ROLE OF SURFACE TOPOGRAPHY IN POOL BOILING SYSTEMS VIA MOLECULAR DYNAMICS SIMULATIONS

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ABSTRACT

In this work we study nucleate pool boiling via non-equilibrium molecular dynamics simulations. We elucidate the effect of nano-structured surface topography on the onset of nucleation and nanobubble growth at the molecular scale, investigating the interplay of the cavity aspect ratio, wall superheat, and wettability by means of a parametric analysis for an atomistic Lennard-Jones system. The solid surface is heated uniformly from the bottom in order to induce the nanobubble nucleation. The role of the cavity size in controlling the vapor embryo formation is highlighted, and its dependence on the other investigated parameters is summarized in a phase diagram. Our results show that heterogeneity at the nanoscale plays a key role in the pool boiling heat transfer performance, and constitute a promising way to link the molecular scale results to continuum models (e.g., computational fluid dynamics) at much larger length- and time-scales in a more general multiscale modelling approach.

1. INTRODUCTION

Pool boiling is a central feature of several thermal management systems applications [1,2] from nano/micro cooling devices in electronics [3] to heat exchangers in the energy industry [4]. Due to the complexity of the phenomena exhibited in pool boiling, molecular dynamics (MD) is emerging as a robust and powerful tool to model the boiling process at the nanometre scale; here, molecular solid-fluid interactions play a fundamental role in driving the nanobubble formation. In the present work, we study the onset of nanobubble nucleation and transition to film-like boiling regimes by means of non-equilibrium molecular dynamics (NEMD). We investigate the surface topography effects on pool boiling using a cavity on the solid surface for an atomistic Lennard-Jones (LJ) system [5]. The solid surface is heated uniformly from the bottom to induce the nanobubble nucleation. The interplay of the cavity aspect ratio, surface wettability and wall superheat are investigated to explore the main mechanisms that control nanobubble formation and rationalized using a classical nucleation theory-based model. This constitutes a promising way to link the current results to larger-scale models in a more general multi-scale framework. NEMD results are summarized in a phase diagram which captures the main phenomena observed at the different operating conditions. We also investigate the impact of the simulation box size on the boiling process, showing how the flow field evolution over space and time can be captured in small subdomains (or chunks) during the MD simulation.

2. SIMULATED SYSTEM AND MAIN INVESTIGATED PARAMETERS

The simulated system is shown in Figure 1. It consists of 105 Lennard-Jones (LJ) particles which interact through a pairwise Lennard-Jones (LJ) potential:

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$$\Phi(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad (1)$$

where ε_{ij} and σ_{ij} represent the energy and the distance parameters between two generic atoms *i* and *j*, at distance r_{ij}, respectively.

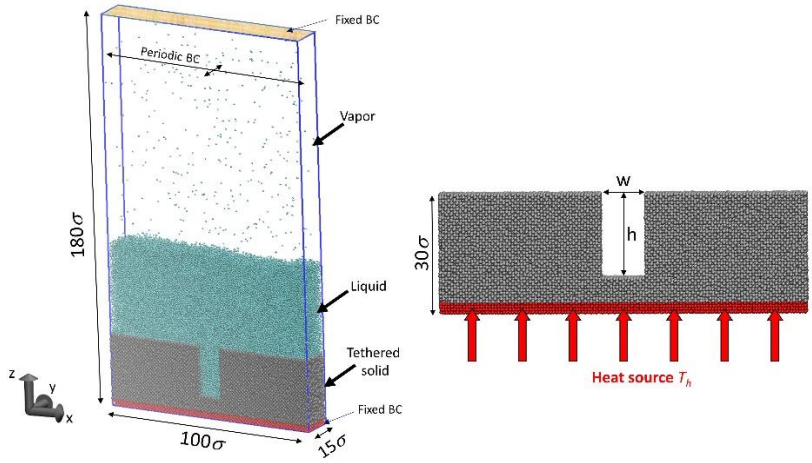

Figure 1: Simulation box, left, and geometry of the solid wall, right, with cavity size of width *w* and depth *h*. The aspect ratio is defined as AR = *w* /*h*. The solid surface is uniformly heated from the bottom (red).

Details of the simulation box geometry and corresponding boundary conditions are schematically represented in Figure 1. All physical quantities are expressed in terms of reduced LJ units. The size of the cavity is characterized by its aspect ratio, AR:

$$AR = \frac{w}{h} \quad (2)$$

where the range of AR = [0.25-2.0] is investigated. Hydrophobic, neutral, and hydrophilic surfaces are studied, and modelled through the corresponding solid-fluid (s-f) LJ parameters and, more specifically, by the ratios ($\varepsilon_{sf}/\varepsilon_{ff}$, σ_{sf}/σ_{ff}) as reported in Table 1. The wall superheat is defined as $\Delta T_{wall} = T_{wall} - T_{sat}$, where T_{wall} represents the average wall temperature and T_{sat} is the fluid saturation temperature. All MD simulations are performed with LAMMPS simulations package and the graphical results postprocessed with the VMD software.

