Separation criteria of nanoscale water droplets from a nozzle plate surface

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Abstract. This paper studies the water nanojet ejection process using molecular dynamics simulation. The results show that nanoscale water droplets cannot separate from the nozzle plate surface when the nozzle aperture has a diameter of 27.5 Å or smaller. The maximum height of the produced water nanojet is reduced after reaching to its highest position when the jet does not separate from the plate surface. Separation phenomenon between the water nanojet and the nozzle plate surface is the most obvious with the 27.5-Å-diameter nozzle aperture for this simulation setup. In addition, initial findings on the characteristics of nanoscale water droplets (width and contact angle) impinging onto a fixed plate surface are revealed in preparation for future investigation.

1 Introduction

Nanofluid ejection technology is employed in many industrial applications such as high precision print heads in the printing industry, cooling systems in metallic processing, printed circuit board manufacturing industry, and many more. In the nanofluidic ejection process, the formation of the fluid nanojet and the separation of the nanoscale fluid droplet have attracted research attention for the design and the accurate operation of micro and nanofluidic devices.

The molecular dynamics (MD) simulation method has been adopted to investigate the physics of nanoscale fluid ejection systems. The MD method employed to perform a number of simulations for propane nanojet ejection with a range of exit nozzle orifice diameters between 2 and 6 nm. In their work, various nozzle size conditions were applied to characterize the necking of the fluid nanojet. The effects of viscosity, wetting, and nozzle configuration factors on nanojet formation were discussed [1]. The MD simulation method also used to simulate the ejection process of water nanojets and the formation of nanoscale water droplets. The effects of nozzle aperture diameters, pressing force, system temperature and fluid flow dynamics on the formation and shape of the nanoscale water droplet were investigated [2, 3].

The formation of fluid droplets during the nanojet ejection process is affected by the nozzle size, temperature system, pressing force, and the properties of the fluid. The MD simulation is applied to study the role of thermal fluctuations on the formation and stability of nanoscale fluid droplets in drug delivery, printing, nanoscale manufacturing and conduct nanojet ejection simulation using non-equilibrium molecular dynamics in a high pressure environment [4, 5].

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Some characteristics of the breakup and formation of fluid nanojets are mentioned in previous researches. The model to simulate the thermal induced breakup of liquid nanojets [6], phenomena of liquid thread breakup and nanoscale droplet formation in the nanoscale ejection process for various pushing periods of oscillation. The simulation results revealed that the sizes of nanoscale droplets are linear depending on the pushing periods [7].

Experimental method has also been used to empirically study the formation of nanoscale fluid droplets. The formation of a nanoscale liquid droplets from a wettable nozzle, the effects of nozzle size and fluid flow rate on the various behaviors of the droplets were investigated and discussed [8]. For inkjet printer heads [9], a moving piezo element which covered with thin foil is adopted to deform the ink channel and eject droplets from the nozzle opening.

Another method of nanofluidic ejection is via bubble expansion. A numerical method is used to describe the three-dimensional Navier-Stokes equation for ink motion both inside and outside of the nozzle by growing bubbles on the chamber wall [10].

In order to observe the phenomenon of the impingement process between the nanoscale fluid and solid molecules. The nanojet ejection process is investigated by spreading droplets on a solid surface using molecular dynamics simulation. The results showed that the spreading width increased as time increased, and the droplet's contact angle varied within a range when the atoms in the ejection process reached a relatively steady state [11]. In another study, the MD simulation based on Lennard-Jones potential is employed to study the nanoscale droplet ejection process and the impingement of the fluid nanojet onto a solid surface [12, 13]. The collisions of two opposed liquid argon nanojets is described. Nanojet exit velocities are the highest for non-wetting surfaces and decrease as solid-liquid interactions are enhanced [14].

Most of the above mentioned research works concern the simulation and experimental studies of the fluid nanojet ejection process, fluid nanojet breakup, and the formation of the nanoscale fluid droplets. However, the effects of the nozzle aperture diameter, various pressing forces on the ejection of the water molecules and separation of the nanoscale water droplets have rarely been investigated. This paper is a continuation of a previous study [15] using MD simulation methods to investigate the separation of nanoscale water droplets from the nozzle plate surface and the causes of separation of the nanoscale water droplet from the nozzle plate surface were also investigated and discussed. Furthermore, cursory observations on the impingement of nanoscale water droplets onto a fixed metallic plate are described.

