Molecular dynamics simulation of bubble nucleation in hydrophilic nanochannels by surface heating

Manish Gupta and Shalabh C. Maroo

Department of Mechanical Engineering and Aerospace Engineering, Syracuse University, Syracuse, NY, USA

ABSTRACT

Bubble nucleation in liquid confined in nanochannel is studied using molecular dynamics simulations and compared against nucleation in the liquid over smooth surfaces (i.e., without confinement). Nucleation in liquid argon is achieved by heating part of a platinum surface to high temperatures using a surface-to-liquid heating algorithm implemented in LAMMPS. The surface hydrophilicity of nanochannels is increased to understand its effect on nucleation behaviour. Liquid structuring is found to play a significant role in altering thermodynamic properties of density and pressure in the nanochannels, which in turn changes the enthalpy of vaporisation. Increased surface hydrophilicity in nanochannels results in the delay of bubble formation as more energy is required for nucleation. Thus, delayed bubble nucleation in hydrophilic nanochannels can dissipate higher heat fluxes and can potentially be used for the thermal management of hot spots in power electronics.

Heat dissipation from a hot spot is the primary challenge in thermal management [1,2] of power electronics and high precision instruments in order to maintain a safe and desired surface temperature. Recent literature shows a significant amount of work is being done to dissipate high heat flux from such electronics, and solutions include creating micro/nano-patterns on the surface [3–7] coupled with liquid–vapour phase change as it is one of the most efficient processes in heat transfer [8]. A few studies have suggested nanochannels can significantly enhance heat flux dissipation from surfaces [3,9]. Nucleation in confined liquid can be different from that without confined liquid due to changes in thermodynamic properties and liquid atoms structuring near the surface [10]. An experimental study by Lin [11] investigated the formation of a bubble in microchannels and concluded that homogenous bubbles are more likely to form in microchannels. Even though the classical theory predicts the formation of heterogeneous nucleation due to the presence of surfaces, a highly smooth surface may not be able to initiate bubble nucleation [11,12]. At nano-length scales, liquid structuring at the surface can affect nucleation behaviour while keeping the surface wet at higher temperatures. Studies have shown that heat transfer is higher when surface is wetted [13,14] due to evaporation of liquid on heated spots. When dry region forms, the local heat flux suddenly drops [15,16] and can cause thermal failure of the surface.

Heat transfer in MD at the nanoscale has been a topic of research and few mechanisms are commonly used in literature. The most straightforward is to couple the domains directly to thermostats, which however have shown to result in unpredictable and unphysical dynamics [17]. The study by Bernadi et al. [18] with various types of thermostats in confined liquid concluded that when thermostats are used on fluid it does not represent the real experimental setup where heat dissipation happens through a wall. The mechanical properties such as shear stresses and dynamic properties such as Lyapunov spectra show significant variations due to thermostat scaling [18]. They also concluded that irrespective of the type of thermostat, the confined fluid should always be kept at constant temperatures by managing heat exchange at the walls (rather than using a thermostat on the fluid) as it mimics real-world experimental setups where heat is transferred through the wall (i.e., surface). Nowadays, the most commonly used heat transfer model in MD, called the ‘Phantom wall method’ [19], is based on several layers of surface atoms being connected with high stiffness springs and coupled with a Langevin thermostat corresponding to the surface temperature while the last layer is kept fixed as a phantom layer to prevent the centre of mass movement of the entire wall. A similar approach was also used in other MD studies with a different number of layers and a Nose–Hoover thermostat [20]. The mathematical model in these methods may depict a thermal bath where the surface is maintained at the desired temperature, but it does not reflect the actual physics of heat transfer from a surface to a liquid. The main reason is that motion of both solid and liquid atoms are integrated over the same timestep even though atomic vibration frequency within the solid is at least ten times faster than the vibrational frequency of liquid atoms [21]. Hence, if the movement of solid surface atoms is modelled as part of the system, a smaller time step would be required for the entire simulation domain (including the liquid atoms), and such a simulation would become computationally exhaustive. Therefore, simulating non-equilibrium transient

CONTACT Shalabh C. Maroo scmaroo@syr.edu

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heat transfer processes like evaporation and condensation in MD using widely available open-source platforms may lead to unphysical results as surface-to-fluid heat transfer models in the literature are based on approximations and assumptions. Further, such models have not been validated in the literature.

