International Communications in Heat and Mass Transfer 97 (2018) 118–124

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

A molecular dynamics investigation on effects of nanostructures on thermal conductance across a nanochannel

T. Lin, J. Li, X. Quan*, P. Cheng

MOE Laboratory for Power Machinery and Engineering, School of Mechanical Engineering, Shanghai Jiao-Tong University, Shanghai 200240, PR China

ARTICLE INFO

Keywords:
Nanochannel
Fin-confinement
Coordinate number
Thermal conductance

ABSTRACT

Molecular dynamics simulations are conducted to investigate effects of nanofins on thermal conductance of a nanochannel with two opposing walls at different temperatures. The nanochannel and nanofins are made of *Pt* with liquid Argon filled in between. It is found that the degree of thermal conductance enhancement across the nanochannel depends on combined effects of (i) confinement of liquid atoms in the nanogap between fins and (ii) lowering of coordinate number of fin atoms at the solid-liquid interface, both of which depend on the fin's width for a fixed pitch distance. It is also found that the thermal conductance across the nanochannel is increasing monotonously with fin's height, and that a notable temperature gap between confined liquid in the nanogap between fins and bulk liquid exists when the effect of fin-confinement is strong and the fin is sufficiently long. The existence of this temperature gap is because the enhanced interfacial thermal heat transfer at nanofin's sidewalls and the enlarged liquid conductive resistance between confined and bulk liquid. Due to the temperature gap between the confined liquid and the bulk liquid, the method chosen to compute the interfacial temperature difference can significantly influence the result of interfacial thermal resistance when nanofins are tall.

1. Introduction

The miniaturization and integration of microelectronic devices have placed an increasing demand for efficient heat dissipation. In nanosystems and devices, thermal transport is usually hindered by resistances at interfaces of two different materials [1]. When heat is transferred across a solid-liquid interface, a discontinuity in temperature profile is established at the interface due to the significant difference in thermal properties between solid and liquid. This temperature jump is known as Kapitza resistance [2], which is defined as:

$$R_k = \Delta T/q \tag{1}$$

where ΔT is the temperature jump at the interface.

Owing to the nanoscale of the solid-liquid interface, it is difficult to carry out experiments to investigate heat transfer at the interface. On the other hand, molecular dynamics simulation can track the position and velocity of every atom, making it a powerful tool to study nanoscale interfacial thermal resistance R_k. In the past decades, numerous studies have been carried out to study characteristics of thermal resistance at solid-liquid interfaces. It is widely accepted that main factors influencing R_k include: the liquid-solid interaction strength (wettability) [3–6], interfacial roughness [7–10], degree of liquid confinement [11, 12], temperature [5, 13, 14], pressure [4, 5, 15, 16], and atomic mass [17]. Recently, several methods such as nanopatterned surfaces [18, 19] and surface functionalization [20, 21] have been proposed to reduce the Kapitza resistance. Nagayama et al. [7] found that the interfacial heat flux increases almost linearly proportional to the surface area, and they noticed that variation of nanostructure morphologies led to fluctuations in the interfacial heat flux. Chen and Zhang [8] pointed out that surface roughness weakens the mobility of liquid atoms near the interface, resulting in liquid atoms in contact with the solid surface for a longer period of time. Shibahara and co-workers [9, 10] found that there was an optimal structural clearance (i.e., gap between fins) to reduce the thermal resistance of solid-liquid interface, which was attributed to the change of structures of adherent liquid molecules and the longer residence time of liquid molecules at interface.

