International Journal of Heat and Mass Transfer 127 (2018) 237–243

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

Molecular dynamics simulation of carbon nanotube-enhanced laser-induced explosive boiling on a free surface of an ultrathin liquid film

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ARTICLE INFO

Article history:
Received 1 March 2018
Received in revised form 21 May 2018
Accepted 29 June 2018

Keywords:
Explosive boiling
Carbon nanotube
Molecular dynamics
Phase transition

ABSTRACT

Molecular dynamics (MD) simulations are conducted to investigate laser-induced explosive boiling on the free surface of an ultrathin liquid film filled with carbon nanotubes (CNTs). The following two atom systems are developed: (i) Ar system, which is composed of argon vapor and liquid argon and (ii) Ar-CNT system, which is composed of argon vapor, liquid argon, and vertically-arranged CNTs. The effects of laser energy fluence and CNTs on phase transition are investigated by the temporal variation of temperature and net evaporation rate and the spatial profiles of temperature and atoms. Results show that phase transition shifts from normal evaporation to explosive boiling. The results of the Ar-CNT system indicate significant increases in the maximum temperature of a laser-absorptive region and the net evaporation rate compared with that of the Ar system. The net evaporation rate is 1.5–2.0 times higher in the Ar-CNT system than in the Ar system. Furthermore, rapid and steady explosive boiling is achieved for the Ar-CNT system in accordance with the monotonic increase in the net evaporation rate and appropriate dispersion of the vapor atoms. These results imply that vertically arranged CNTs effectively affect the laser-induced explosive boiling on the free surface of an ultrathin film.

1. Introduction

Explosive boiling is the process of ultra-fast liquid-to-vapor-phase transition, which can be triggered by rapid superheating or depressurization. The explosive boiling of ultrathin films in short pulse laser processing is an interesting issue given its various applications in the newly emerging technologies, such as pulsed laser deposition [1,2], micro- and nanostructuring [3–7], and laser surgery [8,9]. The development of these previous technologies is rooted in an improved understanding of the mechanism and fundamental science of the explosive boiling phenomena in laser processing (laser-induced explosive boiling).

Molecular dynamics (MD) simulations [10–18] are important for providing an atomic-sized level and a sub-femtosecond time scale understanding of the phenomena to understand the complex and highly non-equilibrium mechanism involved in the laser-induced explosive boiling phenomena. Seyf and Zhang conducted MD simulations to investigate the explosive boiling of a thin liquid argon film adsorbed on solid metal surfaces, which were structured by nanoscale spherical array [12] and nanocone array [13]; their results showed a significant effect of nanostructured surfaces on explosive boiling. Wang et al. [14] carried out similar MD simulations to investigate the effect of cubic nanostructured aluminum surfaces on explosive boiling. Zhang et al .[15] also investigated the effects of nanochannels on the explosive phase transition of ultrathin liquid argon film over the copper surface using the MD simulations. Shavik et al. [16] performed MD simulations to reveal the effect of solid–liquid interfacial wettability on the boiling of the thin liquid argon film placed over a solid flat platinum wall with no nanostructures. Hasan and Shavik et al. [17] also performed MD simulations to reveal the effect of interfacial wettability and nano-sized internal recesses platinum wall on the boiling of thin liquid argon film. In these previous studies [12–17], all-atom potentials were used to describe the atomic interactions. Furthermore, the laser energy deposition was simulated by jump temperature increases in the solid surfaces (called substrate-assisted), which induced the phase transition through normal evaporation or explosive boiling at the solid–liquid interface. The results predicted by these studies showed that a reasonable nanostructure of a solid surface can enhance explosive boiling. In addition, Zhigilei et al. [18] performed MD simulations to investigate the effect of the target structure and composition on the ejection and transport of polymer molecules and carbon nanotubes (CNTs) in a matrix-assisted pulsed laser evaporation (MAPLE) process. These researchers used a coarse-grained MD model to simulate the frozen matrix polymer, a mesoscopic model to the embedded CNTs, and the Lennard-Jones (L-J) potential to the interaction between the matrix

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https://doi.org/10.1016/j.ijheatmasstransfer.2018.06.152
0017-9310/

molecules and CNTs. Moreover, laser irradiation was simulated by depositing quantum of energy equal to the photon energy into the kinetic energy, which is based on the breathing sphere model developed for simulating laser interactions with molecular targets.

Numerous investigations have been conducted to predict laser-induced explosive boiling using MD simulations. However, to the best of the authors' knowledge, the MD study of laser-induced explosive boiling on the free surface of a transparent liquid has not been explored. High intensities and tight focus are required in a pulse laser processing given the nonlinear absorption of light energy in the transparent materials [4]. In addition, the energy transfer processes and physical mechanisms of the laser-induced explosive boiling on the free surface of a transparent liquid are significantly different from the substrate- and matrix-assisted cases. CNTs have attracted considerable attention for the emerging thermal management applications [19–24] given their ultra-high thermal conductivities. Therefore, the explosive boiling is expected to be different when CNTs are arranged in a liquid.