In typical cases, the bubble forms at preferred nucleation sites on the surface instead of in bulk due to the availability of an initiation site for nucleation. The bubble can be formed by reducing the pressure in the liquid, or in a more practical way, by heating the surface. Maruyama et al. [22] studied bubble nucleation inside a channel, by moving the top surface away and hence creating reduced pressure. In their study, they used liquid argon between two parallel solid plates. As the distance between these plates is increased the bubble forms on the surface. They showed that the shape of the bubble depends on the wall-argon interactions as the three-phase boundary line behaves as it would behave for a droplet on the surface. Yi et al. [19] performed MD simulations on thin liquid argon over a solid surface to study the vaporisation and phase change of liquid. They found that at high surface temperatures, vapour forms between liquid and surface, and liquid layers changes to a spherical droplet. They also showed gradual evaporation for lower surface temperatures. A similar observation was found in the study done by Mao et al. [23] where they performed MD simulations to study rapid boiling in water film on a heated copper plate. In their study, the entire liquid film moves up, and vapour forms between surface and liquid. They also found that liquid film moves up and down in the simulation domain similar to a piston. Nagayama et al. [24] investigated the bubble behaviour in confined nanochannels for liquid argon. They concluded that bubble behaviour changes significantly based on the hydrophilicity of the surface. They found that if the surface is very hydrophilic, the bubble forms above the liquid layer in the bulk and resembles homogenous nucleation. In the case of hydrophobic surfaces, they showed a three-phase contact line and heterogeneous nucleation on the surface. Many studies (She et al. [25], Liu et al. [26], Mukherjee et al. [27]) showed that bubble formation also depends on the surface structures and imperfections on the surface. Hens A. et al. [20] investigated the vapour bubble formation in liquid argon with surface textures. The study shows that when the wall is uniformly heated, the vapour forms between the surface and liquid at high superheat, but when the surface is partially heated, the bubble forms quicker on a heated surface. They concluded that a more wettable surface can increase the heat transfer from the surface. Yu et al. [28] used molecular simulations to show that bubble nucleation temperature increases when the size of the channel is reduced, as the effect of increasing confinement is similar to having surface-liquid interaction dominate the interatomic interaction resulting in a dense structured layer. Hydrophilic surfaces can increase the wettabiliy of surfaces [14] and delay the formation of a dry region by keeping the liquid layers on a heated surface through a surface-driven passive liquid flow [29]. Novak et al. [14] investigated homogenous and heterogeneous nucleation at the surface using molecular simulations and showed that nucleation occurs at lower temperatures when surface-liquid interaction is weak.

This work focuses on studying heterogeneous bubble formation inside nanochannels, using molecular dynamics (MD) simulation, as a potential solution for hot spot thermal management. In real-life settings, usually, a spot gets overheated due to heat generated from the transistor, which remains a challenge for microchip cooling. This study shows the effects of surface-liquid interactions on such hot spots. A fixed geometry nanochannel is used and confinement effects are varied by changing the strength of surface-liquid interaction. We identify the variation in thermodynamic properties and heat transfer characteristics of nucleation in nanochannels compared to that in non-confined liquid over smooth surface. As heat from the surface is removed by evaporation, change in enthalpy of fluid before nucleation and after nucleation is also estimated as it serves as an important parameter [8] to predict heat dissipation characteristics.

