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MOLECULAR WATER LAYER EVAPORATION & CONDENSATION

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KEY WORDS

Molecular dynamics, nanopore evaporation, two-phase cooling

ABSTRACT

The past decade has seen a considerable growth in portable devices with mobile connectivity. This growth has been enabled by the development of high capacity telecommunication networks globally. Individuals require high data transfer capabilities to remotely stream large information sets (i.e. HD video) and this is leading to greater demands for next generation networks (i.e. 5G). To ensure this growth continues, hardware devices must be smaller, more energy-efficient and provide greater functionality. This requirement poses a thermal management challenge, increasing heat transfer density significantly. Novel materials and cooling methods, which are engineered at the micro- and nanoscale, are necessary to address this.

The overall aim of this project is to examine and maximize the heat transfer performance capabilities in an enclosed two-phase micro-system architecture.

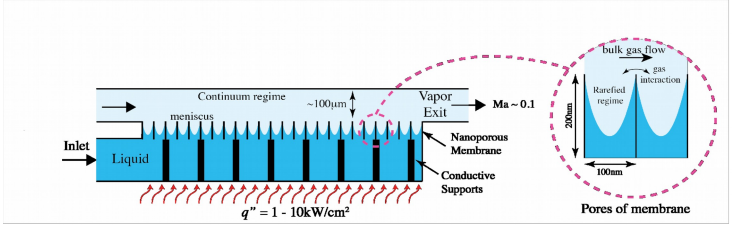

Figure 1: Nanopore evaporation

A very promising cooling technique for the increasing heat transfer density is the method depicted in Fig. 1. In this two-phase cooling system, the liquid phase evaporates from the nanopores to the gas phase [1]. The latent heat of vaporization is the dominant mode of heat transfer while the nanopore geometry generates the requisite capillary pressure to drive the liquid flow to the heat source. This will be studied numerically (to increase the fundamental understanding of the phenomena) and be used to inform detailed experiments and system level design. Therefore, various solids (Si, SiO_2,...), gases (Ar, H_2O, N_2,..) and rarefaction levels will be studied numerically.

In order to study the two-phase cooling system, we start with a simplified model of evaporation and condensation of a water layer system as shown in Fig. 2. We use Molecular Dynamics to investigate different properties of the simulation such as the temperature profile, heat flux, velocity distribution, water molecule orientation (WMO) [4] and the density distribution.

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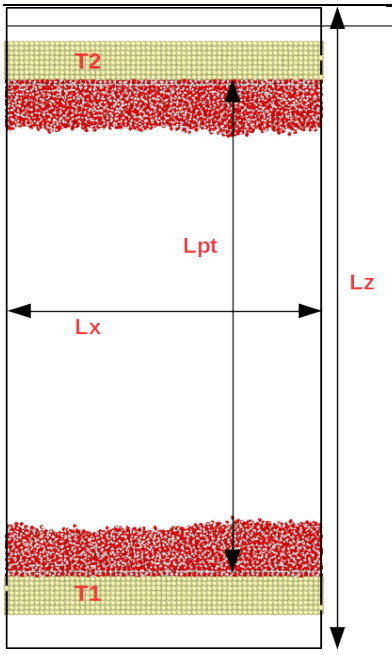

Figure 2: Simulation model for evaporation and condensation of a water layer

The dimensions of the simulation model are Lx, Ly = 121 Å, Lz = 260 Å and Lpt = 200 Å. The temperature at the bottom and top walls are kept constant using a Nose-Hoover thermostat with T1=368K and T2=278K. Periodic boundary conditions are applied in x,y and z direction. The water molecules are modeled using the TIP4P/2005 model [2] and the interaction between the 8 layers of platinum atoms are modeled using harmonic springs [3].

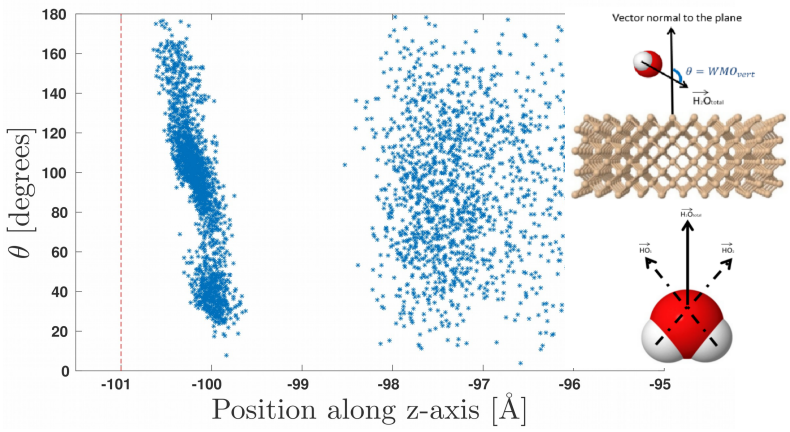

Figure 3: WMO near the bottom wall. Red line: begin of the bottom wall. Right insert: definition of water molecule orientation (WMO).

The results obtained so far are the WMO and the density distribution. It is observed in Fig. 3 that there exists a preferred water molecule orientation around 80°-120° and 40° near the bottom wall. A similar observation can be made near the upper wall. In the bulk no preferred WMO is observed. This could influence the liquid-vapor interface and evaporation.

The density distribution along the z-axis shown in Fig. 4 indicates the high density in the walls and a decay near the liquid vapor interface.

The temperature profile, which is under investigation at the moment, will give us the opportunity to see possible temperature jumps near the solid-liquid and/or liquid/vapor interface and thereby provide us detailed information on the evaporation resistances.

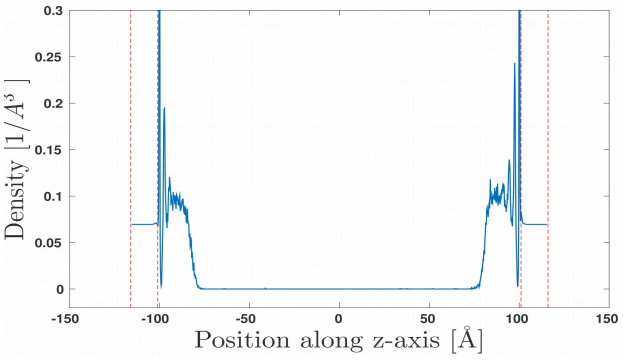

Figure 4: Density distribution along the z-axis. Red lines indicate the walls

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