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Molecular dynamics simulation of the thermal transport on holey copper substrates

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Abstract

The mechanism behind heat transfer at the nanoscale is different from that at macroscale as the size of the surface structure reaches the phonon mean free path. In this work, we investigate the effect of the presence of a nano hole on the solid-liquid heat transfer. To this end, we perform molecular dynamics simulations of a water film in contact with a copper substrate with nanoscale surface structures–here represented by nanoholes. Our results indicate that the presence of a nanohole with diameter of 20 Å increases significantly the transfer of thermal energy from the copper substrate to the water film.

Introduction

- The size of the hole on the surface and the solid-liquid heat transfer are the key factors governing the bubble formation [1]. Moreover, the formation process of the bubble is always triggered by the presence of the nanohole in the substrate [1].
- The phonon transport occurs in the ballistic regime in the hole path-to-surface region thus phonons can carry heat without internal scattering as the size of the substrate is smaller than its phonon mean free path.
- In nanoconfinement, phonon propagation in the ballistic regime can dominate the heat exchange allowing the manipulation of the thermal energy transport which is of key importance for potential application of phononics/phonon engineering in nanoscale heat transfer [2].

Results and discussion

The water temperature variation

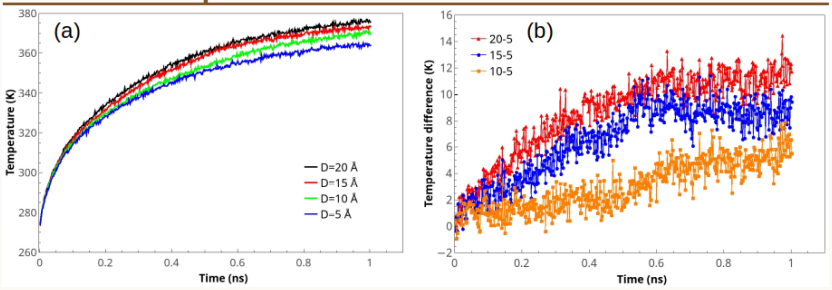


Fig.1. The water temperature variation. (a) variation in mean water temperature using four different hole diameters (D = 5, 10, 15, and 20 Å); (b) The temperature difference of the water region for three cases (10, 15 and 20 Å) compared to the case of 5 Å.

The copper-water energy difference

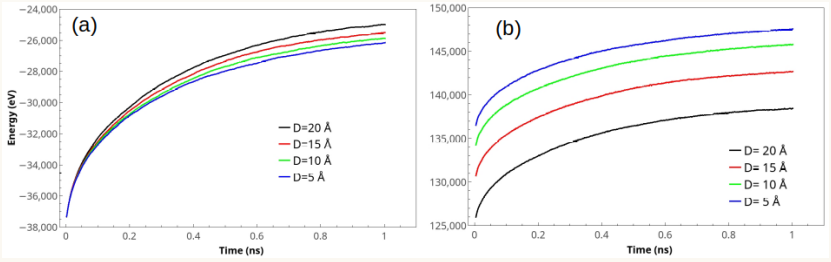


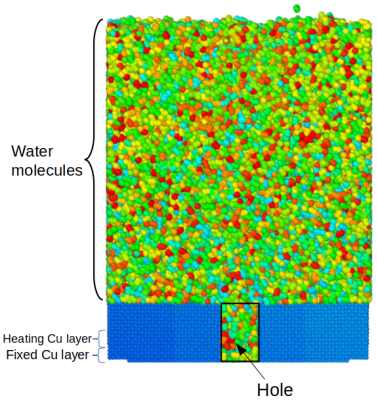
Fig.2. (a) The comparison of the water energy and (b) the total energy difference between the copper and the water region for four cases.

Result comparison and conclusion:

- The presence of the holes facilitate the heat transfer from copper substrate to water region for all cases studied.
- The hole in the copper substrate have a significant influence on the enhancement of heat transfer between copper wall and water region.
- Within 20 Å, the enhancement increases with the increasing hole diameter. The temperature of the water region increase faster in the case with a lager hole.
- The larger hole leads to the lower energy difference of copper substrate and water region in the process of solid-liquid heat transfer, and giving a better capacity for absorbing the energy from copper substrate.

Simulation methodology

Simulation box: 14.0×14.0×80.0 nm



Potential parameters	ε (eV)	σ (Å)	q (e)
O-O	0.0067389	3.166	-0.8476
O-H	0.0	0.0	0.4238
H-H	0.0	0.0	--
Cu-O	0.0524	2.7519	--
Cu-H	0.0	0.0	--

- **Copper potentials - embedded atom model (EAM)**: the face-centered cubic (FCC) structure with the lattice constant of 3.61 Å.

$$E_{tot} = \frac{1}{2}\Sigma_{ij}\Phi_{ij}(r_{ij}) + \Sigma_i F_i(\rho_{i,tot}), \rho_{i,tot} \qquad (1)$$

- **Water potentials - Coulombic and Lennard-Jones 12-6 interaction:** using extended simple point charge (SPC/E) water model. The H-O-H angle and O-H bond are 109.47^o and 1 Å, respectively.

$$U_{ij} = 4\varepsilon_{ij}[(\frac{\sigma_{ij}}{r_{ij}})^{12} - (\frac{\sigma_{ij}}{r_{ij}})^{6}] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} \qquad (2)$$

- Water-copper: Lennard-Jones 12-6 interaction

Simulation setup

- We conduct simulations of four cases wherein systematically nanoholes with different diameters (D=5, 10, 15 and 20 Å) are generated in the copper substrate.
- **Equilibration:** simulations in NVT ensemble for 0.1 ns
- **Verification:** simulations in NVE ensemble for 1.0 ns
- **Heating process:** NVT ensemble heating the copper layers

Reference:

[1] Y. Gao, Q. Liu, and B. Xu, Lattice mismatch dominant yet mechanically tunable thermal conductivity in bilayer heterostructures, ACS nano, vol. 10, no. 5, pp. 5431–5439, 2016.

[2] A. A. Balandin and D. L. Nika, Phononics in low-dimensional materials, Materials Today, vol. 15, no. 6, pp. 266–275, 2012.