First, bubble nucleation on a surface without any nanochannel confinement is studied as the baseline case. The simulation domain consists of 30 nm thick liquid argon over 25 nm × 5 nm platinum surface (Figure 1a). A 20 nm region of argon vapour atoms along with 2 nm of liquid argon on an identical platinum surface is placed over liquid argon to help stabilise bulk properties during the simulation run. The simulation was initially run for 5 ns at 110 K using Nosé–Hoover thermostat to attain equilibrium with the following Lennard-Jones parameters [29]: \( \varepsilon_{\text{Ar-Ar}} = 1.0179672 \text{kJ/mol}, \sigma_{\text{Ar-Ar}} = 0.34 \text{nm} \), and \( \varepsilon_{\text{Ar-Pt}} = 0.5385 \text{kJ/mol}, \sigma_{\text{Ar-Pt}} = 0.3085 \text{nm} \), where \( \varepsilon \) is the depth of the potential well and \( \sigma \) is the distance at which potential between two atoms is zero. The subscripts Ar and Pt represent argon and platinum respectively. The time step was 5 fs and all simulations were run in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software [30]. After 5 ns, the thermostat was turned off and all the platinum surfaces were kept at a constant temperature of 110 K for 1 ns using an in-house implemented surface-to-fluid heat transfer algorithm [31,32]. Our heating algorithm achieves proper thermodynamic heating or cooling of liquid/vapour at the solid-fluid interface rather than capturing heat transfer within the solid. The uniqueness of the heating algorithm allows liquid/vapour on different parts of the same surface to be heated/cooled to different temperatures. The surface-to-liquid heat transfer model is based on two conditions; first,
the liquid atom should be within a certain distance from the surface (defined as Rcr), and the force on the liquid atom must be surface dominated ($\sum F_{Ar-wall} > \sum F_{Ar-fluid}$). If these conditions are met, it is assumed that atom will collide on heated surface and exchange energy corresponding to the surface temperature.

A part of the platinum surface ($W_T$) is heated to a higher temperature to initiate nucleation in the liquid; the heat transfer algorithm enables heating/cooling different parts of the same surface to different temperatures. A total of 10 cases are run for varying widths from 3.5 nm to 6.5 nm and heated surface temperatures varying from 250 K to 350 K. For a lower temperature of the heated surface ($T_h$) and smaller heating width, the bubble is found to initially grow but it eventually collapses. An analytical model [31] is used to predict such a heterogeneous nucleation behaviour and for comparing against our simulation results. The thermodynamic properties of model and detailed validation can be found on our previous work [20].

As seen in Figure 1(b), the heating width and surface temperature conditions below the analytical model result in the bubble collapsing over time. The bubble remains stable for conditions around the model prediction while it grows for conditions above the analytical model line. This phenomenon shows the existence of critical radius of nucleation as predicted by the classical theory of nucleation [8]. The obtained results show that the simulation results are in good agreement with the analytical model prediction.

Next, to study bubble nucleation inside a nanochannel with varying hydrophilicity, the strength of surface-liquid interaction is increased through the parameter $\varepsilon$ and captured using a non-dimensional parameter $\varepsilon^* = \frac{\varepsilon}{\varepsilon_{Ar-Pt}}$, where $\varepsilon_{Ar-Pt} = 0.5385$ kJ/mol as defined earlier. However, changing surface-liquid interaction also affects the critical distance $Rcr$ used to achieve the desired surface temperature in the surface-to-fluid heat transfer algorithm as $Rcr$ depends on the strength of surface-liquid interaction [32] (See supporting information). Thus, to determine the critical distance required to heat the surfaces of different hydrophilicities, a MD simulation domain shown in the inset of Figure 2 is used where liquid argon is sandwiched between two platinum surfaces. The temperature of the lower wall and upper wall are maintained by the heat transfer algorithm. Initially, both the wall temperatures are at 90 K for equilibration following which the upper wall temperature is increased to 140 K while the lower wall temperature is kept at 90 K. Four cases are run for $\varepsilon^*$ equalling 1, 2, 4, and 6, and variation of the average temperature of liquid argon is plotted against time. As the domain resembles a 1D heat conduction problem, the temporal variation of average temperature of liquid argon for all cases are compared with the analytical solution of the 1D heat equation (Figure 2) and are found to be in good agreement. The corresponding $Rcr$ values used for these four cases are plotted in the inset of Figure 2 and the critical distance is found to decrease with increasing hydrophilicity. Thus, these values of $Rcr$ can be used to simulate heat transfer from such surface with varying hydrophilicity (i.e. $\varepsilon^*$), and are used next to study bubble nucleation in nanochannels.