2 Methodology

2.1 Details of simulation model

The configuration of the simulation model was arranged as illustrated in Fig. 1. Periodic boundary conditions of the simulation box are applied along the x-, and y-directions. Water molecules are confined in the space between the nozzle and back plates. The distance between the nozzle and back plates is 60.872 Å. The dimensions of the box are 101.9 Å along both the x-, and y-directions. The model contains 20 691 water molecules having density of 0.999972 g/cm³ at 310 K. The oxygen atoms of the water molecules are arranged into simple cubic crystal lattices with lattice constant $a = 3.104$ Å.

The nozzle and back plates are composed of gold (Au) atoms and arranged into face-centered cubic (fcc) crystal lattice structures with the lattice constant $a = 4.076$ Å. The nozzle plate is fixed while the back plate can move vertically when subjected to a pressing force in the +z-direction. The thickness of the nozzle and back plates is 8.152 Å, each having 5 layers of gold atoms. The number of atoms of the back plate is 6 503. The nozzle plate has an aperture in the center. The number of atoms for the nozzle plates are 6 200, 6 144, 6 060, 5 924, and 5 772 gold atoms for the 25-, 27.5-, 30-, 35-, and 40-Å-diameter nozzle apertures, respectively.

The simulation of impingement of the nanoscale water droplets onto a fixed metallic plate is also performed. The dimensions of the fixed metallic plate are 150.812 Å along both the x and y-directions.

The thickness of the fixed metallic plate is 6.114 Å, consisting of 11 250 gold atoms arranged into a FCC structure with 4 layers of gold atoms.

LAMMPS software and C++ code were used as the tools for the simulation work and the data analysis.

Figure 1. Molecular dynamics simulation model.

2.2 Interaction between atoms

The MD simulation method was used for analyzing the structure of the flexible three-centered (F_3C) water molecules, and provided insight into the features of the nanoscale structure and the dynamics of the fluid nanojet flow. Specific potential model was also employed to represent the interaction among the atoms in the water molecules. In this paper, the shifted Lennard-Jones 12-6 potential was applied to the model of the intermolecular interactions for $H_2O - H_2O$ and $H_2O - Au$ components of the system. Harmonic potential function was used to model the vibrations of the liquid water molecules. The equilibrium values of the oxygen-hydrogen bond length and the H-O-H bond angle were 1.0 Å and 104.5 degrees, respectively.

In the F_3C water molecular model [16], the complete form of the energy function used here to represent the water molecules is given as the sum of the bonding, the bending, the van der Waals and the Coulomb terms and can be expressed as:

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

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

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

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

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

where A_{sc} , K_b^{OH} , K_θ^{OH} , r_i , r_{eq} , θ_i , θ_{eq} , r_{ij} and r_c are the coefficients that adjust the short distance force, the harmonic force constant, the angle bending force constant, the i th O-H bond length, the equilibrium length of the O-H bond, the i th 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. Terms q_i and q_j are the partial charges of O or H.

The interactions between the water molecules and the gold atoms are represented by the Spohr potential functions of

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

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 $S_2(r)$ has the form of

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

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

2.3 Simulation scheme

In this paper, 11 simulation cases with 5 nozzle aperture diameters were studied. A random initial velocity was assigned to each atom of each water molecule. The atomic velocities were scaled such that the system temperature was 310 K. The pre-run time for each simulation was 10 000 time steps for the water molecules to reach an equilibrium state, with one time step being 1 femtosecond (fs). After the pre-run, the back plate is subjected various upward pressing forces to eject the water molecules out of the nozzle aperture. The magnitudes of the pressing force were 9.25×10^{-10} , 10.0×10^{-10} , 11.0×10^{-10} , and 12.0×10^{-10} N for 25-Å-diameter nozzle aperture. The force magnitudes were 9.0×10^{-10} , 10.0×10^{-10} , 11.0×10^{-10} , and 12.0×10^{-10} N for the 27.5-Å-diameter nozzle aperture. The magnitudes of the minimum pressing forces were 7.5×10^{-10} , 6.5×10^{-10} , and 5.75×10^{-10} N for the 30-, 35-, and 40-Å-diameter nozzle apertures, respectively.

The simulation scheme is listed in Table 1. The simulation length in each case is 150 000 time steps. The data output frequency is once per 2000 time steps.

Table 1. Simulation scheme.

