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Molecular dynamics investigation on enhancement of heat transfer between electrified solid surface and liquid water

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ABSTRACT

Interfacial nanolayer acting as a bridge linking a bulk solid phase and a bulk liquid phase has a crucial impact on the heat transfer from the solid to the liquid. In this work, we proposed a promising method to enhance the heat transfer between a Cu surface and liquid water by applying surface charges to the surface, which was expected to change the structure of the interfacial nanolayer. We employed molecular dynamics simulations to verify the effectiveness of the method. Our simulations showed that applying surface charges led to an orientational alignment of water molecules, reducing the spacing between the solid surface and the interfacial nanolayer and increasing the number of water molecules located at the interface nanolayer. Meanwhile, the presence of surface charges also improves the mismatch of vibrational density of states between solid atoms and water molecules. As a results, the heat transfer was enhanced as compared with that without surface charges and the enhancement becomes more remarkeble when applying more surface charges to the Cu surface.

1. Introduction

The liquid in contact with a solid surface is found to be more ordered than the bulk liquid, and the liquid density at the solid-liquid interface is pronouncedly higher than that of the bulk liquid [1,2]. This solid-like nanolayer at the solid-liquid interface, acting as a bridge linking the bulk solid and the bulk liquid, has been shown to improve significantly the thermal transport between nanoparticles and base liquid and hence enhance the thermal conductivity of nanofluids [3–5]. Therefore, optimizing the interfacial nanolayer structure at a solid-liquid interface is expected to be an effective method for enhancing heat transfer between the solid and the liquid.

The studies [6–8] focusing on the structure of water nanolayer at charged solid surfaces showed that water arrangement considerably changes when surface charges are applied to the surfaces, and water molecules are reordered in the interfacial nanolayer extending several molecular diameters from the charged surfaces. However, these studies did not discuss the effect of the nanolayer structure changing on the thermal transport at solid-liquid surfaces. It is therefore interesting to determine whether the structure change in the interfacial nanolayer caused by surface charges affect the thermal transport between the charged solid surfaces and liquid, which is in favor of developing a new approach for enhancing heat transfer between the solid and liquid.

Molecular dynamics (MD) simulation is a powerful tool for investigating nanoscale thermal transport, providing valuable insights into energy transfer mechanisms at solid-liquid interfaces. Applying surface charges to solid surfaces was proposed to suppress the formation of vapor layer on high-temperature solid surfaces in our recent MD work [9]. The results showed that boiling heat transfer coefficient is enhanced significantly as compared with the case without the surface charges. However, the work did not analyze the effect of the changing of the interfacial nanolayer structure on the thermal transport, and hence the mechanism of heat transfer enhancement was not fully revealed.

In this work, a new method is proposed to enhance the heat transfer between a Cu solid surface and liquid water by applying surface charges to the surface. Molecular dynamics simulations

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are employed to verify the effectiveness of the method. The density profiles, orientation, and structure of water near the charged surface are analyzed to understand thermal transport mechanisms between the surface and water. At the nanoscale, the transmission of thermal energy across a solid-liquid interface is hindered by the acoustic mismatch between the atoms in the solid and liquid [10,11]. Therefore, the thermal mismatch of vibrational density of states between Cu atoms and water molecules is also calculated and discussed.

2. Model

The initial configuration of the system is shown in Fig. 1. The simulation cell is a cuboid box with dimensions of $12.80 \times 3.46 \times 3.46$ nm^3. A Cu plate with 3.80 nm thickness and 4200 atoms is placed in the center of the cell, and 3360 water molecules are placed on the two sides of the plate. Periodical boundary conditions are applied to all three direction of the box. The Cu plate is modeled by the face-centered cubic (FCC) unit with a lattice constant of 0.362 nm, and the Cu atoms in the center of the plate with 2.00 nm thickness are used as thermostat.

The extended simple point charge (SPC/E) water model is chosen because it adequately captures the properties of liquid water in MD simulations [12]. The H—O—H angle of 109.47° and the O—H bond length of 0.1 nm remain constant. The interaction of water molecules consists of the Lennard-Jones 12-6 and Coulombic potentials [9], expressed as,

$$U_{ij} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} \qquad (1)$$

where U_{ij} and r_{ij} are the potential energy and distance between particles i and j, q_i is the electric charge associated with site i, ε_0 is the vacuum permittivity, ε_{ij} is the well depth of the LJ potential, and σ_{ij} is the characteristic diameter. The interactions of Cu-Cu and Cu-water are modeled by Lennard-Jones 12-6 potentials. A spherical truncated method is adopted for the short-range and long-range forces with truncated distances of 10 Å. The particle-particle particle-mesh (PPPM) method [13] with an accuracy of 10^{-4} is used to modify the long-range Coulombic interaction. The SHAKE algorithm [14] is applied for water molecules to maintain their bond length and angle. The parameter values for water-water, Cu-Cu and Cu-water interactions are listed in Table 1.

