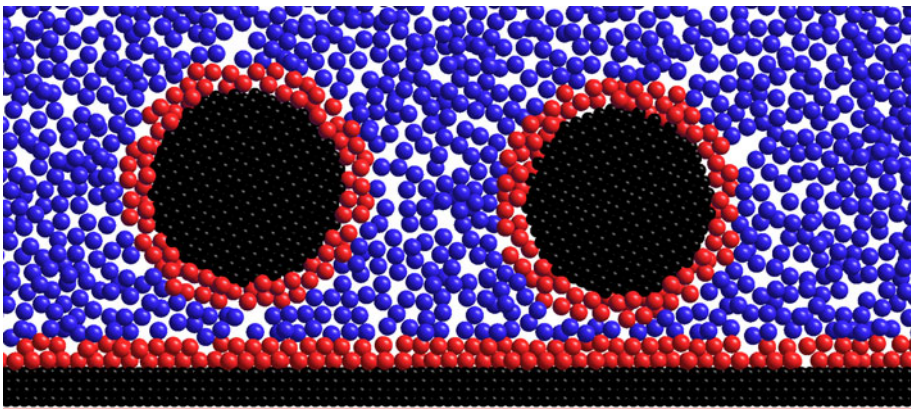

Fig. 4 Argon atoms nearby a nanoparticle or plate would be absorbed to the surface of solid and form an absorption layer. The thickness of the absorption was about 0.5 nm. The screenshot was at simulation time of 1,400 ps. (Color figure online)

of liquid argon, as shown in Fig. 4. The forming reason of the absorption layer was that the interactions between copper and argon atoms were much stronger than those between homogeneous argon atoms. And that made argon atoms nearby a nanoparticle or plate be absorbed to the surface of solid. In the meantime, influenced by the even distribution of the solid surface, the distribution of argon atoms in the absorption layer was more even and more like a solid. When tracking the movements of a nanoparticle, it would be found that once the absorption layer forms, the argon atoms in it would not leave the nanoparticle anymore, and would accompany with the nanoparticle to move forward. Those ones near the plates appeared similar case.

The observed phenomenon of absorption layer agreed with the study of Li et al. (2008). In their study, the diameter of copper nanoparticle was 1.75 nm and the thickness of the absorption layer was about 0.5 nm. In this study, 4 nm copper nanoparticle was used and the absorption layer was found to be the same thickness. So the thickness of absorption layer was unrelated with the diameter of nanoparticle. Merely two layers of argon atoms were absorbed to the solid surface; those in more remote areas would not be affected.

The absorption layer might be effective to heat transferring for the even-distribution layer was believed to have a much higher thermal conductivity than that of liquid and would become a "bridge" of heat conducting between solid nanoparticle and liquid argon. However, the effective diameter of nanoparticle was increased for the existence of the absorption layer and the nanoparticle became heavier. So the absorption layer might obstruct flow and had almost no contribution to enhance flowing of nanofluid.

During the simulation, nanoparticles would translate along with liquid argon on y-axis as a main flow. The translational velocity of nanoparticles in the top layer was the fastest for the influence of the moving upper plate. That

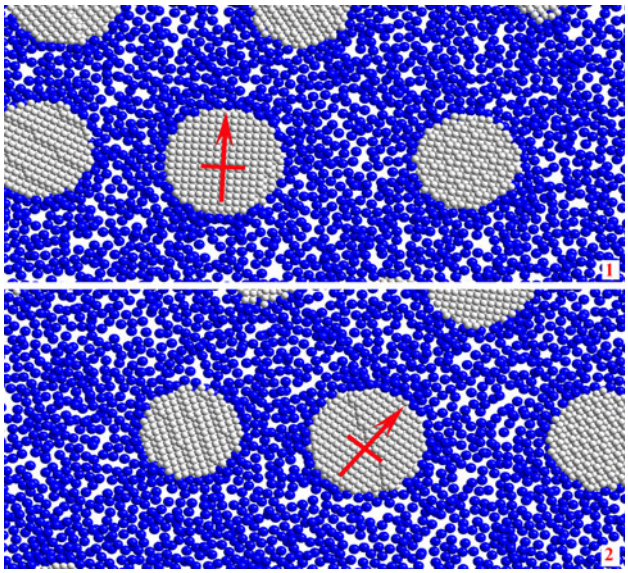

Fig. 5 The rotation of one nanoparticle in the middle layer when the translational velocity of upper plate was 50 m/s. The *top part* was at simulation time of 1,400 ps and the *lower part* was at 1,500 ps

of nanoparticles in the bottom layer was the slowest as affected by the fixed lower plate. And the situation in the middle layer was in between.