Table 1: Parameters of the experimental program.

($\varepsilon_{sf}/\varepsilon_{ff}$, σ_{sf}/σ_{ff})	Wettability
(0.5, 1.05)	Hydrophobic
(1.0, 1.0)	Neutral
(1.7, 0.93)	Hydrophilic

3. RESULTS

MD simulations results are summarized in a phase diagram, shown in Figure 2 for $\Delta T_{wall} = 0.2$. All the points enclosed in each colour border are characterized by the same common property (stated in the corresponding label). The nucleation time is also depicted as a counter plot in the background. The amount of liquid/vapor inside the cavity is qualitatively shown for each investigated case with a circle: a blue fully-filled circle corresponds to the cavity filled with the liquid phase; white corresponds to the vapor phase. Figure 2 captures the main trends observed in this work: small cavity AR (e.g. AR = 0.25) show high nucleation times and provides less control on the nucleation site. The onset of nucleate boiling is promoted by larger cavity AR, which, however, are also associated with the possibility of complete dry-out, undesirable for heat transfer applications. For some operating conditions, multiple nanobubbles may form eventually and coalesce before growing and expanding (light blue region).

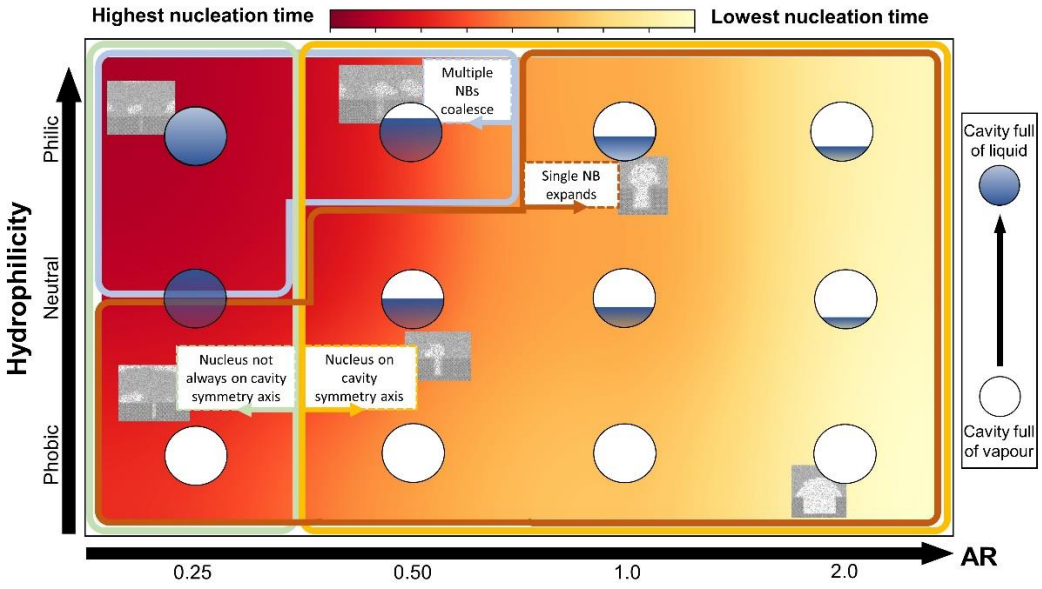

Figure 2: Phase diagram which summarizes the main results and the key mechanisms observed in the MD simulations carried out in this work, at ΔT_{wall} = 0.2.

In order to evaluate the impact of the system size on the dynamics of bubble formation and growth we also show a comparison between the system size investigated in this work and a similar system but three times larger. Larger simulations (three times in size, 2.5×10^6 atoms) have been carried out, and we report here one case simulated at heating temperature T_h = 1.5 and a hydrophilic wall in Figure 3 as a demonstrative show-case. Some similarities can therefore be reached, at least in terms of nucleation time and dynamics of nanobubble formation (yellow line in Figure 3); however, the dynamics of the nanobubble growth is substantially different.

We also report the density field stored in subdomains (or chunks) during the simulation time for both the simulated system and the three-times bigger one previously analysed. The chunks size is $1x1x1\sigma^3$. The simulation box is divided in a finer grid and the trajectories of the discrete atoms are stored in it and eventually time-averaged every $2 \cdot 10^4$ timesteps in order to smoothen the statistical error due to the property fluctuations. This represents a powerful tool to link the flow fields at the molecular scale directly to a continuum scale model. The properties stored in these subdomains can be passed to a CFD code and used as boundary conditions to study the bubble growth and frequency departure at much larger length scales at a reasonable computational cost. Along with the aforementioned properties, also other relevant parameters can be directly calculated from the MD framework, such as viscosity, contact

angle and thermal conductivity, of paramount importance to close the mathematical models at the continuum scale.

