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Temperature and heat flux dependence of thermal resistance of water/metal nanoparticle interfaces at sub-boiling temperatures

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ABSTRACT

Molecular dynamics simulations of heat transport through nanoscale metallic systems in contact with water are performed to investigate the effects of temperature and heat flux on thermal resistance across the interface. Non-equilibrium MD simulations are performed using 4 different metals: gold, silver, copper, and aluminum. The simulation space is composed of a 5-nm wide nanochannel of water between two parallel metallic walls, with one wall serving as a heat source and the second serving as a heat sink. 60 simulations are performed at heat source temperatures spanning from 300 K to 650 K at intervals of 25 K, and fixed heat sink temperatures of 250 K. Steady-state wall and fluid temperatures at the interfaces and the imposed energy required maintaining each wall temperature are recorded to measure system heat flux. The interfacial thermal resistance is calculated for each wall temperature and metal combination, and the wall temperatures, heat fluxes, and resistance data is presented for all cases where the interfacial water temperature is below 373 K. Using two-dimensional least squares regression, linear fit coefficients for the calculation of interfacial thermal resistance as a function of wall temperature and heat flux are compiled. These fitting coefficients may be used to implement temperature and heat flux-dependent interfacial resistances for each metal for a variety of thermal applications.

1. Background

Heat transfer through two dissimilar materials results in a form of thermal contact resistance that is manifested as a discontinuous temperature jump across the interface. This temperature jump is caused by a mismatch between the vibrational density of states between the solid and liquid [1–3,17,20–23,27]. Current understanding of phonon transport across solid–liquid interfaces is based on the acoustic mismatch model (AMM) and the diffusive mismatch model (DMM). The AMM [2,3] assumes no phonon scattering at the interface, where the DMM assumes that all phonons are scattered at the interface. These models serve as upper and lower extremes of interfacial thermal resistance, with the AMM predicting the highest theoretical thermal resistance (low thermal conductance) and the DMM predicting the lowest theoretical thermal resistance (high thermal conductance). Molecular dynamics simulations are used to calculate the level of resistance between these two extremes by directly calculating the heat flux across the system and the temperatures at each boundary.

A common measurement for interfacial thermal resistance (ITR) is the Kapitza resistance, named after P.L. Kapitza who carried out the first systematic study of thermal interface behavior in liquid helium in 1941 [10]. It is defined as $R_K = \Delta T/q$, where ΔT is the discontinuous temperature drop at the interface, and q is the heat flux through the interface. This resistance is often quantified in terms of a length term called the Kapitza length, which is the length of fluid that would result in an equivalent ΔT based on the local temperature gradient of the fluid. It is expressed mathematically as $L_K = \Delta T/(\delta T/\delta z)$ where $\delta T/\delta z$ is the temperature gradient of the liquid portion of the liquid/solid interfacial system.

Recent studies have suggested that the interfacial thermal resistance of an interface is not static but can be dependent on a variety of local conditions such as the surface temperature and geometry [3,9,24,28]. In 2009, Merabia conducted a molecular dynamics study of the heat transfer from laser-induced heated gold nanoparticles in water at three different power levels: 350 nW (10^{-9} W), 525 nW, and 700 nW. The spherical gold particle had a radius of 1.3 nm and consisted of 494 gold atoms arranged in a face-centered cubic (FCC) lattice [17]. The water consisted of 10,000 SPC/E molecules in a cubic simulation cell with periodic boundary conditions and water held to a constant temperature of 450 K at 20 Å from the nano-particle surface. He measured interfacial

