Chemical Physics Letters 695 (2018) 112–118

Contents lists available at ScienceDirect

Chemical Physics Letters

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

Research paper

Molecular dynamics simulation of wetting and evaporation characteristics for sessile nanofluid nanodroplets

Weili Qiang [a], Baohe Wang [a,*], Qun Li [a], Wei Wang [b]

[a] State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian, PR China
[b] School of Chemical Machinery and Safety, Dalian University of Technology, Dalian, PR China

ARTICLE INFO

Article history:
Received 21 November 2017
In final form 1 February 2018
Available online 2 February 2018

Keywords:
Molecular dynamics simulation
Evaporation
Wetting
Nanofluid
Sessile nanodroplet

ABSTRACT

Wetting and evaporation characteristics of sessile nanofluid nanodroplet (SNFND) were investigated by molecular dynamics simulation. Results show that for lyophilic surface, with the increase of nanoparticle energy coefficient, contact angle of SNFND increases and total evaporation decreases. Effects of nanoparticle volume percentage on the wetting and evaporation behaviors of SNFND are related to surface wettability. For lyophilic surface, the greater the nanoparticle volume percentage, the greater the contact angle, and the slower the evaporation. For neutral and lyophobic surfaces, nanoparticle volume percentage has obviously strengthening effect on evaporation, and the strengthening effect decreases as nanoparticle volume percentage increases.

1. Introduction

It is well known that evaporation characteristics of sessile nanofluid droplet are critical in the field of electronic chip cooling, firefighting, pesticide spraying, inkjet printing, medical diagnosis and so on [1–4]. Up to now, studies on evaporation of sessile droplets or nanofluid droplets are mainly focused on experiments, theories and computer simulations for millidroplets or microdroplets [5–16]. In order to better understand wetting and evaporation mechanism of millidroplets or microdroplets, it is necessary to study the nano-size droplets. With the rapid development of computer and the emergence of molecular dynamics (MD) simulation technology, it is possible to determine the contact angle (CA) and evaporation characteristics of nanodroplets or nanofluid nanodroplets. So far, a large amount of research has been done for wetting or evaporation behaviors of sessile pure component nanodroplets by MD simulations [17–20]. However, a few of study has been made for wetting or evaporation behaviors of sessile nanofluid nanodroplets by means of MD simulations [21–27]. Lu et al. [21] investigated the dynamic wetting of water nanodroplets containing gold nanoparticles on a gold substrate and observed that the addition of nanoparticles hinders the nanodroplet wetting process. Li et al. [22] indicated that volume percentage and surface wettability of nanoparticle would effectively influence the spreading behaviors of nanofluid nanodroplets, and a competitive mechanism analysis of spreading was proposed. Lu et al. [23] studied the effects of evaporation on wetting kinetics of sessile water nanodroplet, and presented micromechanism by analyzed contact line mobility and water molecules absorption–desorption behavior in the vicinity of the contact line region. Chen et al. [24] investigated the evaporation behaviors of sessile nanodroplets containing colloidal nanoparticles by MD simulations and a comparison was made with the pure L-J nanodroplets. Wang et al. [25] studied the effect of salt type and concentration on the evaporation rate of nanodroplets with dissolved salts via MD simulation. They found the presence of salts results in a slower evaporation rate compared to pure water nanodroplets; and the higher the salt concentrations, the slower the evaporation rate. Zhang et al. [26] explored the wetting and evaporation characteristics of salt-water nanodroplets on platinum surfaces. They revealed the CA of salt-water nanodroplets increases with the increase of salt concentration while the evaporation rate of nanodroplets was declining. Li et al. [27] proposed three motion styles of contact line and three ways to regulate contact line pinning. As well, they explained the driving mechanism of the nanoparticle confined in the contact line, which provide a theoretical basis for the contact line pinning issues in spreading or evaporation process.

In this work, we attempt to investigate the wetting and evaporation characteristics of SNFNDs via molecular dynamics simulation. Furthermore, the effect of nanoparticle energy coefficient or volume percentage on CA and evaporation rate of SNFNDs will be discussed.

* Corresponding author.
E-mail address: wbaohe@dlut.edu.cn (B. Wang).

https://doi.org/10.1016/j.cplett.2018.02.001
0009-2614/

2. Simulation details

2.1. Simulation models

A certain number of gold nanoparticles were added to argon nanodroplet (base fluid) to form the argon-base SNFND, which is shown in Fig. 1. The size of simulation box is 25.2 nm × 25.2 nm × 25 nm. In the initial configuration of argon SNFND, the red is argon atom, and the blue is gold nanoparticles with a diameter of 0.8 nm that is distributed evenly in the argon SNFNDs. The initial diameter of the SNFND is 10 nm, and it is located in the center of the cube simulation box. In order to simulate the heat transfer process of the solid wall, the bottom wall uses the Phantom virtual wall model [28–31], while the black line in the middle of the simulated box is virtual reflect wall. The height of the solid wall is 1.5 nm, which is composed of the real wall atomic layer, the virtual wall atomic layer and the fixed wall atomic layer, see the literature [28] for details.

2.2. Potential energy function

Since argon and nanoparticle and solid atoms are simple ones, the interaction between them is described by the LJ (12-6) potential function, as shown in Eq. (1) [32].

