

The Influencing Mechanism of Surface Wettability on Convective Heat Transfer in Copper Nanochannel

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ABSTRACT

Non-equilibrium molecular dynamics simulation is employed to probe the convective heat transfer of water flowing through a nanochannel. The wall-fluid interaction is considered as different values to characterize nanochannel wall with various surface wettability. The atomic microstructure, flow behavior and heat transfer characteristics are investigated. The results show that wall-fluid interaction plays an important role in interfacial fluid structure, density distribution, velocity slip, velocity distribution and temperature distribution as well as interfacial heat transfer. Adjusting the surface wettability of nanochannel wall will bring a significant impact on the heat transfer performance and flow properties. The increase of wall-fluid interaction enhances the first peak value of density and the main peak value of static structure factor. Thus, the interface velocity slip decreases, which is not beneficial to the reduction of flow resistance. In contrast, the nanochannel wall with the strong wall-fluid interaction is more similar to hydrophilic surface, and the heat transfer performance is better.

Keywords: nanochannel, surface wettability, water flow, heat transfer, molecular dynamics

NONMENCLATURE

Symbols

μ	Shear viscosity of fluid, Pa·s
u_x	Fluid velocity, m/s

L_s	Slip length, m
u_s	Slip velocity, m/s
$T_m(x)$	Fluid mean temperature, K
c	Specific heat capacity, J/kg·K
ρ	Fluid density, kg/m ³
$h(x)$	Heat transfer coefficient, W/(m ² ·K)
λ	Thermal conductivity, W/(m·K)
D_h	Hydraulic diameter, m
T_w	Wall temperature, K
L_k	Temperature jump length, m
<i>Greek symbols</i>	
ε	Energy parameter, J
σ	Length scale, m
<i>Subscript</i>	
x, y, z	Coordinate direction
s	Slip
w	Wall

1. INTRODUCTION

Due to the rapid development of industry and economy, countries all over the world are generally facing the severe energy situation. In addition to the development of new energy, how to increase the efficiency of current energy utilization has also attracted widespread attention. In various thermal energy utilization systems, the heat transfer enhancement is crucial for saving energy and reducing the cost of investment as well as improving the productivity [1]. Especially, with the wide application of micro/nano heat transfer devices, the mechanism investigation on micro/nanoscale heat transfer

enhancement is particularly urgent. As a form of nanoscale convective heat transfer, employing nanochannels for cooling is a promising method of thermal control in energy systems [2]. In conventional scale, heat transfer enhancement is usually at the cost of increasing flow resistance. Therefore, how to enhance heat transfer and reduce flow resistance is of great significance, which is also true for micro/nanoscale heat transfer. In addition, compared with the conventional heat transfer used in macroscale systems, the nanoscale heat transfer shows different flow and heat transfer characteristics. Specifically, the no-slip boundary condition gives way to the development of interfacial slip, and temperature jump derived from interfacial thermal resistance will not be ignored. Besides, the wall-fluid interaction becomes more prominent at the nanoscale, which will significantly affect the flow behavior and interfacial heat transfer in channel [3].

To further probe the microscopic mechanism of micro/nano scale heat transfer, molecular dynamics simulation has become a powerful tool to investigate flow behavior and heat transfer characteristics from the atomic level because of the limitation of experimental technology at the nanoscale. For example, Markvoort et al. [4] found that strong wall-gas interaction was conducive to convective heat transfer in nanochannel. Ge et al. [5] pointed out that the strong wall-fluid interaction was beneficial to heat transfer enhancement as well. Similar result was also demonstrated in the work of Sun et al. [6]. Wang et al. [7] probed the effect of wall material properties on the flow behavior and interfacial heat transfer in nanochannel. Song et al. [8] studied the effects of nanostructures on convective heat transfer in nanochannel with different periodic sinusoidal structures.

