International Journal of Science and Research (IJSR)
ISSN: 2319-7064
ResearchGate Impact Factor (2018): 0.28 | SJIF (2018): 7.426

Investigating the Influence of Ejection Diameter Size Parameter to Liquid Ejection by Molecular Dynamics Simulation Method

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Abstract: ***The research adopts the molecular dynamics simulation method to simulate the liquid molecule ejection through different ejection diameter sizes of 25 Å and 40 Å and pushing force 11.0 $\times 10^{-10}$ N. The obtained simulative results conclude that almost liquid molecules eject out through the hole diameter of 40 Å to build up liquid jet and then produce nanoscale droplets. Contrarily, the liquid molecules after ejecting out the container could not go away the top plate for the hole diameter of 25 Å under same the magnitude of pushing force.***

Keywords: Molecular dynamics simulation method, ejection diameter size, liquid ejection

1. Introduction

From the requirements on developing the equipments as about reducing device size and facilities to apply for the medicine and industry fields that the nanotechnology is a suitable solution for these requirements.

The gold material with nanomet size is studied for manufacturing on the oxit membrane Fe_2O_3 [1]. The simulation works for the propane ejection is simulated with the nozzle diameters from 2 to 6 nm by the molecular dynamics simulation method [2].

The formation of the liquid jets were mentioned in the discussion about influences of nozzle diameters, system temperature and fluid flow [3-6].

The ejection and formation of fluid jets have also been used to study by the experimental method. The effects of nozzle size, and fluid flow rate on the formation and characteristics of the liquid jets were discussed [7-9].

Almost the above researches primarily mention to the simulation and experimental studies of the liquid ejection, the formation and breakup of the jets. However, the liquid ejection and movement up under the effects of different hole diameters and pushing forces have little been researched. This study is a development of a previous research [10] for describing the effects of different hole diameters and pushing forces to liquid ejection by the molecular dynamics simulation method.

2. Methodology

2.1 Simulation Model

The simulation model was built as in Figure 1 with the liquid molecules are contained at the position between the top and bottom plates. The height and width of the container are 77.176 and 101.9 Å, respectively. The periodic boundary conditions are applied for bounding along the x-, and y-directions of the liquid block.

The top and bottom plates are built by gold (Au) atoms and arranged into face-centered cubic (fcc) crystal lattice structures. The bottom plate designs to move vertically in the +z-direction when subjected to a pressing force while the top plate is fixed and designing an aperture in the center.

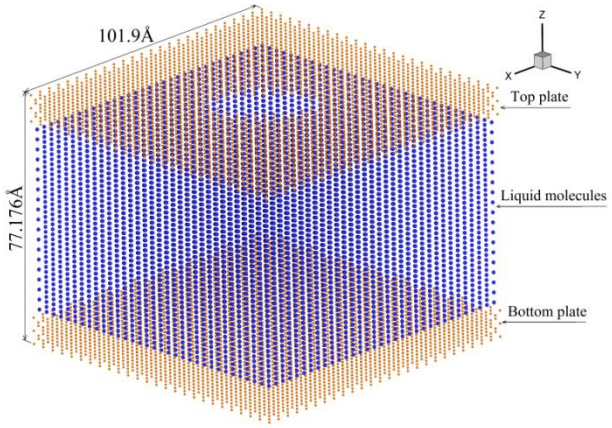

Figure 1: Simulation model

2.2 Interaction between Atoms and Molecule

The interaction among the atoms of the liquid molecules was represented by specific potential model. The form of the energy function of the F_3C molecular model [11] is represented as equation (1). With the value is the sum of the bonding, the bending, the van der Waals and the Coulomb terms.

$$U = U_{bond} + U_{bend} + U_{vdw} + U_{els}$$
$$= \sum K_b^{OH}(r_i - r_{eq})^2 + \sum K_\theta^{HOH}(\theta_i - \theta_{eq})^2$$
$$+ \sum [A_{SC}\varepsilon_{ij}\left(\frac{r_0^{ij}}{r_{ij}}\right)^{12} - 2\varepsilon_{ij}\left(\frac{r_0^{ij}}{r_{ij}}\right)^{6} - S_{vdw}(r_{ij})] + \sum [\frac{q^i q^j}{r_{ij}} - S_{els}(r_{ij})], \quad (1)$$

where $S_{vdw}(r_{ij})$ is the truncation shift function of the van der Waals force, which is showing as equation (2):