To study the effects of surface charges on the heat transfer between the Cu plate and liquid water, the first Cu layers contacting with the liquid water are charged [15]. The surface charge density (σ) in our simulations is taken to be 0, ±0.27, ±0.54, and ±0.80 C m^{-2}, respectively. Liquid water and Cu plate with various surface charge densities are simulated in an NVT ensemble at T = 298 K to

Table 1
Values of L-J potential parameters and particles charge.

Particles i, j	$\sigma_{i,j}$ (Å)	$\varepsilon_{i,j}$ (eV)	q (e)
O—O	3.1660	0.0067	−0.8476
H—H	0.0000	0.0000	+0.4238
O—H	0.0000	0.0000	–
Cu—Cu	2.3377	0.4093	–
Cu—O	2.7519	0.0524	–
Cu—H	0.0000	0.0000	–

reach the equilibrium state using LAMMP (large-scale atomic/molecular massively parallel simulator) [16]. A run of 800 ps can ensure the equilibrium of the simulation system. When the system reaches equilibrium state, the temperature of Cu atoms near the heat source rises rapidly up to 360 K by a Nose-Hoover thermostat [17,18]. Single-phase heat transfer between the solid and the liquid water takes place, and the average temperature of the water is calculated to compare the difference of the heat transfer between the water and solid surface with or without surface charges. In the simulations, the particles motion is solved by the velocity-Verlet a lgorithm [19] with a time step of 1 fs, the positions and velocities of the particles are stored every 1 ps to analyze the results.

3. Analysis and discussions

Time evolutions of the water temperature for the Cu plates with or without surface charges are shown in Fig. 2. The water temperature is calculated based on Eq. (2) by summing the kinetic energy of water molecules.

$$\frac{1}{2}N_f kT = \sum \frac{1}{2}m_i v_i^2 \qquad (2)$$

where N_f is the total number of degrees of freedom of water molecules, k is Boltzmann constant, m_i is the mass of water molecule, and v_i is the center-of-mass velocity of water molecule. As shown in Fig. 2, the initial water temperature at t = 0 is 298 K for either the uncharged or the charged surface. Because the water is heated by the Cu plate with high temperature of 360 K, its temperature increases up to 355 K at 230 ps for the uncharged surface. However, for the Cu plates with surface charges of 0.27, 0.54, and 0.80 C m^{-2}, the water temperature increases to 355 K at 200 ps, 150 ps, and 120 ps, respectively. For the Cu plates with surface charges of −0.27, −0.54 and −0.80 C m^{-2}, the water temperature increases to 355 K at 190 ps, 130 ps, and 90 ps, respectively. It is noted that the water temperature increases more quickly for the higher positive or negative surface charges, indicating an increased heat transfer rate between the Cu plate and water due to the surface charges. In addition, applying negative surface charges yields a stronger heat
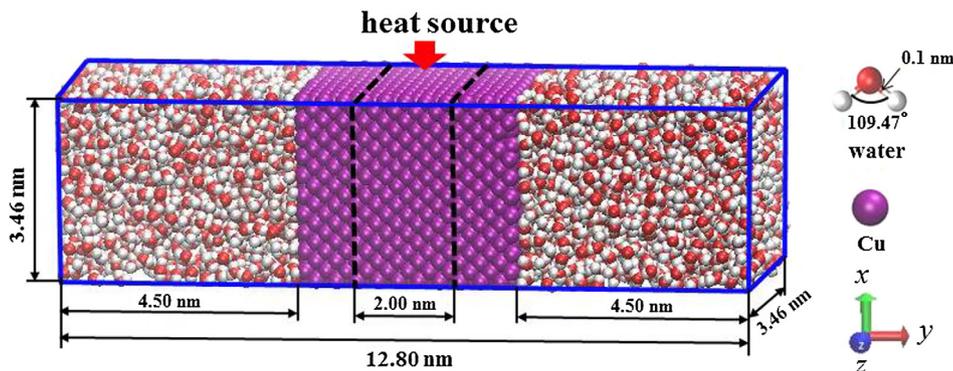

Fig. 1. Schematic of the simulation system.