The Diffuse Mismatch Model (DMM) has been used to study phonon transport at the interface [22]. It is assumed that phonons are scattered at the interface, and the Kapitza resistance is owing to the mismatch in vibrational density of states (VDOS) of two neighboring materials at the interface [23]. For a solid-liquid interface, the vibration frequency of solid atoms is far higher than that of liquid atoms. There are two options to improve the vibrational match of liquid atoms and solid atoms

* Corresponding author.
E-mail address: quan_xiaojun@sjtu.edu.cn (X. Quan).

https://doi.org/10.1016/j.icheatmasstransfer.2018.05.025

at the interface in order to reduce the interfacial thermal resistance: either by raising the vibration frequency of liquid and/or by lowering the vibration frequency of solid. Liang and Tsai [11] showed that the interfacial thermal resistance between *Ag* particles and *Ar* thin film was about one order of magnitude smaller when the liquid film contained only one liquid monolayer, and the resonance of solid and liquid atoms is responsible for the low thermal resistance. Hu et al. [12] reported that freezing of water molecules at extremely confined conditions, and the excellent matching of vibrational states can remarkably enhance the thermal conductance of water quartz interface. Hu and Sun [18] concluded that the increase of width-to-spacing ratio of nanopatterns could reduce the Kapitza resistance by diminishing the mismatch between the VDOS of water and gold.

It is known that lower coordination numbers of solid atoms led to higher amplitude of vibration at low frequencies because of a softer force field [24, 25]. The coordination number of an atom is defined as the number of its nearest neighbors. In the study of vibrational properties of metallic nanocrystals, Kara et al. [26] and Derlet et al. [27] observed an enhancement in the VDOS at low frequencies for smaller size of crystals as compared to that for an atom in the bulk crystal. It should be noted that the percentage of solid atoms at crystal boundaries increases with decreasing crystal size, and solid atoms at crystal boundaries have lower coordination number. Recently, Issa and Mohamad [19] demonstrated that lower coordination number of solid atoms near the interface was beneficial to enhance the solid-liquid interface heat transfer because of better matching of vibrational of liquid and solid atoms at interfaces.

It is widely accepted that liquid confinement in a gap can enhance conduction heat transfer, although this enhancement is effective only when the distance between two walls is extremely small. This is because the VDOS of liquid atoms became bulk-like quickly when the gap becomes larger [11]. In most situations where the walls are separated by a much greater distance, the nanoconfinement effect diminishes.

In this paper, we investigate effects of nanofins on the walls of a nanochannels for the purpose of enhancing heat conduction across the nanochannel. It will be shown that higher thermal conductance can be obtained by smaller fin spacing (fin-confinement effect of liquid atoms in nanogap) or by smaller fin width (lower coordination number of solid atoms). These two effects (which are in opposite directions with regard to fin width for a fixed pitch distance) result in a non-monotonously increase in conduction heat flux with respect to fin width (or fin spacing). Furthermore, the local thermal resistance at the solid-liquid interface of nanosfins is analyzed to show how heat conduction and temperature distribution can be affected by the fin width or fin spacing. In addition, two existing methods of calculating the temperature difference at solid-liquid interfaces of nanofins are compared. Results obtained from the present study can provide a valuable guide for the design of nanostructures with solid-liquid interfaces to reduce thermal resistance in nanoscale thermal devices.

2. Simulation methods

A schematic of the simulation system is shown in Fig. 1, where liquid *Ar* (yellow color) is filled in a nanochannel where two parallel walls are made of *Pt* (light red color) separated by a nano-distance H (i.e., a nanochannel). An array of nanofins also made of *Pt* (light red color) with height h, width w at a spacing s or at a pitch distance p (where $p = w + s$), are fabricated on the walls. The dimensions of the computational domain in the X, Y and Z directions are $L_x = 58.3$ Å, $L_y = 38.5$ Å and $L_z = 90.3$ Å, respectively. The nanofins on the walls are constructed by adding atoms on base walls, and the spacing formed between successive fins serves as confined spaces for liquid *Ar*.