In order to study bubble nucleation inside a nanochannel, a new platinum wall is placed at a distance of 5 nm above the lower wall in the simulation domain of Figure 1(a). The modified domain is shown in Figure 3(a). The other domain parameters are the same as the previous simulation of Figure 1(a). Four simulation cases are run with increasing hydrophilicity of the surface based on $\varepsilon^*$ values of 1, 2, 4, and 6. Each simulation is equilibrated for 2 ns using Nose–Hoover thermostat at 110 K followed by turning off the thermostat and maintaining surface temperatures at 110 K for another 1 ns using the surface-to-fluid heat transfer algorithm. In the equilibrium state, the density and pressure of liquid argon in the nanochannel are plotted in Figure 3(b); the same properties of liquid argon without the nanochannel are also included in the same plot (estimated from Figure 1 simulations).

![Figure 2](image1.png)  
**Figure 2.** (Colour online) Average bulk liquid temperature variation over time using implemented surface-to-fluid heat transfer algorithm and compared with 1D heat condition equation to determine critical distance $Rcr$, for increased surface-liquid interaction $\varepsilon^*$.  

![Figure 3](image2.png)  
**Figure 3.** (Colour online) Equilibrium simulations with 5 nm-height nanochannel showing (a) simulation domain, (b) density and pressure variation with $\varepsilon^*$, and (c) absolute enthalpy of liquid argon variation with $\varepsilon^*$.  


Compared to the no-channel case (marked as ‘NC’), the liquid pressure and density slightly increase when the channel is present (marked as ‘5 nm C’) due to liquid structuring. This effect is enhanced within the channel with increasing liquid-surface interaction \( \varepsilon^* \). Figure 3(c) shows the absolute enthalpy values of liquid argon with confinement during the equilibrium period. As the liquid is more structured for higher values of \( \varepsilon^* \), the magnitude of enthalpy increases. Thus, thermodynamic properties in confinement obtained by changing hydrophilicity show that more hydrophilic surfaces mimic the behaviour of increasing confinement, i.e. smaller channel heights where liquid structuring further dominates the overall properties.

After equilibration, the 5 nm width \( W_T \) of the lower and upper walls of the nanochannel, shown in Figure 3(a), is increased to a higher temperature of 350 K to initiate bubble formation in the nanochannel. The rest of the surfaces in the domain are maintained at the initial equilibrium temperature of 110 K. A bubble nucleates and forms at the heated part of the walls. The evolution of a vapour bubble is shown in Figure 4 for the no-channel case (with \( \varepsilon^* = 1 \), Figure 4a) as well as nanochannel cases with \( \varepsilon^* = 1 \) (Figure 4b). The density distribution is calculated by dividing the domain into \( 0.25 \text{ nm} \times 0.25 \text{ nm} \) rectangular bins and averaging the fluid properties over every 50 ps. In MD simulations, the liquid–vapour interface is tracked using local densities [8]. The rectangular bins with density below 300 kg/m\(^3\) are considered as vapour, and above 1000 kg/m\(^3\) as liquid. Area between 300 kg/m\(^3\) to 1000 kg/m\(^3\) is considered as liquid–vapour interface. The bubble vapour volume is defined by the number of bins classified in vapour region. The bubble grows with time for the no-channel case and the dry region forms over the heated area. At 0.1 ns (Figure 4a1), the bubble size is smaller but distinct, and grows to a much bigger bubble at 1.0 ns (Figures 4a3); the corresponding density contours confirm this observation. However, for the same surface-liquid interaction (\( \varepsilon^* = 1 \)) in the nanochannel, the bubble does not distinctly form at 0.1 ns (Figures 4b1 and b2). Thus, this clearly shows that nucleation is difficult to achieve in nanochannel because of higher density and pressure (Figure 3b) in the confined liquid. It can also be seen that at 1 ns (Figures 4b3 and b4), vapour bubble forms but with a density higher than the no-channel case (Figures 4a4 vs. b4). Thus, such effects are expected to become more prominent as surface hydrophilicity is increased.