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

in which U is potential energy; σ and ε are length and energy parameters between atom i and j, respectively; r_{ij} represents the distance between atoms. The potential energy parameters of each atom are shown in Table 1 [22,33,34]. Among them, the interaction energy parameter between argon and surface atom $\varepsilon_{\text{Ar-Solid}}$ is defined as $\alpha \times 0.24$, where α is called the surface energy coefficient [35]. When surface energy coefficients equal to 0.2, 0.4 and 0.6, the three surfaces (lyophobic, neutral, lyophilic) will be modeled separately. Just like the surface energy coefficient α, nanoparticle energy coefficient β represents nanoparticle wettability and is defined as $\beta = \varepsilon_{\text{NPs-Ar}}/\varepsilon_{\text{Ar-Ar}}$. The greater the nanoparticle energy coefficient is, the better the wettability of nanoparticle becomes. For $\beta = 1.0$, nanoparticle-argon interaction equals to argon-argon interaction. For $\beta < 1.0$, nanoparticle-argon interactions are weaker than argon-argon interaction, and the nanoparticles are lyophobic. For $\beta > 1.0$, nanoparticles are lyophilic within nanofluid nanodroplets. In order to explore the effect of nanoparticle wettability on the wetting and evaporation properties of SNFNDs, β is taken as 0.5, 1.0, 1.5 and 2.0. Due to the relative strong force between metal atoms, these small nanoparticles tend to agglomerate during the evaporation process. Generally, it is believed that the energy parameter is a key factor in the agglomeration of nanoparticles [36]. In this paper, the energy parameter between nanoparticle atoms is selected as 0.01 kCal·mol^{-1} [36]. In addition, the length parameters are obtained by LB combination rule [32].

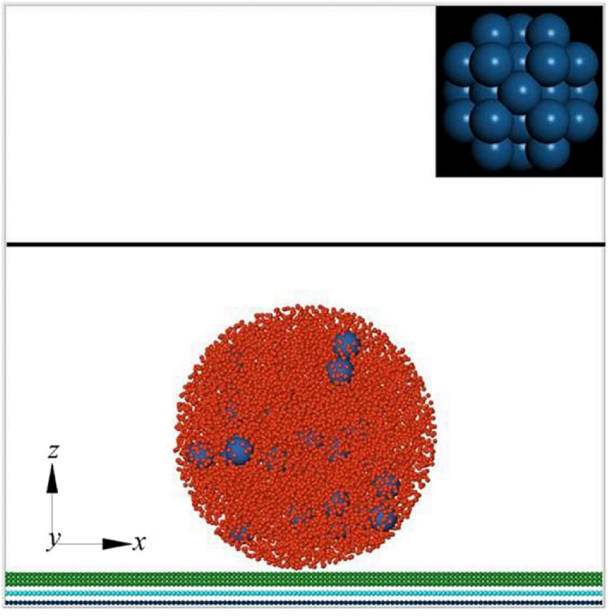

Fig. 1. Initial configuration of sessile argon-base nanofluid nanodroplet.

Table 1
Potential parameters of argon, nanoparticles and solid atoms.

Interaction types	ε (kCal·mol^{-1})	σ (Å)
Ar-Ar	0.24	3.405
Ar-Solid	$\alpha \times 0.24$	2.93
Ar-NPs	$\beta \times 0.24$	3.405
NPs-NPs	0.01	3.405
NPs-Solid	0.144	2.93
Solid-Solid	12	2.45

The cutoff radius of the LJ potential function between the argon atom and the solid surface atom is 1.2 nm [37]. Since the nanoparticle diameter is 0.8 nm and the volume of the nanoparticles cannot be neglected, the cutoff radius of interaction force between nanoparticle and other atom is set to 2.0 nm.

2.3. Simulation method

The whole simulation process is divided into two phases: equilibrium MD simulation and non-equilibrium MD simulation. In equilibrium MD simulation, the system with the initial configuration is simulated in an NVT ensemble. And Nose-Hoover thermostat was used to control the temperature of nanodroplet in the vicinity of 100 K. For solid substrates, Langevin thermostat is used to keep the temperature constant at around 110 K. In non-equilibrium MD simulation process, the NVE ensemble is selected. During the equilibrium MD simulation, the nanofluid nanodroplet on the solid surface has a stable CA and reaches the vapor-liquid equilibrium state. Then the virtual reflect wall is removed and a vacuum layer with a height of 10 nm is added in $z+$ direction, and non-equilibrium evaporation process begins. The equilibrium and non-equilibrium MD simulations run 3 million and 5 million steps, respectively. The time step for the Velocity-Verlet integrator is 0.5 fs.

All the MD simulations were performed with the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software [38]. Periodic boundary conditions were applied in the x, y directions, while fixed boundary conditions were adopted in the z directions. We constantly adjusted the mass center of the system in order to ensure that the total momentum of the nanodroplet is zero. The "Oxford" method [39] was used to count the number of argon atoms in the SNFND, and then to calculate the evaporation capacity per unit time (measured in atomic number).

3. Results and discussions

3.1. Effects of nanoparticle energy coefficient

For hydrophilic surface ($\alpha = 0.6$), under the condition of the same nanoparticle volume percentage ($\psi = 7\%$), two-dimensional mass density profiles and contact angles of SNFNDs at different