$$S_{vdw}(r_{ij}) = \begin{cases} U_r - U_{r_c} - (r - r_c)\left(\frac{dU}{dr}\right)_{r_c} & \text{for } r < r_c, \\ 0 & \text{for } r \geq r_c \end{cases} \quad (2)$$

and $S_{els}(r_{ij})$ is the shift function for the Coulomb's force and is showing as equation (3):

$$S_{els}(r_{ij}) = (r - r_c)\left[\frac{q^i q^j}{r_c^2}\right], \quad (3)$$

where $A_{sc}, K_b^{OH}, K_\theta^{OH}, r_i, r_{eq}, \theta_i, \theta_{eq}, r_{ij}$ and r_c are the coefficients of the short distance force, the harmonic force constant, the angle bending force constant, the ith O-H bond length, the equilibrium length of the O-H bond, the ith H-O-H bond angle, the equilibrium angle of the H-O-H bond angle, the interatomic distance, and the cutoff distance (10 Å), respectively.

The q_i and q_j are the partial charges of O or H. The Spohr potential functions are showing for interaction between the liquid molecules and the gold atoms as equation (4):

$$U_{Au-H_2O} = U_{Au-O}(r_{Au-O}) + U_{Au-H_1}(r_{Au-H_1}) + U_{Au-H_2}(r_{Au-H_2}), \quad (4)$$

with

$$U_{Au-O}(r) = S_2(r)D_0[\exp(-2\alpha_0(r - r_{e1})) - 2\exp(-\alpha_0(r - r_{e1}))] \quad (5)$$

and $$U_{Au-H}(r) = \gamma D_0 \exp(-2\alpha_H(r - r_{e2})). \quad (6)$$

The switch function $S_2(r)$ is showing as equation (7):

$$S_2(r) = \begin{cases} 1 & \text{for } r \leq r_{on} \\ \frac{(r_{off}^2 - r^2)^2(r_{off}^2 + 2r^2 - 3r_{on}^2)}{(r_{off}^2 - r_{on}^2)^3} & \text{for } r_{on} < r < r_{off} \end{cases}, \quad (7)$$

where r_{on} and r_{off} are the start and end distances of the switch function with magnitudes of 7.0 and 11.0 Å, respectively.

2.3. Simulation Scheme

The research performs 2 simulation cases with 2 nozzle hole diameters under same the magnitude of pushing force 11.0 $\times 10^{-10}$ N and system temperatures of 310 K. A random initial velocity was assigned to each atom of each liquid molecule. The list of simulation scheme is showed as in Table 1.

Table 1: Simulation scheme

Cases	Ejection diameter (Å)	Temperature (K)	Pushing force (N)
1	25	310	11.0 $\times 10^{-10}$
2	40	310	11.0 $\times 10^{-10}$

3. Results and Discussion

3.1. Liquid Ejection Results of different Ejection Diameter Sizes

The snapshots of the liquid nanojets for the different ejection diameters at 100000 fs are shown as in Figure 2. Figures 2(a) shows the snapshot of the liquid jet ejected through 25-Å-diameter size under the pressing force of 11.0 $\times 10^{-10}$ N and the system temperature of 310 K. Figures 2(b) is the snapshot of the jet for 40-Å-diameter size under same above pushing forces and system temperature.

In these research cases, the indispensable parameters to eject all the liquid molecules out of container to build up the nanojet that include the smallest ejection diameter of 25 Å, the system temperature of 310 K and pushing force of 11.0 $\times 10^{-10}$ N. However, the liquid jet could not continue to establish droplet for going up at 100000 fs as shown in Figure 2(a).

Contrarily, When increasing the values of ejection diameter from 25 to 40 Å and still maintain the magnitudes of pushing force and temperature, the liquid jet after build up that continue to establish droplet for going up at 100000 fs as shown in Figures 2(b).

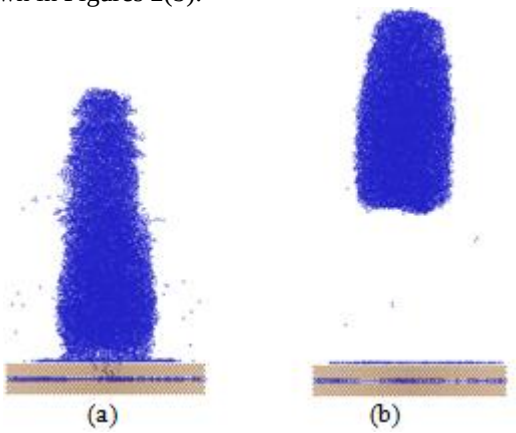

Figure 2: Snapshots of the liquid nanojet of 25- and 40 Å-diameters ejection at 100000 fs.