Figure 5 shows the growth of the bubble in the nanochannel for \( \varepsilon^* = 6 \). At 0.1 ns, the liquid argon heats up but does not lead to bubble formation (Figures 5a1 and a2). With time, the bubble grows between the heated walls resulting in an elongated oval shape (Figures 5a3 and a4). Interestingly, a liquid monolayer exists on the surface unlike the other cases of Figures 4(a and b); the presence of the monolayer is due to the very strong surface-liquid interaction.

At steady state, the phase change continues with evaporation happening over heated parts of the walls and condensation at the relatively cooler ends of the bubble (See supporting document for more information). It is expected that heat transfer would be higher in the channels where the surface is more hydrophilic. The qualitative analysis of heat dissipation is done by estimating the change in enthalpy of vapourisation as follows:

\[
\Delta h = \frac{\sum (\varepsilon^* (h_v - h_0))}{\sum (N_v)}
\]

where, \( N_v \) is the number of vapour atoms, \( h_v \) is enthalpy of vapour atoms, and \( h_0 \) is the initial enthalpy of liquid argon in the channel before heating was started. Further, enthalpy
channel and condensation occurs at the liquid–vapour interface away from the surface. The change in thermodynamic energies of the system is shown in Figure 6(b), where $\Delta h$ is calculated by equation (1) with the help of equation (2). The change in $U$ and $PV$ are statistically obtained from MD simulations and are also plotted separately to show the importance of each term during nucleation. The change in expansion energy term ($PV$) remains almost the same for all cases, slightly decreasing for higher $\varepsilon^*$ cases as the vapour bubble volume $V$ decreases (Figure 6a) enough to counteract the increase in pressure $P$. The internal energy part of enthalpy change is greater for the nanochannel than nucleation in without confinement for the same surface-liquid strength ($\varepsilon^* = 1$), and it increases almost linearly with increase in $\varepsilon^*$. Similarly, the change in enthalpy of the system follows the internal energy trend. The increase in enthalpy of vapourisation for such confined nanochannels coupled with hydrophilic surfaces shows that heat dissipation can be enhanced by over 30%, and such a combination can potentially be utilised towards the thermal management of electronics.

To summarise, molecular dynamics simulations are used to study vapour bubble nucleation and heat transfer in 5 nm height nanochannels with increasing surface hydrophilicity while comparing against bubble nucleation in without confined liquid. Nanochannel confinement and increase in strength of surface-liquid interaction results in change in liquid density and pressure as more liquid structuring occurs next to the surface. Nanochannel confinement is found to require more energy to convert liquid into vapour atoms and is captured through an increase in enthalpy of vapourisation. The effect is more visible when the relative strength of surface-liquid interaction is increased based on multiples of 2, 4 and 6. Hence, nucleation in nanochannels can result in higher energy dissipation from the surface with increasing confinement effects and can be used to advance thermal management solutions.

**Data availability**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

**Disclosure statement**

No potential conflict of interest was reported by the author(s).

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$H$ is the sum of internal energy $U$ and work required to achieve its pressure $P$ and volume $V$ as follows [8]:

$$H = U + PV \quad (2)$$

The change in enthalpy represents the heat gained in the fluid from the heated walls, and a higher value of $\Delta h$ implies higher heat dissipation from the walls. The enthalpy of vapour atoms and initial liquid atoms were calculated by a statistical ensemble of atomic properties in 0.25 nm $\times$ 0.25 nm rectangular bins. Enthalpy is calculated by using the expression $h = u + pv$, where $u = ke + pe$, is internal energy, $p$ is pressure and $v$ is the volume of the bin. Density is directly calculated based on the number of atoms present in the bin and the molecular mass of atoms. Temperature and kinetic energy are determined by the velocity of atoms. Pressure distribution is derived from the stress tensor measured in each bin. The variation of vapour bubble volume with time is shown in Figure 6(a). In the case of no-channel, a larger bubble forms early due to a sudden increase of surface temperature and lack of confinement. The unsteady large bubble leads to immediate condensation of vapour at the bubble top resulting in a slight decrease in bubble size. Once a quasi-steady state is reached, the bubble continuously grows over time as the fluid gains energy from the heated surface. In the case of nanochannel, once the bubble reaches a steady state, the bubble size remains almost similar for all cases as the bubble is restricted inside the

![Figure 6.](image-url)
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