Case	Nozzle aperture diameter (Å)	Temperature (K)	Pressing force (N)
1	25	310	9.25×10^{-10}
2	25	310	10.0×10^{-10}
3	25	310	11.0×10^{-10}
4	25	310	12.0×10^{-10}
5	27.5	310	9.0×10^{-10}
6	27.5	310	10.0×10^{-10}
7	27.5	310	11.0×10^{-10}
8	27.5	310	12.0×10^{-10}
9	30	310	7.5×10^{-10}
10	35	310	6.5×10^{-10}
11	40	310	5.75×10^{-10}

3 Results and discussion

3.1 Water nanojet ejection process results of various nozzle aperture diameters

Snapshots of the oxygen atoms of the water nanojets corresponding to various pressing forces and nozzle aperture diameters at 150 000 fs are shown in Figure. 2. Figures 2(a)-(d) and (e)-(h) respectively show the snapshots of the water nanojets ejected through 25- and 27.5-Å-diameter nozzle apertures with the different pressing forces. In these simulations, the minimum pressing forces to eject all the water molecules though the 25- and 27.5-Å-diameter nozzle apertures were 9.25×10^{-10} and 9.0×10^{-10} N, respectively, as shown in Figures. 2(a) and (e). The water nanojets after ejection through the 25- and 27.5-Å-diameter nozzle apertures did not separate from the nozzle plate surface and form a nanoscale water droplet, regardless of pressing force. Figures 2(i)-(k) show the snapshots of the nanoscale water droplets ejected through the 30-, 35-, and 40-Å-diameter nozzle apertures with the minimum pressing forces of 7.5×10^{-10} , 6.5×10^{-10} , and 5.75×10^{-10} N, respectively. The nanoscale water droplets separated from the nozzle plate surface into jets in these cases.

Table 2 shows circumference-length-to-area ratios for the 25-, 27.5-, 30-, 35-, and 40-Å-diameter nozzle apertures in cross-section. The respective minimum pressing forces were 0.04, 0.036, 0.033, 0.029, and 0.025. The water molecules ejected through the nozzle apertures form water nanojets at these ratios. Based on a combination of the circumference-length-to-area ratios and the simulation results, criteria of the circumference-length-to-area ratios for the separation of the nanoscale water droplets from the nozzle plate surface in the water nanojets can be established as follows:

First, when the circumference-length-to-area ratio (L/A) is in a range from 0.036 to 0.040, the water molecules are ejected out through the nozzle aperture. The water nanojets are formed on top of the nozzle plate surfaces. However, the water nanojet does not separate out from the nozzle plate surface to produce droplets.

Second, if the L/A is less than or equal to 0.033, the formation of the water nanojets is similar to the first scenario however, the nanoscale water droplets are formed when the nanojet separates from the nozzle plate surface.

The ejection process of the water nanojets is affected by the diameter of the nozzle aperture. In order to determine the causes of the phenomena, the typical simulation cases of water nanojets ejected through the 27.5- and 40-Å-diameter nozzle apertures with respective 9.0×10^{-10} and 5.75×10^{-10} N pressing forces are analyzed in this study. The 27.5-Å-diameter nozzle aperture is chosen because the separation phenomenon of water nanojet from the nozzle plate surface is the most obvious, though nanoscale water droplet did not separate out from the nozzle plate surface. Furthermore, this

case is also employed to compare with the case of the 40-Å-diameter nozzle aperture where the water droplet can separate from the nozzle plate surface. The following analysis focuses on these simulation cases.

Figure 2. Snapshots of the water nanojet at 150 000 fs. (a)-(d) Water nanojets of the 25-Å-diameter nozzle aperture for various pressing forces (e)-(h) Water nanojets of the 27.5-Å-diameter nozzle aperture for various pressing forces (i) 30-Å-diameter nozzle aperture water nanojet (j) 35-Å-diameter nozzle aperture water nanojet (k) 40-Å-diameter nozzle aperture water nanojet.

Table 2. Features and circumference-length-to-area ratios of the nozzle apertures.

Nozzle aperture diameter (Å)	Minimum pressing force (N)	Circumference length of nozzle aperture in cross-section (L)	Area of nozzle aperture in cross-section (A)	Ratios of circumference Length to area (L/A)
25	9.25×10^{-10}	78.540	1963.494	0.040
27.5	9.0×10^{-10}	86.394	2375.827	0.036
30	7.5×10^{-10}	94.248	2827.431	0.033
35	6.5×10^{-10}	109.956	3848.448	0.029
40	5.75×10^{-10}	125.664	5026.544	0.025

3.2 The separation or non-separation of the nanoscale water droplet

Snapshots of the oxygen atoms of the water nanojets through the 27.5-Å-diameter nozzle aperture with a 9.0×10^{-10} N pressing force at 60 000 and 100 000 fs are shown in Figure. 3. The trajectories of the molecules in the water nanojet ejection process are used to analyze the formation of the water nanojet and explain why the nanoscale water droplet cannot separate from the nozzle plate surface and the increase of the water nanojet base diameter. For clarification, only oxygen atoms are shown.