As shown in Table 3, the liquid nanojet could not movement up from the top plate surface to establish the droplets for the hole diameter of 25 Å under magnitude of pushing force of 11.0 $\times 10^{-10}$ N and system temperatures of 310 K. While, the droplets is easy to manufacture to move up for the hole diameter of 40 Å under same above magnitude of pushing force and system temperature.

Table 3: Effect of hole diameter to movement up of liquid jet

System temperature	Pushing force	Ejection diameter of 25 (Å)	Ejection diameter of 40 (Å)
310 (K)	11.0×10-10 (N)	Not movement up	Movement up

3.2 Effects of Different Ejection Diameter Size on the Ejection and Movement up of Liquid Jet

Snapshots of the liquid nanojets eject through the 25 and 40-Å-diameter holes under the pressing force of 11.0 $\times 10^{-10}$ N with the system temperature of 310 K at 180000 fs are shown in Figure 3.

The simulation gives the results that the liquid jet have downwards movement for the 25-Å-diameter size in comparison between the Figures 2(a) and Figures 3(a).

Contrarily, the droplet after be manufactured continue to move up for the 40-Å-diameter size with the same

magnitudes of pushing force and system temperature in comparison between the Figures 2(b) and Figures 3(b).

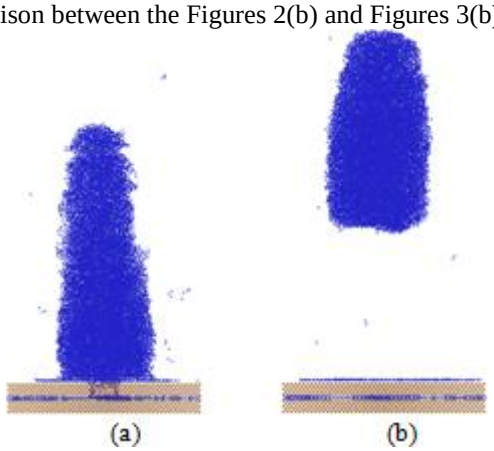

Figure 3: Snapshots of the liquid nanojet of 25- and 40 Å-diameters ejection at 180000 fs.

In order investigating the influence of the different ejection diameter sizes to the liquid ejection, the molecular number and location inside the ejection hole volume are analyzed and discussed. The molecular number inside the ejection hole volume is divided into two groups along the z-direction as shown in Figure 4. The group A is an annular volume close to the hole wall with a annular radius of 3 Å. The group B is the rest with the radius depends on the magnitude of the hole diameter. Thus, the molecular number at each group can know for each time step for each different influence parameters of the hole diameter sizes.

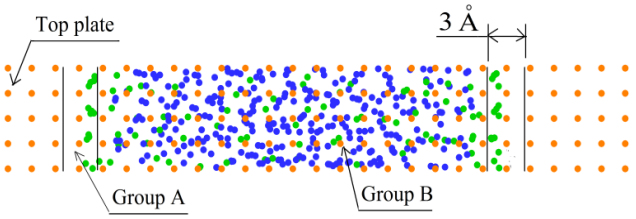

Figure 4: Molecular number between two groups inside the ejection hole volume.

The molecular ratios between the two groups along the z-direction inside the hole volume at each 10000 fs instant are shown as in Figure 5. The group A is an annular volume close to the hole wall with a 3-Å-annular radius. The group B is the rest. The curves in Figure 5 respectively show the molecular ratios for the 25- and 40-Å-diameter size under the action of the pushing force of 11.0 $\times 10^{-10}$ N and the system temperature of 310 K. There are two observations of the molecular ratio during the ejection process of molecules through the ejection hole. In the first stage, these ratios change in a narrow band and increase at the end of this stage. The ratio value of curves marked by the ejection diameter of 25 Å is greater than the diameter of 40 Å under same the magnitude of pushing force and temperature. The curves show a high density of molecules in the annular volume resulting in many collisions on the wall of the 25-Å-diameter size. This influences the velocity and moving direction after ejecting out of the ejection hole. In the second stage, almost of the molecules eject out of the ejection hole already. At this point, the low velocity molecules close to the nozzle aperture dropped back into the hole. Thus the molecular ratio significantly increases at this stage.