In this study, molecular dynamics simulation will be carried out to study heat conduction in a nanochannel with nanofins on opposing walls at different temperatures as shown in Fig. 1. Five different spacings of nanofins ($s = N_s(a_0)$, where $N_s = 1, 2, 3, 4, 5$, and $a_0 = 2.77$ Å is the thickness of one *Pt* atomic layer in X direction), and four different fin heights ($h = N_h(c_0)$, where $N_h = 2, 3, 4, 5$, and $c_0 = 2.27$ Å is the thickness of one *Pt* atomic layer in Z direction) are considered in this paper. Note that $N_h = 0$ is for a smooth nanochannel. In all simulations, it is assumed that the separation distance of the nanochannel $H = 54.1$ Å, pitch distance of the nanofins $p = 7a_0$, and each base wall consists of eight layers of *Pt* atoms arranged as FCC structures with the lattice constant of 3.92 Å, and its ⟨111⟩ crystal plane is in contact with liquid. The two outermost monolayers (white) in the Z-direction are fixed at its lattice sites, which guarantees a constant volume during simulation. The two monolayers immediately adjacent these fixed atoms are bath atoms, to which energy can be added from bottom (dark red heat bath at 120 K) or removed from the top (blue cold bath at 100 K) to establish a temperature gradient in the Z-direction across the nanochannel. At the beginning of a simulation, *Ar* atoms are also arranged by FCC lattice with a density of 1.31 g/cm^3, corresponding to the saturation temperature of liquid *Ar* at 100 K. Periodic boundary conditions are applied to X and Y directions, while fixed boundary condition is adopted in the Z-direction. In this study, only heat conduction is considered.

All interactions between atoms in this paper are described by the 12–6 LJ potential:

$$U(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \tag{2}$$

where r is the distance between two interacted atoms, σ and ε are the length and energy parameters. For liquid-liquid interaction, $\sigma_{ll} = 3.405$ Å and $\varepsilon_{ll} = 0.24$ kcal/mol, while for solid-solid interaction, $\sigma_{ss} = 2.475$ Å and $\varepsilon_{ss} = 12.02$ kcal/mol. The Lorentz-Berthelot combining rule is used for the cross interaction, i.e.$\sigma_{sl} = (\sigma_{ll} + \sigma_{ss})/2$, and $\varepsilon_{sl} = \alpha\sqrt{\varepsilon_{ll}\varepsilon_{ss}}$, where $\alpha = 0.14$ is the potential energy factor, which determines the interaction strength between solid and liquid. For computational efficiency, the potential function is truncated and shifted at $4\sigma_{ll}$. All simulations are performed by LAMMPS [28], a large-scale atomic/molecular massively parallel simulator, and visualizations are done by OVITO [29]. During simulations, the equation for motion of atoms are integrated using the Velocity-Verlet algorithm with a time step of 5 fs. Before data acquisition, liquid and solid atoms are first equilibrated at 100 K in an NVT ensemble with Nose-Hoover thermostat for 2 ns individually. After that, nonequilibrium molecular dynamics (NEMD) simulations are carried out with an NVE ensemble applied to the entire system. To establish a temperature gradient through the simulation cell, the Berendsen thermostat [30] is used to maintain temperatures of heat bath and cold bath atoms at 120 K and 100 K, respectively. A stable temperature profile is established after 3 ns, followed by another 10 ns for data acquisition.

The cell domain is divided into grids of 0.566 Å in Z-X plane to capture the local density distribution of the liquid. Temperature data is recorded over bins of size 2.27 Å along the Z axis. The local temperature of each bin can be obtained by:

$$T = \frac{2}{3k_B}\frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}m_i\left(\sum_{j=1}^{3}v_{i,j} - \overline{v_j}\right)^2 \tag{3}$$

where N is the number of atoms in each bin, k_B is the Boltzmann constant, m_i and v_i are the mass and velocity of the ith atom respectively, and $\overline{v}$ is the mean velocity of all atoms ($\overline{v} = 0$ in this study). The total thermal resistance of the entire nanochannel can be calculated from:

$$R_t = \Delta T_{ss}/q \tag{4}$$

where q is the conduction heat flux across the nanochannel, and ΔT_{ss} is the temperature difference between two solid walls, which equals to the temperature difference between the heat and cold bath (20K) minus the temperature drop along the base wall.

From the view of DMM, Kapitza resistance is owing to the mismatch in VDOS of two neighboring materials at the interface. The VDOS of