Figure 3. Snapshots of the water nanojet through the 27.5-Å-diameter nozzle aperture at (a) 60 000 fs and (b) 100 000 fs.

Figure 4. Trajectories of water molecules at 60 000 fs.

Figure 4 shows the trajectories of a few oxygen atoms at 60 000 fs. The water molecules close to the nozzle aperture moved with a zigzag trajectory. Their trajectories become straight after ejecting out of the nozzle aperture. Most of these molecules are ejected at the beginning and then move away

from the nozzle plate surface form the upper half of the water nanojet. The distance between any two adjacent dots on each trace expresses the velocity of the particle. The velocities of the molecules are reduced along the top of the water nanojet. In addition, a few molecules with low velocity after ejection through the nozzle aperture moved sinuously near the nozzle plate surface, and then fall down to form a wetting molecular layer on the nozzle plate surface.

The trajectories of a few oxygen atoms at 100 000 fs are shown in Figure. 5. Some water molecules adjacent to the wall of the box and far away from the nozzle aperture are ejected out at this time. When subjected to a pressing force, most of the molecules move up with high velocity. Shortly after, these velocities rapidly low and move along the box wall. After having collisions with the bottom of the nozzle plate, the direction of the molecular trajectories is changed from the vertical direction to the horizontal direction, and then move towards the nozzle aperture before ejecting out with low velocity. Hence, a large number of molecules sinuously move near the nozzle plate surface. The attraction force among the molecules and the cohesion in water contribute to pull the water nanojet downward. Therefore, the water nanojet cannot separate from the nozzle plate surface because many molecules with low velocity move equivocally near the nozzle plate surface in a short period and thereafter, drop on the wetting molecule layer which was formed by the previous stage.

Figure 5. Trajectories of water molecules at 100 000 fs.

Figure 6 presents the molecular ratios between the two water molecular groups inside the nozzle aperture at each 10 000 fs instant. The molecules are divided into two groups along the z-direction as shown in Figure. 7. The first group is an annular volume close to the wall of nozzle aperture with a 2 Å annular radius. The second group is the rest. The curves in Figure. 6 marked by triangles and circles respectively show the molecular ratios for the 27.5- and 40-Å-diameter nozzle apertures. There are two observations of the molecular ratio during the ejection process of molecules through the nozzle aperture. In the first stage, these ratios change in a narrow band and increase at the end of this stage. The ratio value of 27.5-Å-diameter nozzle aperture is greater than that of 40-Å-diameter nozzle aperture. The curves show a high density of molecules in the annular volume resulting in many collisions on the wall of the 27.5-Å-diameter nozzle aperture. This affects the velocity and moving direction after ejection out of the nozzle aperture. This also induces an increasing diameter at the bottom of the water nanojet and affects the separation ability of the water nanojet from the nozzle plate surface. In the second stage, almost all of the molecules are ejected out of the nozzle aperture already. At this point, the low velocity molecules close to the nozzle aperture dropped back into the nozzle aperture. The attraction force of the gold atoms constituting the nozzle plate pulls most of these molecules towards the wall of the aperture, thus the molecular ratio significantly increases at this stage.

Figure 6. Plot of the molecular ratio between two sections inside the nozzle aperture.

Figure 7. The number of molecules of two groups inside the nozzle aperture volume: (a) view in projection from top to bottom; (b) view in vertical projection.

Figures 8 (a)-(b) show the snapshots of the water nanojets at 200 000 fs through the 27.5- and 40-Å-diameter nozzle apertures, respectively. In comparison to the snapshot of the 27.5-Å-diameter nozzle aperture at 150 000 fs (Figure. 2(e)), the snapshot at 200 000 fs (Figure. 8(a)) shows a downwards movement, an increasing diameter and a formation of necking of the water nanojet. The molecular velocity in horizontal direction inside the nozzle aperture and the molecular density inside the simulation box are used to explain these phenomena. In contrast, Figure 8 (b) shows the continued upward movement of the water nanojet.

Figure 8. Snapshots of the water nanojet at 200 000 fs: (a) 27.5-Å-diameter nozzle aperture; (b) 40-Å-diameter nozzle.