Besides translational motion with liquid argon, nanoparticles vibrated, and rotated driven by Brownian motion. In Fig. 5, the rotation of one nanoparticle in the middle layer was shown. In order to be clearly observed, only one layer of atoms on x-axis was selected when creating the screenshot. And on the nanoparticle a red crossed arrow was used to mark the rotation of the nanoparticle. In the figure, the state of the nanoparticle at simulation time of 1,400 ps was numbered as 1, and that at 1,500 ps was numbered as 2. In the figure, it could be clearly found that nanoparticle rotated weakly during the moving process which made micro-flow effect in the partial region nearby the nanoparticle. Figure 6 and 7

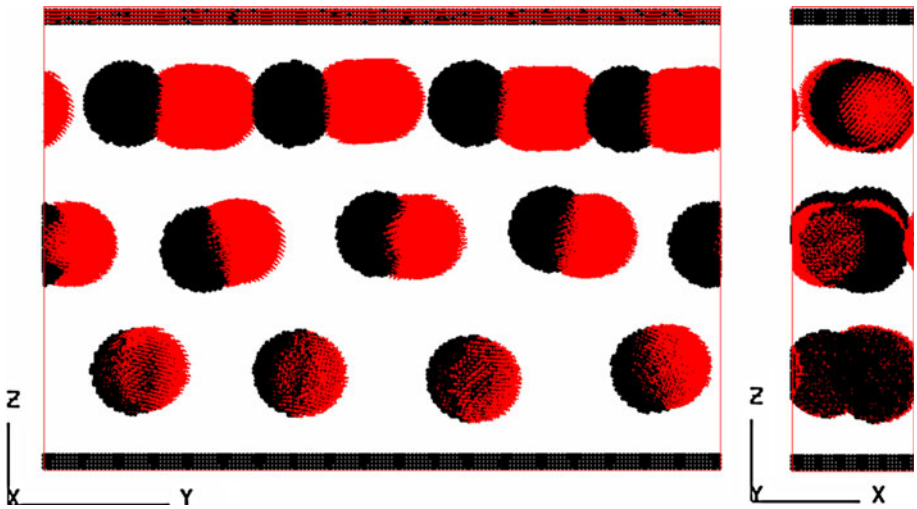

Fig. 6 Trajectories of nanoparticles from 1,400 to 1,500 ps when the translational velocity of upper plate was 10 m/s. (Color figure online)

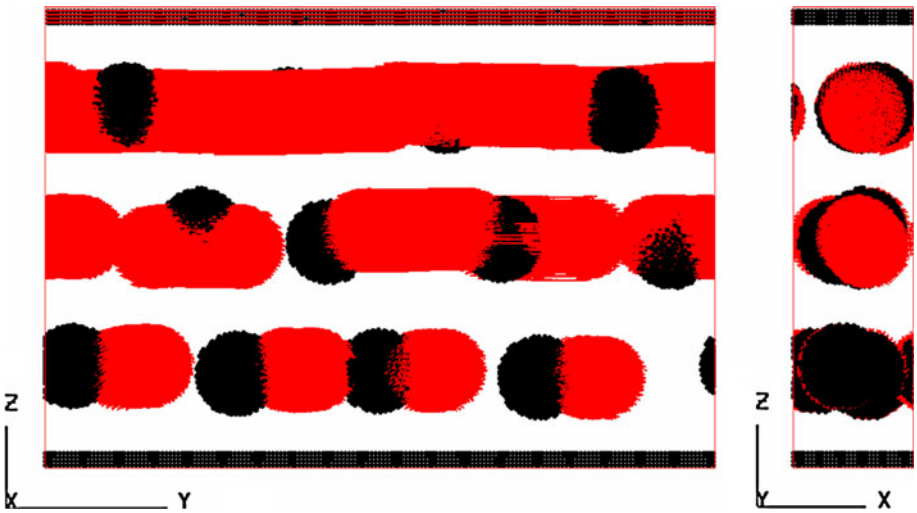

Fig. 7 Trajectories of nanoparticles from 1,400 to 1,500 ps when the translational velocity of upper plate was 50 m/s. (Color figure online)

showed the trajectories of nanoparticles from 1,400 to 1,500 ps with translational velocities of 10 and 50 m/s, respectively. As illustrated, nanoparticles vibrated on both *x*- and *z*-axis. With the increase of translational velocity, the vibration became more obvious. The compositive effects of vibration and rotation of nanoparticles enhanced flowing of nanofluids.

It is generally known that one main reason of the high thermal conductivity of solid was its even distribution of atoms. As argon atoms in absorption layer distributed more like solid, the thermal conductivity of argon in the layer would be much higher than that of liquid argon. Nanoparticle and its absorption layer enhanced heat-conducting property of nanofluids synthetically. In addition, the vibration and rotation of nanoparticles in nanofluids would bring about partial micro-flow which made chaos in the flowing process. So the convection heat transfer between wall and fluid was strengthened, thus the heat transferring was enhanced further.

4 Conclusions

Molecular dynamics model of nanofluid between flat plates under shear flow conditions was built. The model consisted of several 4-nm copper nanoparticles and liquid argon as base fluid. The LJ potential function was adopted to deal with the interactions between atoms. Through the comparative analysis of simulation results, the following conclusions were obtained:

(1) Absorption layers consisted of argon atoms were found near surfaces of nanoparticles and plates. This layer had a much higher thermal conductivity and would enhance heat-conducting property of nanofluids together with nanoparticles.
(2) In the process of shear flowing, the nanoparticles would vibrate and rotate besides main flowing with liquid argon and these micro-motions could strengthen partial flowing nearby nanoparticles. The convection heat transfer between solid and fluid was strengthened.

Acknowledgments This study was supported by the National Natural Science Foundation of China (Grant No. 50876016 and 51006015) and China Postdoctoral Science Foundation (Grant No. 20100470070).

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