However, there are few studies on interfacial velocity slip and its effect on flow resistance in nanochannel. Actually, the low hydraulic diameter of nanochannel will cause a rather high flow resistance, and the effects of wall-fluid interaction on velocity slip and energy loss are unclear as well. Thus, one of the most significant issues concerning employing nanochannel for enhancing heat transfer is how to decrease the energy consumption to run the fluid through the nanochannels. Although in the work of Sun et al. [6], the effect of surface wettability on pressure drop in smooth nanochannel was discussed, the wall roughness was not considered. As the system dimension decreases, the roughness effect will be

amplified. Therefore, the flow resistance of convective heat transfer in rough nanochannel was investigated comprehensively in our previous work [9]. It was found that the strong wall-fluid interaction and rough nanostructure were beneficial for heat transfer enhancement, but were not conducive to the drag reduction.

It is worth mentioning that our previous studies [7, 9] concentrate on the heat transfer of simple LJ fluids in nanochannels. Generally, complex fluid such as water and solution are used as the most common heat transfer medium in practical applications. In this context, based on our previous studies, the convective heat transfer of water flowing through the copper nanochannel is performed in present work. The impacts of surface wettability on the atomic structure, velocity distribution, velocity slip as well as the temperature distribution and heat transfer in nanochannel are probed. The microscopic mechanism of surface wettability influencing water flow behavior and interfacial heat transfer are investigated. It will provide some new insights into the surface design of nanochannel and control of water flow behavior, which is beneficial to the application of nanochannel cooling in the field of energy efficient utilization.

2. GOVERNING EQUATIONS AND SIMULATION DETAILS

2.1 Basic governing equations

The velocity along the x -direction (flow direction) can be defined as Eq. (1):

$$\mu \frac{\partial^2 u_x}{\partial z^2} = \frac{\partial p}{\partial x} \quad (1)$$

Where μ is shear viscosity. u_x is fluid velocity along the x -direction, $\frac{\partial p}{\partial x}$ is pressure gradient in x -direction.

Generally, the slip length L_s is given by:

$$L_s = \frac{u_s}{\left. \frac{\partial u_x}{\partial z} \right|_{z=w}} \quad (2)$$

Where u_s and $\left. \frac{\partial u_x}{\partial z} \right|_{z=w}$ are the slip velocity and velocity gradient at the wall-fluid interface, respectively.

For convective heat transfer, the local mean fluid temperature $T_m(x)$ over the cross-section at different x position is defined as Eq.(3), and the local heat transfer coefficient $h(x)$ can be obtained as Eq. (4). The local

Nusselt number Nu_x can be calculated from Eq. (6) by combining Eq. (4) and Eq. (5).

$$T_m(x) = \frac{\int_0^H c\rho u_x(x,z)T(x,z)dz}{\int_0^H c\rho u_x(x,z)dz} \quad (3)$$

$$h(x) = \frac{\lambda}{(T_m(x) - T_w)} \left. \frac{\partial T}{\partial z} \right|_{z=w} \quad (4)$$

$$Nu_x = \frac{h(x)D_h}{\lambda} \quad (5)$$

$$Nu_x = \frac{D_h}{(T_m(x) - T_w)} \left. \frac{\partial T}{\partial z} \right|_{z=w} \quad (6)$$

Where c is specific heat capacity, $T(x,z)$ is fluid temperature along the x -direction. D_h is hydraulic diameter, ρ is fluid density, λ is thermal conductivity, T_w is wall temperature.

$\left. \frac{\partial T}{\partial z} \right|_{z=w}$ is temperature gradient at the wall-fluid interface.

The temperature jump length L_k can be defined as:

$$L_k = \frac{\Delta T}{\left. \frac{\partial T}{\partial z} \right|_{z=w}} \quad (7)$$

Here, ΔT is temperature jump at the wall-fluid interface.

2.2 Simulation details

The geometry of the system is presented in Fig.1, the channel wall is placed along the x and y direction with a length of $L_x=220\text{\AA}$ and $L_y=43\text{\AA}$, respectively. Each solid wall consists of ten layers with the total number of 14640 copper atoms. The channel height between the copper walls is $H=50\text{\AA}$. Water molecules are confined between two channel walls with the total number of 16128, and the fluid density is 1000kg/m^3 . Periodic boundary conditions are applied in the x - and y -directions, while the fixed boundary condition is applied in the z direction. Based on the previous study, the thermal pump method [10, 11] is introduced to the fluid domain and the convective heat transfer of cold fluid flowing through the hot nanochannel is achieved. Specifically, as shown in Fig.1, the force region is applied to the x -directional coordinates of $-18\text{\AA} < x < -11\text{\AA}$ and a driving force of $F_{\text{ext}}=1.4\text{pN}$ is imposed to water molecules located in force region. Moreover, the inlet temperature of 300K is generated in temperature resetting region of $-11\text{\AA} < x < 0\text{\AA}$ without disturbing the

directional flow [5, 12]. Besides, the temperature of channel walls is controlled at specified value of 350K.

