Advanced Powder Technology 26 (2015) 180–187

Contents lists available at ScienceDirect

Advanced Powder Technology

journal homepage: www.elsevier.com/locate/apt

Original Research Paper

Effect of Morse potential as model of solid–solid inter-atomic interaction on the thermal conductivity of nanofluids

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ARTICLE INFO

Article history:
Received 7 June 2014
Received in revised form 29 August 2014
Accepted 15 September 2014
Available online 26 September 2014

Keywords:
Nanofluid
Molecular Dynamics simulation
Thermal conductivity
Lennard-Jones potential
Morse potential

ABSTRACT

Over the last years a body of studies has been proposed by several authors to calculate the thermal conductivity of nanofluid, using the molecular dynamics (MD) simulations based on the Green Kubo formalism applying the well-known Lennard-Jones potential. The present work shows the influence of the solid–solid inter-atomic potential type on the thermal conductivity of nanofluids. The effective thermal conductivity obtained from the conventional models is compared with the present simulation, by varying nanoparticles concentrations and the system temperatures. The present results follow considerably the theoretical models integrating the Brownian motion of nanoparticles inside the base fluid. Our mainly findings suggest that the thermal conductivity of (Ar-Cu) nanofluid is influenced by the type of potential used in the simulation. Furthermore introducing Morse potential, which is recommended for metallic's interactions between (Cu-Cu) atoms, enhances significantly the simulation results of nanofluid thermal conductivity and shows a good agreement with the existing literature data.

1. Introduction

Nanofluids have received much attention, over the last past decades. Researchers have used nanofluid as a new class of high efficiency heat exchange media, to overcome the limited heat transfer capacities of traditional fluids such as water, engine oil, and ethylene glycol (EG). For instance, experiments have shown that nanofluids exhibit very high thermal conductivity even at low concentrations of suspended nanoparticles [1–4]. Furthermore, some experimental studies have revealed that the nanofluids thermal conductivity increases as temperature increases [5–7], making nanofluids even more attractive as a cooling fluid for devices at high temperature. The traditional understanding of the effective thermal conductivity of mixtures originates from the continuum formulation that includes only the particle volume fraction, size and shape. In addition this approach assumes a diffusive heat transfer in both solid and fluid phases. Also gives a good result for the micrometer solid fluid system, but it fails to highlight the anomalous heat transfer characteristics of nanofluids [1,8–12]. To predict the thermal conductivity of such materials, conventional analysis requires several simplifications and assumptions to find simple equations. Moreover, they are unable to take into account deep details at the atomic level. Those methods are limited to special cases and give underestimate results for the new and complex materials at the nanometer scale. In fact, various numerical models were proposed to explain the unusual enhancement of the thermal conductivity at the nano-metric level such as lattice Boltzmann method [12,13], Monte Carlo simulation [14–16] and molecular dynamics (MD) simulation [6,17–27]. From the microscopic point of view, the (MD) consist of solving Newton's equation of motion for a system of particles interacting with each other under atomics potentials [28]. As MD simulation predict directly and accurately the trajectories as well as the motion of particles at the atomic level, it gives to scientist's a very innovative technique to predict macroscopic properties via statistical mechanics. Due to the accuracy and the quality of results, in addition to the faster development of the computers capacities, the molecular dynamics simulation has been widely used in the literature to study the thermal conductivity in the nanofluids via the Green Kubo or Einstein formalism. A number of studies have been oriented to develop novel models able to explain the anomalous enhancement of the thermal properties of nanofluid and its mechanisms [29–31]. Bhattacharya et al. [32] carried out Brownian dynamics simulation with equilibrium Green–Kubo method to calculate effective thermal conductivity of nanofluid and they found good agreement with experimental results [9]. Vladkov and Barrat

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http://dx.doi.org/10.1016/j.apt.2014.09.006