In the present work, MD simulations are performed to investigate the laser-induced explosive boiling on the top free surface of an ultrathin argon liquid film with embedded CNT. The liquid and vapor argon and the single-walled (5, 5) CNT are described by the all-atom potentials. In addition, the pulsed laser excitation is simulated by depositing thermal energy to the atoms in the upper layer of the liquid argon. Then, the effects of the laser fluence and CNT on explosive boiling on the free liquid surface are explored by discussing the temporal variation of the temperature and net evaporation rate and the spatial profiles of the temperature and atoms.

2. Simulation method

Two simulation systems, namely, the Argon (Ar) and Ar-CNT systems, are developed (Fig. 1). The initial energy-minimized simulation domain is a cube with the size of 10.52 nm (x) × 10.52 nm (y) × 92 nm (z) for both systems. The liquid argon atoms are initially arranged by a solid state on a face-centered cubic (FCC) lattice that corresponds to the density at zero temperature, and the region above the liquid argon is filled with FCC vapor argon atoms. The Ar-CNT system is created by inserting the CNT molecule into the Ar system, thereby removing the argon atoms that overlap with the CNT. For the Ar system, the total number of argon atoms is 56,240. The height of the bottom liquid region with 56,000 atoms is 17.6 nm, and the remaining domain is filled with 240 vapor atoms. For the Ar-CNT system, the inserted CNT with the length of 18.8 nm and the atom number of 1500 are vertically arranged with its axis that is parallel to the z-direction and completely immersed into the bottom liquid argon. A total of 55,720 liquid and 240 vapor argon atoms exist in the Ar-CNT system.

The C—C interatomic interactions in a CNT are modeled by a covalent-bonding potential developed by Tersoff [25], as follows:

$$E_b = \sum_i \sum_{j(i<j)} \{V_R(r_{ij}) - B_{ij} V_A(r_{ij})]\}, \tag{1}$$

where E_b is the sum of the C—C bonding energy of each bond between carbon atom i and atom j. V_R and V_A are the repulsive and attractive pair terms, respectively, and r_{ij} is the intermolecular distance. B_{ij} is the many-body interaction parameter, which represents the many-body coupling between the bond from atom i to atom j and the local environment of atom i. This potential has been successfully used to simulate a CNT with sufficient accuracy [26–28]. The Ar—Ar and Ar—C interatomic interactions are modeled by the 12-6 L-J potential, which is described by the van der Waals forces between atoms, as follows:

$$\Phi(r_{ij}) = \begin{cases} 4\varepsilon[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^{6}], & r \leqslant r_{\text{cut}} \\ 0 & r > r_{\text{cut}}, \end{cases} \tag{2}$$

where ε and σ are the energy and distance parameters, correspondingly, and r_{ij} is the distance between atoms i and j. The L-J potential parameters for the Ar—Ar and Ar—C interactions are obtained from Ref. [29] and listed in Table 1. Moreover, r_{cut} = 1.20 nm is the overall cut-off distance for the L-J potential.

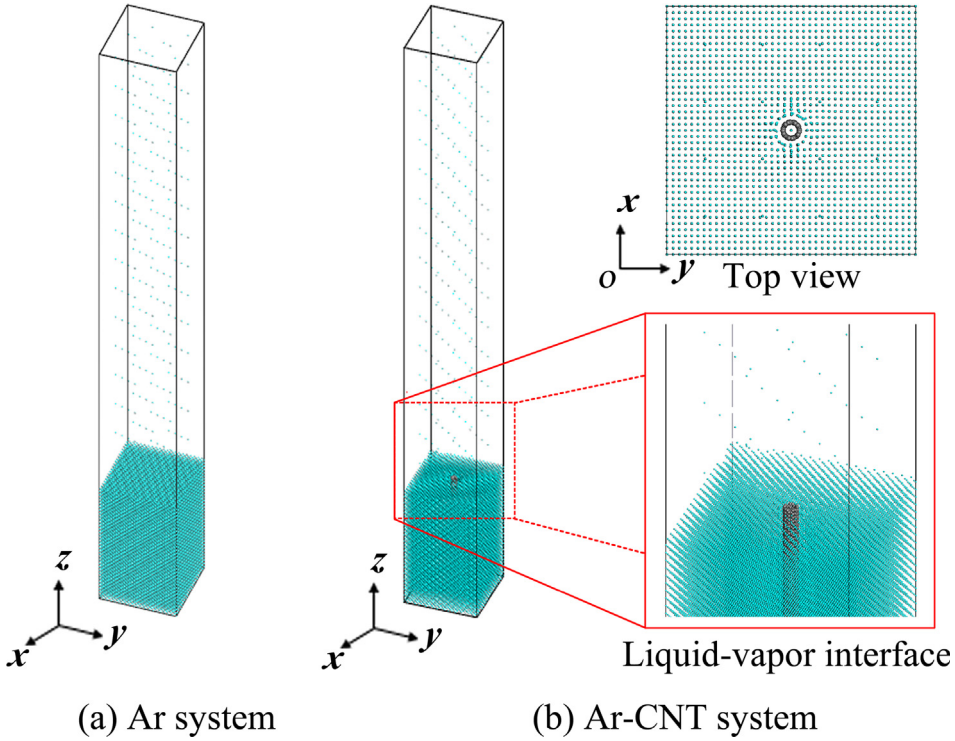

Fig. 1. Schematic of the initial configuration.