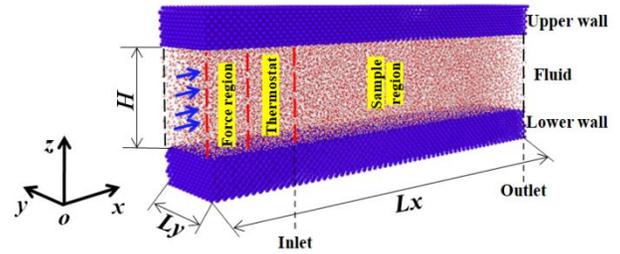


Fig 1 The schematic of the computational model

The TIP4P/2005 model is employed to describe the water molecule and the bond lengths and angles are fixed using the SHAKE algorithm. The interaction between water molecules and copper atoms are obtained by the Lennard-Jones (LJ) 12-6 potential based on the Lorentz-Berthelot rule. As shown in Tab.1, ϵ is energy parameter and σ is length scale for LJ potential.

Tab.1 LJ parameters of the solid and fluid atoms

	$\epsilon(\text{eV})$	$\sigma(\text{\AA})$	mass(g/mol)
Cu	0.410	2.338	63.5
O	0.0080	3.1589	15.9994
H	0.0	0.0	1.008

To investigate the effect of surface wettability on the flow and heat transfer characteristics, based on the interaction between the copper atoms and water's oxygen atoms $\epsilon_{\text{Cu-O}}=0.05738\text{eV}$ and $\sigma_{\text{Cu-O}}=2.7485\text{\AA}$, the wall-fluid interaction $\epsilon_{\text{sl}} = c\epsilon_{\text{Cu-O}}$ is adjusted to simulate different interfacial wettability with varying the value of c . Here, two cases are considered and presented in detail in Fig.2 with the wall-fluid interaction ϵ_{sl} are $0.25\epsilon_{\text{Cu-O}}$ and $0.025\epsilon_{\text{Cu-O}}$, which characterizes the hydrophilic and hydrophobic surfaces. As shown in Fig.2, a higher ϵ_{sl} characterizes a more hydrophilic wall surface, whose contact angle θ is smaller.

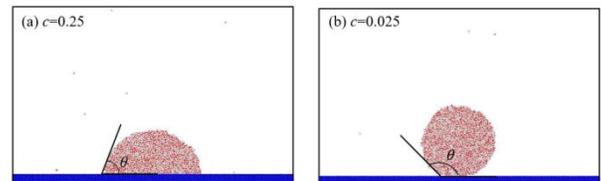


Fig 2 Contact angles with various surface wettability

All simulation cases are performed with a timestep of 1fs. Velocity Verlet method is used for integration of the Newton's equation. The entire system is firstly relaxed in canonical ensemble at 300K with 1 ns. Then, the second run of 2ns is performed to reach the steady

state with an external driving force. After that, the data collection is obtained over the last 6 ns.

2.3 Validation of numerical model

To verify the accuracy and reliability of present model, the simulation on convective heat transfer of argon fluid in smooth nanochannel was performed in our previous study [9]. As shown in Fig.3, the local Nusselt number obtained by present simulation model is in good agreement with that of literature results [5], which indicates that the present numerical model of convective heat transfer is accurate and reliable.

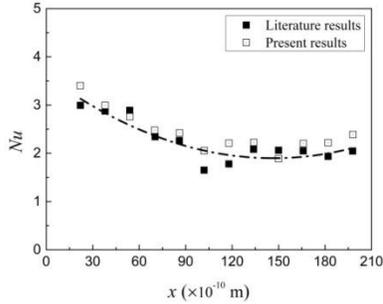


Fig 3 Comparison between the present model and the literature results.