Nomenclature

C_p	heat capacity [J K^{-1} kg^{-1}]
D	the depth of the potential well [J]
d_p	the diameter of the nanoparticle [m]
E	excess energy [J]
F_{ij}	force between the pair atoms i and j [N]
h^k	the average enthalpy per atoms of species k [J]
HF^{α}	the partial enthalpy flux of species α [J m s^{-1}]
J	heat current [J m s^{-1}]
$J(0)$	heat current at time zero [J m s^{-1}]
$J(n)$	the heat current at MD time step n [J m s^{-1}]
$J(t)$	heat current at time t [J m s^{-1}]
J^C	heat flux of fluctuation collision [J m s^{-1}]
J^K	heat flux of fluctuation kinetic [J m s^{-1}]
J^P	heat flux of fluctuation potential [J m s^{-1}]
k	thermal conductivity [W K^{-1} m^{-1}]
k_B	Boltzmann constant $k_B = 1.8.6173 \times 10^{-5}$ [J K^{-1}]
m	number of time steps or mass
M	total number of MD time steps for averaging [–]
n	number of time steps [–]
r_0	the equilibrium bond [m]
r_{cut}	cut-off distance [m]
r_i	position of atom i [m]
r_{ij}	distance between atoms i and j [m]
T	temperature [K]
u	potential [J]
V	volume [m^3]
v_i	velocity of atoms i [m s^{-1}]
L	side of box [m]
N	total number of MD simulation time steps or number of atoms

Greek symbols

δ	parameter controlling the width of the Morse potential well [m^{-1}]
ε	the depth of the Lennard-Jones potential well [J]
φ	volume fraction of nanoparticles [–]
ρ	density [kg m^{-3}]
σ	the finite distance at which the inter-particle Lennard-Jones potential is zero [m]
μ	dynamic viscosity [kg m^{-1} s^{-1}]
Δt	time step [s]

Subscripts

f	base fluid
C	fluctuation collision
CC	correlation collision – collision
CK	correlation collision – kinetic
CP	correlation collision – potential
K	fluctuation kinetic
KC	correlation kinetic – collision
KK	correlation kinetic – kinetic
KP	correlation kinetic – potential
nf	nanofluid
p	nanoparticle
P	fluctuation potential
PC	correlation potential – collision
PK	correlation potential – kinetic
PP	correlation potential – potential
α, β	copper or Argon atoms
L-J	Lennard-Jones potential
M	Morse potential

[33] used molecular dynamics simulation to calculate the thermal conductivity of nanofluid; they found that in the absence of collective effects, the thermal conductivity of the nanofluid can be described by the classical Maxwell-Garnet [34] equation. Another interesting numerical investigation was conducted by Xue et al. [35] using non-equilibrium MD simulations. They studied the effect of the liquid–solid interface on the interfacial thermal resistance and they conclude that the simple monatomic liquid around the solid particle showed no influence on the thermal transport either normal or parallel to the surface. Furthermore, they suggested that the large thermal conductivity enhancement of nanofluids couldn't be explained by the thermal transport in the liquid–solid interface layer. Many materials have been widely used for this issue and interest in copper nanoparticles arises from the useful properties of this metal such as the good thermal and electrical conductivity and lower cost. Furthermore copper nanoparticles are elaborated with very simple and competitive methods such as chemical reduction [36].

The investigations carried out in the present paper deal with equilibrium molecular dynamics (EMD) simulation of the thermal conductivity of a nanofluid (Ar-Cu) consisting of argon as base fluid and nanoparticles of copper suspended in this fluid, using the Green–Kubo formalism with different type of interatomic potentials. The obtained results shows that the dependence of the thermal conductivity of nanofluids, on both temperature and volume fraction of nanoparticles, is significantly influenced by the type of potential used in the modeling of the atom–atom interactions within the copper nanoparticle.

2. Molecular dynamics model

2.1. Modes of microscopic heat flux fluctuations and decomposition of thermal conductivity

Several mechanisms have been used to calculate the thermal conductivity in the complex material. One of the most fascinating method is the molecular dynamics (MD) simulation since it has been successfully employed in the past to predict solids, fluids and nanofluids thermal conductivity via Green Kubo framework [17,37–40]. The thermal conductivity is defined as the linear coefficient relating the macroscopic heat current J to the temperature gradient (Fourier's law).

$$J = -k\mathrm{grad}(T) \tag{1}$$

In this work the thermal conductivity is calculated using the Green–Kubo method [28,41]

$$k = \frac{1}{3Vk_BT^2}\int_0^{+\infty}\langle J(t)\cdot J(0)\rangle dt \tag{2}$$

The heat current J is defined by [42] as

$$J = \frac{d}{dt}\sum_{i=1}^{N} r_i \cdot E_i \tag{3}$$

Where E_i denotes the excess energy and r_i is the position of atom i. For a two-component system, the heat current J consists of three parts: kinetic, potential and collisional part. [6,43,44].