The sum of the molecular velocities in the x- and y-horizontal directions near the wall of the nozzle aperture is shown in Figure. 9. The velocities rapidly increase at the initial stage of the molecular ejection process and reach to an equilibrium value at 120 000 and 60 000 fs for the 27.5-, and 40-Å-diameter nozzle apertures, respectively. Smaller nozzle aperture diameter yields higher velocity. Thus, direction of molecules is changed after ejection out of the nozzle aperture due to many molecules colliding on the wall. Most of these molecules move perpendicular to the axis of the water nanojet. This is a main reason for an increase of diameter of the water nanojet at the base. After 170 000 fs, the molecular velocity associated with the smaller nozzle apertures increases. This results in the downward movement of the water nanojet after reaching the maximum height but not separating from the nozzle plate surface. This is because the molecules are pulled by the attraction force of the gold atoms and the water molecules on the aperture wall.

Figure 9. Plot of molecular velocity in x- and y-directions inside the nozzle aperture.

Figure 10 shows molecular density inside the water reservoir at each 2 000 fs instant. The initial density value is 0.378 g/cm³. When the back plate moves upward and acts on the water molecules, the molecular density rapidly increases in the beginning and the density of molecules inside the reservoir fluctuates in a wide band with the 27.5-Å-diameter nozzle aperture. These fluctuations affect the continued ejection stream and cause the necking of the water column. The collisions of molecules in the water column increase and thus affect the upward z-direction velocity of the water nanojet. Shortly after, these densities gradually reach the steady values of 0.748 and 0.692 for the 27.5-, and 40-Å-diameter nozzle apertures, respectively. Intuitively, the ejection time is longer when the nozzle aperture diameter is smaller. The density of the molecules inside the reservoir fall back to near the initial value at the end of the molecular ejection process.

Figure 10. Plot of molecules densities inside the reservoir at each 2 000 fs instant.

3.3 Studying the impingement of the nanoscale water droplet onto the fixed plate surface

Impingement of a nanoscale water droplet onto a fixed plate surface was modeled by MD simulation using a 50-Å-diameter nozzle aperture with pressing forces of 8.0×10^{-10} , 10.0×10^{-10} , and 12.0×10^{-10} N under a system temperature of 310 K. Figures 11 (a)-(c) show snapshots of the nanoscale water droplet impingement onto a fixed plate surface at 1 200 000 fs with pressing forces of 8.0×10^{-10} , 10.0×10^{-10} , and 12.0×10^{-10} N, respectively. It can be seen that the number of water molecules on the solid plate surface and the width of the spreading droplet increase as the impingement time increases. Comparing the snapshots of Fig. 11, the results show that the contact angle of the water droplet with the fixed plate surface and the height of the nanoscale water droplet reduce as time and pressing force increase.

Figure 11. Snapshots of the nanoscale water droplets onto a fixed plate surface at 1 200 000 fs.

4 Conclusions

The molecular dynamics method is used in this study to simulate the formation of the water nanojet and the separation or non-separation of the water nanojet from the nozzle plate surface. Furthermore, initial observations on the impingement of a nanoscale water droplet onto a fixed solid surface are given. Based on the simulation results, the following five conclusions were drawn:

1. When the circumference-length-to-area ratio (L/A) is in the range from 0.036 to 0.040, all the water molecules in the reservoir are ejected through the nozzle apertures. However, the water nanojets do not separate from the surface of the nozzle plate. If the L/A is less than or equal to 0.033, the nanoscale water droplets are formed from the separation of the jet from the surface of the nozzle plate.
2. For small nozzle aperture diameters, the attraction force among the molecules and the cohesion in water are the main reasons which pull the water nanojet downward. This is enough to present the separation of the water nanojet from the nozzle plate surface.
3. The distribution and velocity in x-, and y-direction of molecules close to the nozzle wall are large for the smaller aperture diameters. These molecules have many collisions with the wall, so direction of molecules is changed after ejection from the nozzle aperture. Most of these molecules move in direction perpendicular to the axis of the water nanojet. This induces an increasing diameter

at the base of the water nanojet and affects the separation ability of the water nanojet from the nozzle plate surface.

4. The fluctuation of molecular density inside the reservoir is a wide band at the beginning of the ejection process for the 27.5-Å-diameter nozzle aperture. This affects the ejection stream and causes the necking of the water column.

5. The width of the spreading droplet on the fixed plate surface increases as the impingement time increases. The contact angle of the water droplet in relation to the fixed plate surface is reduced when the pressing force increases.

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