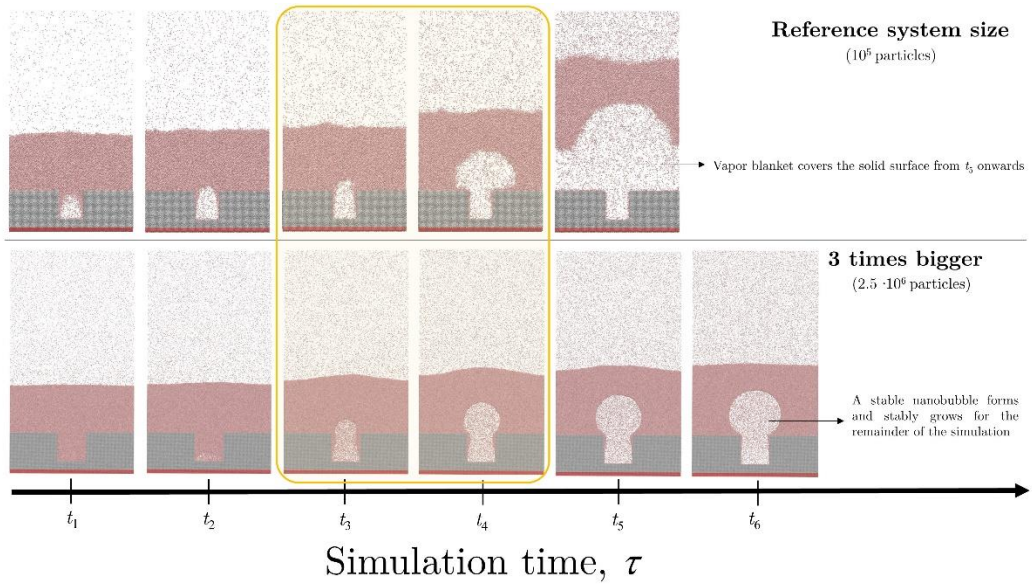

Figure 3: Temporal evolution of the system over the simulation time, in reduced LJ units τ. A comparison between the system size under investigation (first row) and a three-time bigger system (second row) for a hydrophilic wall at T_h = 1.5 and cavity AR = 1. Similarities about the time for nucleation can be shown (yellow line); however, the nanobubble growth dynamics is substantially different.

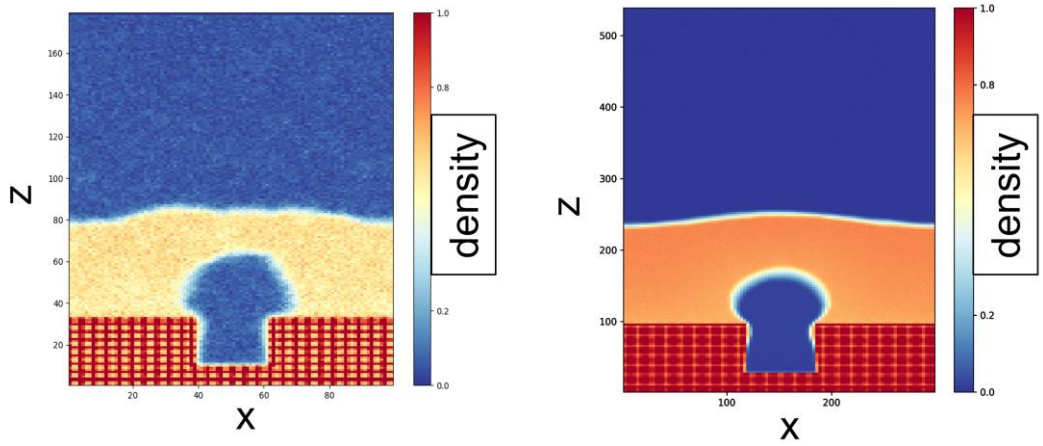

Figure 4: Density field stored in subdomains (or chunks) for the simulated system (left) and the three-time bigger system (right) on a hydrophilic wall, at T_h=1.5 and cavity AR = 1.

4. CONCLUSIONS

We show how molecular scale investigations via non-equilibrium molecular dynamics (NEMD) simulations may represent a powerful tool to study pool boiling systems. Our results can be applied to the design of surface topography to control nanobubble nucleation for the optimization and design of solid surfaces for thermal management systems. They also represent an important step forward for a future link to macro-scale models in a more general multiscale framework. Future work in these directions will focus on the investigations of real liquids, such as water and refrigerants.

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