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Wettability alterations and magnetic field effects on the nucleation of magnetic nanofluids: A molecular dynamics simulation

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ABSTRACT

In this study, the effects of surface wettability and nanoparticle concentration on boiling of ferrofluids were investigated with the application of magnetic field using molecular dynamics simulations. Liquid argon was considered as the base fluid with the use of Lennard-Jones fluid model. Two different surfaces (hydrophilic with contact angle of 40.5° and hydrophobic with contact angle of 130.6°) were taken into consideration to investigate the effect of nanoparticle presence on bubble formation over a uniformly heated wall. According to the obtained results, vapor film formation and nucleation depend on the interfacial wettability of nanoparticles and substrate. Compared to the pure liquid, film boiling does not easily happen in the ferrofluid containing hydrophilic nanoparticles, while it is easy to have vapor film in the nanofluid with hydrophobic nanoparticles. It was found that the momentum change due to external magnetic field dramatically alters the evaporation mechanism, resulting in lower liquid film temperature.

1. Introduction

Boiling is of one of the major heat transfer modes and offers a variety of applications in the industry [1,2]. Methods such as enhanced surfaces and engineered fluids are used to augment boiling heat transfer. Nanofluids are new generation fluids, where conductive nanoparticle (e.g. Cu, CNT) are dispersed in a base fluid (e.g. water). Ferrofluid is one of the popular types of nanofluids, which can be manipulated by an external magnetic field and have a strong potential in applications of electronics cooling, miniature chemical – biological analysis and drug delivery [3].

Accurate modeling of boiling is important for understanding heat transfer mechanisms. The classical theories of two phase flows predict extremely large superheats for nano-bubble formation on the smooth surface, which is not in agreement with most of the experimental studies [4,5]. Obviously, for the case of nanofluid boiling, this is more complicated. In this regard, with the advances in both hardware and software during recent years, computer simulations based on molecular dynamics (MD) have become one of the most useful and prevalent methods to study the phase change phenomena in the atomistic level [6].

Extensive investigations have been done in order to study boiling and bubble formation in the nano-scale [7–11]. Wneg et al. [12] newly studied the boiling of thin water film on an electrified solid surface and the enhancement of the boiling heat transfer. This study also provided a new method to suppress vapor layer formation for rapid boiling and revealed mechanisms on the heat transfer enhancement with charged surface. Based on this study external electric field increases the molecular collision and enhances the heat transfer [12]. Maruyama and Kimura [13] simulated the bubble formation in liquid Argon between parallel solid platinum walls by slowly expanding the surfaces. The change in the volume resulted in pressure reduction, which was due to the growth of a successful patch. Moreover, in order to simulate the wall wettability effects on vapor bubble formation, they changed the potential parameter between the liquid and solid atoms in their molecular dynamics simulations. In another study, Maroo and Chung [14] studied phase change of a liquid argon film on a platinum surface and the colloidal adsorption phenomenon by using molecular dynamics to provide

microscopic characterizations of the dynamic thermal energy transport mechanisms during the liquid film evaporation and also the resulting non-evaporable colloidal adsorbed liquid layer at the end of the evaporation process. This study also provides a creative method to calculate the number of evaporated liquid atoms to quantify the evaporation process. Yamamoto and Matsumoto [15] applied the molecular dynamics simulation technique to observe the initial stage of nucleate boiling for the Lennard-Jones (LJ) liquid model. They examined two cases: the overall heating, where the surface temperature is kept constant all over the area, and the partial (spot) heating. Based on the presented results, in both cases, when the liquid in the vicinity of the heating surface obtains sufficient energy, it thermally expands and its

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Nomenclature

m	Mass (kg)
r	Particle-particle distance (m)
rc	Cut of radius (m)
t	Time (s)
F	Force (N)
i,j	Particle index (−)
L	Simulation box length (m)
$\vec{v}$	Velocity vector (m/s)
e	Energy per atom (J/mol)
S	Stress tensor
J	Heat flux (W/m^2)

Greek

ϕ	Interaction potential function
ε	Potential depth (m)
σ	Quantity of particle diameter
μ_0	Vacuum permeability
$\vec{\mu}$	Magnetic momentum
τ	Torque (N·m)
ω	Angular velocity (raad/s)
θ	Contact angle (degree)
φ	Particle volume fraction

Superscript

dip	Dipolar interaction
w,l	Wall-liquid
mag	Magnetic
LJ	LJ fluid

Subscript

ext.	external
	ll, ww, wl Liquid-liquid, solid-solid and solid-liquid
x,y,z	Cartesian coordinate direction

pressure decreases, leading to the formation of bubble nuclei of atomic size. This study also illustrates that the inception time of nucleation is affected by surface wettability as well as the surface temperature. Hens et al. [6] examined the mechanism of bubble formation in LJ liquid on a Platinum surface. They simulated boiling of liquid argon on the surfaces with different wettability conditions, which were controlled by the changes in energy parameter of the LJ model. Their results showed that film boiling and bubble nucleation occur more quickly on the hydrophilic surface rather than the hydrophobic surface.

