Effects of temperature and aperture size on nanojet ejection process by molecular dynamics simulation

Te-Hua Fang\textsuperscript{a}, Win-Jin Chang\textsuperscript{b,\ast}, Shi-Cheng Liao\textsuperscript{a}

\textsuperscript{a}Department of Mechanical Engineering, Southern Taiwan University of Technology, Tainan 710, Taiwan
\textsuperscript{b}Department of Mechanical Engineering, Kun-Shan University of Technology, Tainan 710, Taiwan

Received 15 March 2004; received in revised form 1 July 2004; accepted 4 July 2004

Abstract

This paper studies the effects of temperature and aperture size on the nanojet ejection process by means of molecular dynamics simulation using the Lennard-Jones potential. According to the analysis, it can be seen that the spurting atoms from the nanojet aperture are more evenly distributed as the temperature is increased. However, as the temperature lowers, the atoms easily concentrate on the central region. Furthermore, when a larger nanojet aperture was used, the amount of spurting atoms increased and concentrated easily into the central region. The phenomenon of the pressure wave was found with the aid of molecular dynamics.

Keywords: Molecular dynamics simulation; Lennard-Jones potential; Nanojet; Nozzle; Ejection

1. Introduction

Jets of macroscopic dimensions have been of great scientific interest in many industrial applications [1–3]. In the nanoworld, nanojets are attracting considerable attentions due to their unique characteristics. However, to actually build a nanojet is still a difficult task and using molecular dynamics [4–10] is an ideal tool to simulate this. Molecular dynamics can recognize the underlying atomistic mechanisms and offer novel insights into nanometer-scale behavior due to their high temporal and spatial resolution. In addition, molecular dynamics can clearly identify the atomic configuration of each nanojet trajectory.

Moseler and Landman [11] performed a molecular dynamics computation for a nanojet squirting propane from nozzles 2 to 6 nm in diameter and found that no steady jet formation was possible. Recently, Eggers [12] studied the breakup of a liquid nanojet. Based on an equation derived by Moseler and Landman, Eggers [12] presented that noise can speed up the breakup phenomena. Temperature and size have an important effect on control of nanojet ejection flow rate and particle distribution. This paper studies the effects of temperature and aperture size on nanojet ejection process with an aperture dimension smaller than 6 nm. This may be useful in the design of a nanosprayer or a nanoprinter.

2. Molecular dynamics methodology

The nanojet ejection process of argon clusters was investigated using molecular dynamics simulations. The initial atomic configuration used in the simulation system is shown in Fig. 1. The Ar atoms inside the housing are liquid and the housing is also made of rigid Ar atoms. F stands for the applied force. In the simulation the interaction of Ar atoms and the housing material was taken into account. For this simulation, the system was set at a microcanonical ensemble model [13]. The nanojet atomic array model is simulated under the condition of constant temperature and volume (i.e., NVT model). Six hundred and twenty four atoms were constructed as a push panel with a velocity of 50 m/s from the back of
the Ar atoms were ejected into a vacuum and formed a bubble.

The total atoms in Table 1 represent the push panel atoms, the housing atoms and the squirtable interior atoms. There are four aperture types in the simulation; they are A, B, C, and D and also represent the four different aperture dimensions as listed in Table 1. In this paper, the Lennard-Jones potential model, which is still widely used, was adopted for the calculation process. It is

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

where $\phi(r_{ij})$ is a pair energy function, $r_{\text{cut}}$ (cut-off distance) is set at 3.5$\sigma$, $\sigma = 3.40 \times 10^{-10}$ m and $\varepsilon = 1.67 \times 10^{-21}$ J.

According to the NTV model the nanojet housing temperature must remain constant, the following correction was required in order to attain a constant temperature.

$$v = v \sqrt{\frac{T_D}{T_A}}$$  \hspace{1cm} (2)$$

where $v_{\text{new}}$ is the velocity of the particle i after correction. $T_D$ and $T_A$ are the desired temperature and actual temperature of system, respectively. The time integration of motion is performed by Gear’s fifth predictor-corrector method [14] with a time step of 1 fs.

3. Results and discussions

The snapshots of the aperture type A nanojet ejection process at a temperature of $T=200$ K and measured at various sampling time are shown in Fig. 2(a)–(d). After 60 ps a steady flux of atoms out of the simulation box is achieved, with a spatial particle distribution constant in time. Over time, it can be seen that

![Fig. 2. Snapshots of nanojet process from the aperture type A at $T=200$ K for various sampling times.](image-url)
the atoms squirted through the aperture increase and reach further away. The spurting numbers at temperature \( T = 200 \) K for various aperture dimension types are shown in Fig. 3. As expected, the spurting numbers increased as time and the aperture dimensions also increased.

Fig. 4 illustrates the pressure variation for the aperture dimension types used in this study. From 0 to 20 ps the pressure remains constant for all four aperture dimensions used, since there were no atoms to be squired. Then the atoms began to squirt and the pressure slightly decreased. However, the pressure in the nanojets with smaller aperture dimensions increased. The reason for this is that the pressure formed by the push panel which is applied at the back of the nanojet assembly is larger than that of the atoms within the housing. Therefore the push panel area is larger than aperture area. Fig. 4 also shows the phenomena of a pressure wave, especially for the nanojets with larger aperture dimensions. The pressure wave is generated from the velocity of panel motion. The pressure variation of aperture type B at \( T = 50 \) K and various velocities of the panel motion is shown in Fig. 5. The period of the cycle for the pressure wave increases when the velocity of the panel decreases.

Fig. 6(a)–(d) show the snapshots of the nanojet ejection process for the four aperture dimensions used at \( T = 50 \) K and taken at 40 ps. It can be seen that the larger aperture dimensions have more spurting atoms and the density of the atoms squirted from the larger aperture dimensions easily concentrated within the central region. The spraying aperture outer housing absorption phenomena become more pronounced as the size of the aperture dimension increased.

The effect of the temperature on the nanojet ejection process are shown in Fig. 7(a)–(d). From these figures, it can be seen that the temperature effect is significant. Under the higher temperature the squirted atoms have a further spurting distance and a wider spurting region. This is because the atoms at the higher temperatures have a higher kinetic energy.
4. Conclusions

The molecular dynamics method is used to analyze the effects of temperature and aperture on the nanojet process. According to the analysis, the following results were obtained:

1. As the temperature increased, the spurting atoms from the nanojet are more evenly distributed.

2. The configuration of the spurting atoms from the nanojet showed that the atoms concentrated within the central region when the larger aperture dimensions were used.

3. The pressure of the atoms in the nanojet housing and the number of spurting atoms varied as the aperture dimension changed. The phenomenon of a pressure...
wave was experienced when the larger apertures were used.

References