3. RESULTS AND DISCUSSION

3.1 Velocity development and atomic structure

The fluid velocity distributions along the flow direction under the various wall-fluid interactions are shown in Fig.4. The mean velocity in nanochannel with weak wall-fluid interaction is greater than that in nanochannel with strong wall-fluid interaction by comparing Fig.4 (a) and Fig.4 (b). In addition, according to the definition of slip length, it can be observed that the slip velocity at the wall-fluid interface is greater under the weak wall-fluid interaction. All these phenomena are attributed to the strength of the interaction between fluid and solid wall. That is, the strong wall-fluid interaction makes more aggregation of water molecules near the wall and further hinders the movement of water molecules, which results in the decrease of the slip velocity and the velocity near wall as well as the mainstream velocity.

Fig.5 shows the density profiles in nanochannel under the strong and weak wall-fluid interactions, which well reveals the aggregation of fluid molecules. Just as shown in Fig.5, under the strong wall-fluid interaction, the density distribution near the wall has a greater peak value, indicating that there are more fluid molecules near the solid wall. As a result, owing to the existence of viscous friction between the fluid layers,

the movement of fluid along the flow direction is impeded, and the lower average velocity in nanochannel with the strong wall-fluid interaction is observed.

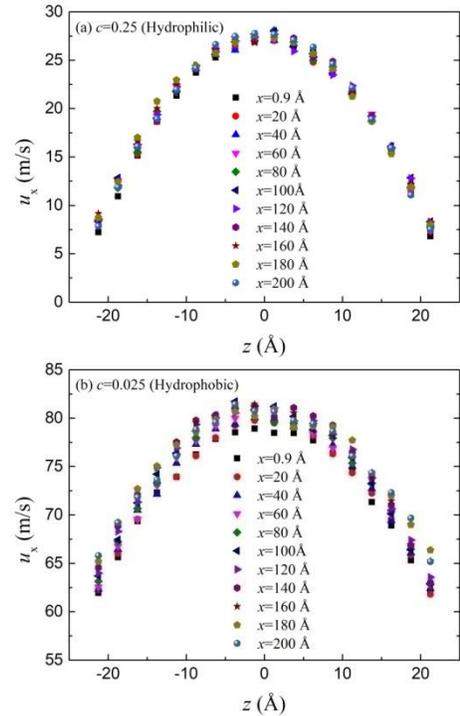


Fig 4 Velocity profiles along the flow direction

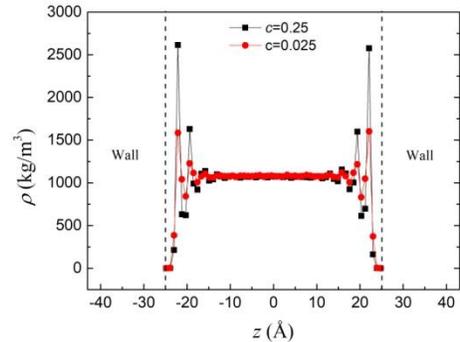


Fig 5 Density distributions along the nanochannel height

In addition, the effect of surface wettability on the slip length can be further proved by the static structural factor. According to the previous research, under the strong wall-fluid interaction, it is easier to form a "solid like" layer near the wall. Just as shown in Fig.6, this structural ordering in the first fluid layer near the wall can be quantitatively characterized by static structural factor. The larger the main peak value of static structure factor, the smaller the slip length. Under the weak wall-fluid interaction, the structural ordering is weakened, and fluid molecules move more freely near wall, which has a greater slip and is more conducive to drag reduction.