Many researchers have implemented molecular dynamics simulations to study heat transfer and thermal properties of nanofluids. Aminfar et al. [16] investigated the time dependent behavior of nanofluid flow, and nanoparticle aggregation under magnetic fields using molecular dynamics simulations. They implemented magnetics dipole–dipole interaction potential to the nanoparticle simulation and found that the system with magnetic nanoparticles agglomerates faster relative to non-magnetic nanoparticles. Wang et al. [17] studied the microstructure of ferrofluids for various concentrations and particle dipole moments by using the mesh Ewald summation for long-rage dipolar interactions and considering the rotational and translational degrees of freedom. They also conducted Langevin molecular dynamics (MD) simulations to inquiry the equilibrium properties of ferrofluid systems for different fractions of small and large particle sizes [18].

In the literature, researchers have widely investigated phase change in liquid transport and equilibrium properties in nanofluids as well as the effects of magnetic fields on nanofluid micro-structure. However, the MD studies involving magnetic field effect on phase change of nanofluids have been rarely reported.

In the present study, molecular dynamics simulations were carried out to illustrate the magnetic field effects on the nucleation and explosive boiling of a LJ ferrofluid considering magnetic dipole-dipole interaction potential for the nanoparticles. The results were compared with pure LJ liquid. Temperature, surface wettability condition, magnetic field intensity and nanoparticles volume fraction were taken as the major parameter effects. The microstructure of the system, temperature of each atoms group, normal heat flux and the number of each phase atoms were obtained.

2. Simulation method

In the present study, the ferrofluid consists of magnetic particles dispersed in the base fluid on a metal crystal structure heater. Translational equations of motion for both particles and the base fluid were considered. The rotational equations of motion for the nanoparticles were considered as well.

By simplifying the interactions of the particles in the system to pairwise interactions, the Newtonian equation for each particle of the simulation model can be written as:

$$m_i \frac{d^2\vec{r_{ij}}}{dt^2} = -\sum_{j\neq i} \frac{\partial\phi\left(\vec{r_{ij}}\right)}{\partial r_{ij}} + \vec{F}_{ext} \tag{1}$$

where $\phi(\vec{r_{ij}})$ is the interaction potential function between particles i, j and $\vec{F}_{ext}$ is the external force due to the presence of magnetic field acting on the particles. For characterizing the interactions between the particles, various potential functions have been proposed [16,19]. In this study, the liquid argon was chosen as the base fluid to reduce the computational costs and to eliminate the additional interatomic interactions, which are undesirable. Thus, the Lennard-Jones (LJ) potential, as the most commonly used interatomic interaction potential, has been chosen to model the pairwise atomic interactions as:

$$U_{ij}^{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{2}$$

where r, ε, and σ are the particle-particle distance, the potential depth and the quantity corresponding to the particle diameter, respectively.

Generally, the most important interactions to be considered for magnetic particles are the dipolar interactions, which have anisotropic long-range characteristics. Considering both Lennard-Jones and Dipolar interactions, the equations of motion for the magnetic particles can be written as [16]:

$$\sum_{j\neq i}\left(\vec{F}_{ij}^{dip} + \vec{F}_{ij}^{LJ}\right) = m_i\frac{d\vec{v}}{dt} \tag{3}$$

$$\sum_{j\neq i}\left(\vec{\tau}_{ij}^{dip}\right) = I\frac{d\vec{\omega}_i}{dt} \tag{4}$$

The resultant force and torque by considering the magnetic dipole-dipole interaction potential can be expressed as [20,21]:

$$\phi_{ij}^{dip} = \frac{\mu_0}{4\pi}\frac{1}{|r_{ij}|^3}\left[\mu_i.\mu_j - \frac{3}{|r_{ij}|^2}\left(\mu_i.r_{ij}\right)\left(\mu_j.r_{ij}\right)\right] \tag{5}$$