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Nomenclature

Latin symbols

a	lattice unit length (nm)
A	surface area
Ag	silver
Al	aluminum
AMM	atomic mismatch model
Au	gold
A_{xy}	channel cross-sectional area
$_C$	cold (subscript)
$_{CL}$	cold liquid (subscript)
$_{CS}$	cold solid (subscript)
Cu	copper
C_1	least squares regression coefficient
C_2	least squares regression coefficient
$_{C3}$	least squares regression coefficient
D_{OH}	anharmonic potential (kJ/mol)
DMM	diffuse mismatch model
e	electron charge
ΔE_{cold}	energy added to heat sink (J)
ΔE_{hot}	energy added to heat source (J)
Γ	interfacial conductance (MW/m^2-K)
$_H$	hot (subscript)
$_{HS}$	hot solid (subscript)
$_{HL}$	hot liquid (subscript)
ITR	interfacial thermal resistance (W/m^2-K)
k_w	bulk water thermal conductivity (W/m-K)
L	length (nm)
m	mass of atom (amu)
N	number of atoms
$_O$	oxygen (subscript)
O–H	oxygen–hydrogen bond
q	heat flux (W/m^2)
q_i	charge of atom i in water molecule
q_j	charge of atom j in water molecule
q_z	system heat flux in z direction (W/m^2)
r_{ij}	distance between component i and j (nm)
R_K	Kapitza resistance (m^2-K/W)
R_i	Interfacial thermal resistance (m^2-K/W)
Δr_1	hydrogen–oxygen bond equilibrium displacement (nm)
Δr_2	Hydrogen–Oxygen bond equilibrium displacement (nm)
Δr_3	hydrogen–hydrogen bond equilibrium displacement (nm)
r_{cut}	spherical cutoff distance (nm)
SPC-F	single point charge-flexible water model
T_i	water temperature at interface (K)
T_L	temperature at location L (K)
T_{r1}	temperature at radial location r_1 (K)
T_{r2}	temperature at radial location r_2 (K)
T_w	temperature at nanoparticle wall (K)
v	atomic velocity (nm/ps)
V_{mol}	total intermolecular potential (kJ/mol)
V_{OO}	Lennard-Jones Potential between oxygen atoms of separate water molecules (kJ/mol)
$V_{coulomb}$	electrostatic potential between the atoms in one water molecule to the atoms of a second water molecule (kJ/mol)

Greek symbols

ε	depth of potential well in Lennard-Jones term (kJ/mol)
λ	velocity scaling constant
ρ	density (kg/m^3)
σ	Lennard-Jones potential minimum energy distance (nm)
τ	total time elapsed during simulation run (s)

conductances, G, varying between $G = 170$ MW/m^2-K to 150 MW/m^2-K ($R_K = 5.8823 \times 10^{-9}$ to 6.6666×10^{-9} m^2-K/W). His gold surface temperatures varied between approx. 550 K, 650 K, and 725 K using heat fluxes of 350 nW, 525 nW, and 700 nW, respectively. His study showed a clear dependence of interfacial resistance on temperature with higher resistances at higher surface temperatures.

In 2012, Hu and Sun investigated the effect of nanopatterns on interfacial thermal resistance at a water-gold interface during boiling [8]. They modeled a liquid water film of 7200 TIP4P-Ew water molecules inserted between two flat gold substrates of 13,824 gold atoms. The two substrates served as a heat source and heat sink, and they were used to apply a constant heat flux of 1.33×10^9 W/m^2 across the system.[1] In their most basic case, a flat wall at 470 K, they measured a Kapitza resistance of 8.327×10^{-9} m^{2}K/W. In the presence of a phase change, they measured a Kapitza resistance of 8.271×10^{-9} m^{2}K/W, within 0.7% of the case without phase change, concluding that the liquid-vapor phase transition does not affect the Kapitza resistance of a water-gold interface. For nanopattern heights of 0.8156, 1.631, and 2.447 nm, along with widths and spacing distances of 2.447, 4.894, and 7.341 nm, the Kapitza resistance at the interface ranged from 4.006 to 8.271×10^{-9} m^{2}K/W. They concluded that the Kapitza resistance decreases with increased nanopattern height, and they attributed this change to an increase in interaction energy per unit area, reasoning that "the increase in height of nanopatterns leads to an increase in contact area and thus the interaction energy per unit area becomes larger, thereby reducing the Kapitza resistance."

In 2014, Barisik et al investigated the temperature dependence of thermal resistance at a water/silicon interface [3]. They examined three cases of water in a channel between two walls of silicon using hot wall temperatures of 363 K, 353 K, and 343 K, and cold wall temperatures of 283 K, 292 K, and 303 K, respectively. Their simulations show that interfacial thermal resistance decreases with increased temperature on a surface with good wettability. Examining the liquid structure near the solid, they attribute the decreased resistance to a higher phonon density of state at high temperatures, creating better vibrational coupling.

In this study, we use molecular dynamics simulations to model the heat transfer across a rectangular nanochannel with water confined between two parallel solid metallic walls of 4 different metals. The outer boundaries of each of the two walls serve as the system heat source and heat sink. Direct velocity scaling is used to fix the temperatures at the heat source and sink, while the kinetic energy required for maintaining these temperatures are recorded over the duration of the simulation to calculate the heat flux. Application of the heat flux results in the formation of three distinct temperature gradients that form within the hot wall, the water channel, and the cold wall. The resultant steady-state temperatures that develop at the interfaces are used with the heat flux to directly calculate the interfacial thermal resistance. This process is systematically repeated for each metal, with hot wall temperatures ranging from 300 K to 600 K at intervals of 25 K and cold wall temperatures fixed at 250 K.

[1] 1×10^9 W/m^2 = 1 nW/nm^2.