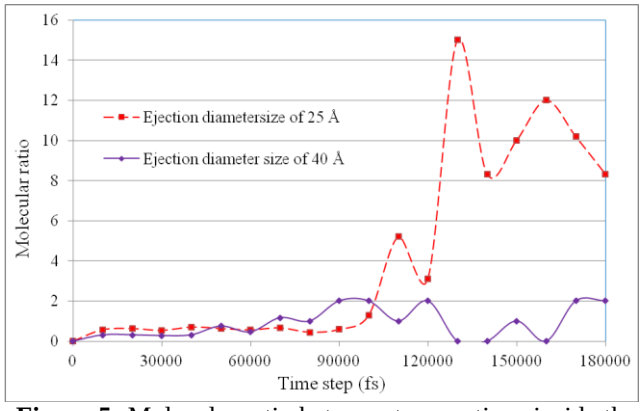

Figure 5: Molecular ratio between two sections inside the ejection hole volume

The sum of the molecular velocities in the x-, and y-horizontal directions at near the ejection hole's wall is shown in Figure 6. The molecular velocities do not increase much at the initial stage of the ejection process for the 25-, and 40-Å-diameter sizes under the action of pushing force 11.0 $\times$ 10^{-10} N and the system temperature of 310 K. The velocities rapidly increase at the next stage of the ejection process for the larger diameter size and they reach the relatively equilibrium value in remained ejection process. The molecular velocities rapidly reduce back to value at initial stage for smaller ejection diameter size. Thus, direction of molecules is changed after ejecting out of the ejection hole due to many molecules colliding on the wall. Most of these molecules move perpendicular to the axis of the liquid nanojet. The result is the downward movement of the liquid nanojet after reaching the maximum height but not separating from the top plate's surface.

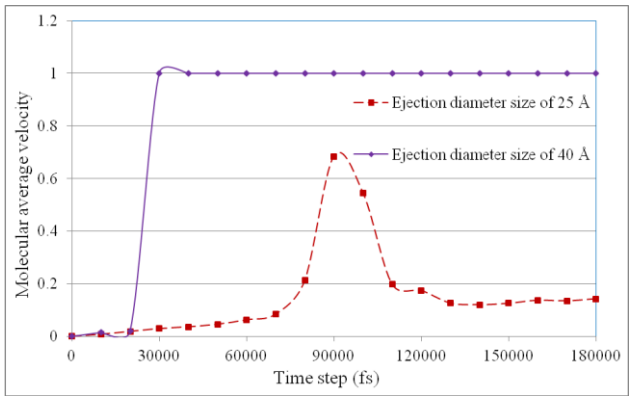

Figure 6: Molecular velocity in x- and y-directions at ejection hole's wall

4. Conclusions

The molecular dynamics simulation method is adopted in this research to simulate the formation of the liquid nanojet and the movement up of the jet under the influence of the different ejection diameter sizes. Based on the obtained simulation results, the following conclusions were shown:

The liquid nanojet is built but it could not movement up from the top plate's surface to establish the droplets for the ejection diameter of 25 Å under same magnitude of pushing force and system temperature. While, the droplets is easy to manufacture to move up for the ejection diameter size of 40

Å under same above magnitude of pushing force and system temperature.

The observations of the molecular ratio during the ejection process of molecules through the ejection hole show that the molecular ratios change in a narrow band and increase at the end of the first stage. The ratio value for the ejection diameter size of 25 Å is greater than the diameter size of 40 Å. Thus, this has many collisions of molecules on the wall of the 25-Å-diameter size. This influences the velocity and moving up of the liquid jet after ejecting out of the ejection hole.

The velocities rapidly increase after the initial stage of the ejection process and reach the relatively equilibrium value for the larger ejection diameter size under same magnitude of pushing force and system temperature.

Meanwhile, the molecular velocities rapidly reduce back to value at initial stage for smaller ejection diameter size. Thus, most of these molecules move perpendicular to the axis of the liquid nanojet. The result is the downward movement of the liquid nanojet after reaching the maximum height but not separating from the top plate's surface for the smaller ejection diameter size.

5. Funding

This research is supported by Department of Sciences and Technology, Hanoi University of Industry, Viet Nam.

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