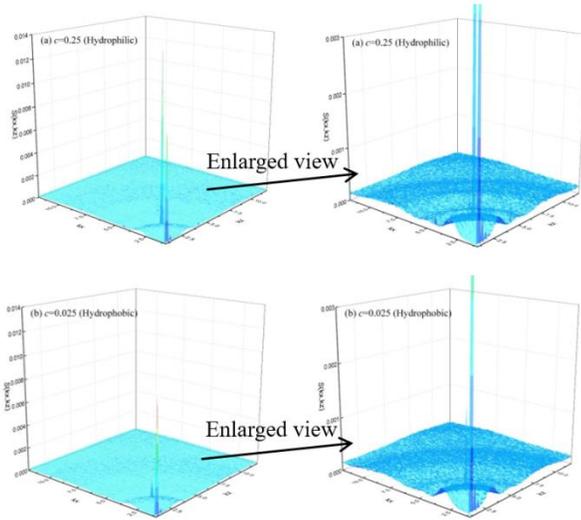


Fig 6 Static structure factor in the first fluid layer

3.2 Temperature development and heat transfer

Fig.7 shows the fluid temperature distribution along the flow direction under the various wall-fluid interactions. Obviously, when the fluid flows along the channel, the flow is in the thermally developing firstly and finally reaches the thermal-fully developed condition. Correspondingly, the fluid temperature along the x direction firstly increases, and then temperature profiles are almost overlapping and invariable.

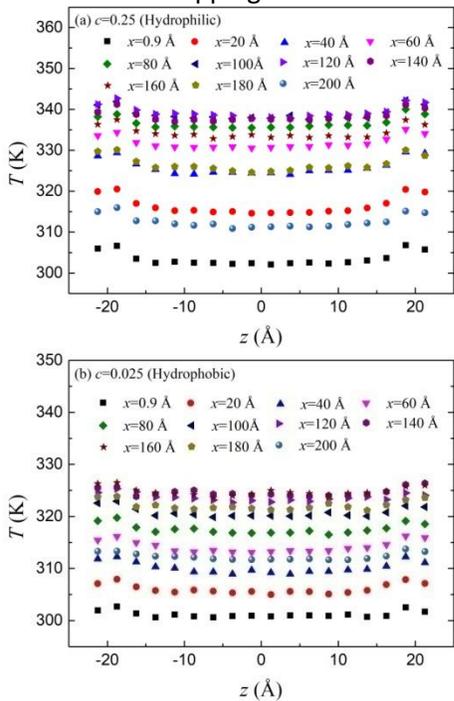


Fig 7 Temperature profiles along the flow direction

Moreover, the fluid temperature at the thermal-fully developed state under the strong wall-fluid interaction is higher, which indicates that the strong wall-fluid interaction is beneficial to interfacial heat

transfer, which makes the heat transfer more sufficient. The local Nusselt number in nanochannel under various wall-fluid interactions are shown in Fig.8. Obviously, with the increase of the wall-fluid interaction, the ‘solid like’ property of fluid molecules is strengthened, the interface thermal resistance is effectively reduced and the temperature jump decreases as shown in Fig.7 (a). Then, the local Nusselt number increases.

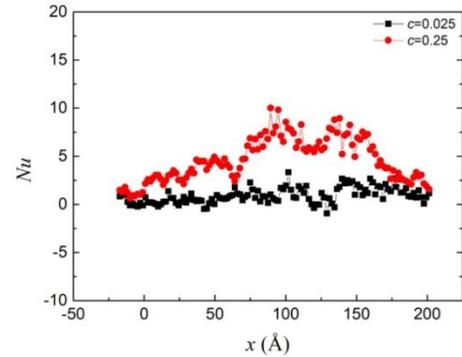


Fig 8 Variation trends of local Nusselt number under different surface wettability

4. CONCLUSIONS

In present work, the convective heat transfer of water flowing through a nanochannel is investigated. The influence of surface wettability on the flow characteristics and heat transfer is probed. Different surface wettability can be achieved by changing the wall-fluid interaction strength. It’s found that the surface wettability plays a significant role in affecting the interfacial fluid structure, flow behavior and heat transfer. With the increase of wall-fluid interaction, the structural ordering of the first layer of fluid molecules near wall is enhanced, the first peak value of fluid density increases, and more fluid molecules are gathered near channel wall. Due to the friction derived from the nanochannel wall and inner friction within fluid molecules, the interface velocity slip and fluid velocity in nanochannel decrease, which is conducive to the sufficient heat exchange between fluid molecules and channel wall. Therefore, the strong wall-fluid interaction is conducive to obtain the better heat transfer, but is not beneficial to the drag reduction.

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