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Nano-scale liquid film sheared between strong wetting surfaces: effects of interface region on the flow[†]

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Abstract

In this paper, we use molecular dynamics (MD) simulations to investigate changes in fluid flow at a solid/liquid interface. The flow is driven by shearing FCC structured solid molecular walls under isothermal conditions using previously developed interactive thermal wall models. For the nano-scale thin liquid film flows, a fluid molecular layer attached to the wall molecules behaves as an extended wall layer, which induces increased shearing in the middle of the fluid by reducing the width of the flow region. Small variations in molecular diameter length at the interface significantly affect flow characteristics. Shear locking on strong wetting surfaces caused by the dynamic structuring of fluid molecules (i.e., the fluid molecules layering on the solid surface due to the wall force field) increases the density and viscosity and decreases the shear rate and the heat dissipation ratio on the interface, which are important in nano-scale fluid flow analysis.

Keywords: Nano-scale fluid flow; Solid-liquid interface; Shear locking; Liquid layering; Boundary slip

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1. Introduction

Nano-/micro-scale liquid flow on solid surfaces is an important part of micro/nano-fabrication processes (i.e., photoresistant coating), liquid film lubrications, drug delivery, and selective absorption [1]. However, the mechanisms of nano-scale thin film flows and interface phenomena on the solid substrates are not fully understood. Experimental evidence [2] shows that a strong wetting surface results in dynamic structuring of the fluid near the solid surface as the thin liquid film flows and advances as a series of distinct molecular layers. For such sub-micro/-nano scale fluid flows, the layering of the fluid molecules on the strong wetting surface is an important factor influencing fluid properties at the solid/liquid interface, including the density, viscosity and thermal conductivity [3, 4]. For nano-scale thin film fluid flows, the surface effects dominate the nano-scale conduits due to their miniscule dimensions compared to the force penetration distance induced by the intermolecular force fields of the wall molecules. Investigations of momentum transport at liquid-solid interfaces have shown velocity-slip and -stick conditions depending on the wall-fluid interaction strength, fluid/wall density, and shear rate [5-9]. Recent studies have shown that the thermal oscillation and crystal bonding stiffness of solid molecules affect the slip length for specific surface wettabilities [10, 11]. In addition, significant variations in the diffusion coefficient, shear viscosity, and thermal conductivity have been reported depending on the wall/fluid interaction strength [12-14]. In particular, the layering of fluid molecules on strong wetting surfaces is a well-known phenomenon. However, the influence of layered liquid molecules on flow properties of strong wetting interfaces has been less frequently studied compared to liquid slips on weak wetting interfaces. Layering (Dynamic structuring) of fluid molecules on the solid surface is not prominent in most macroscopic problems but is important in multi-scale methods or nano-scale fluid flow problems where the continuum approach breaks down and the analysis is sensitive to variations on the interface/flow boundary layer [15, 16].

This study demonstrates variations in viscosity, shear rate, and heat dissipation as a function of wettability caused by the dynamic structuring of fluid molecules on strong wetting surfaces with shear locking (Negative slip). Our MD simulation implements coupled molecular modeling of momentum and heat transport in the flow to calculate the properties above. In order to investigate changes in fluid flow on a molecular scale, we performed molecular dynamics (MD) simulations, driving the flow by shearing FCC molecular walls under isothermal conditions using a previously developed interactive thermal wall mode [17] with various strong surface wettabilities but the same wall shearing conditions.

2. Theoretical background and model description

In the case of shear driven flow, the momentum and heat

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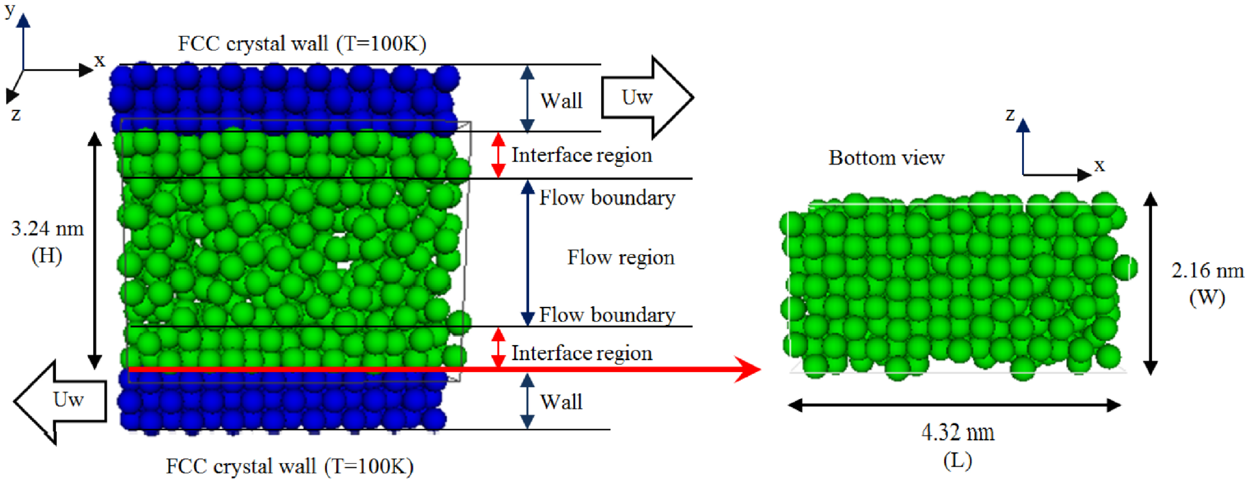


Fig. 1. Schematic and dimensions of MD simulation domain and the bottom view of FCC-like structured first liquid molecule layers for strong wetting walls ($\varepsilon_{wf}/\varepsilon_{ff} = 4$).

transport happen simultaneously. In addition to the slip or locking phenomena on the interface, there is a work done by viscous forces that cause heat inside the flow and that heat is need to be dissipated through the wall. Since the energy imparted on the fluid was dissipated by the fluid as viscous heating, while constant wall temperature applied on the surface enabled heat loss through the walls. Hence, the coupled molecular modeling of momentum and heat transport is essential. In this background, we investigate the coupled momentum and heat transfer in shear driven nano-channels by utilizing a previously developed interactive thermal wall model [17], which efficiently simulates thermal interactions between fluid and wall molecules by modeling the walls with crystal bond springs with stiffness K. A thermostat is applied separately to each wall layer. Higher-order velocity moments are calculated, and the local thermal equilibrium is verified with walls of two different temperatures and imposed thermal gradients.

To conduct MD simulations of shear driven flow with viscous heating, simple molecular liquids were simulated in a 3D channel with height (H) 3.24 nm, width (W) 2.16 nm, and length (L) 4.32 nm, as shown in Fig. 1. The number density ($\rho^* = N\sigma^3/\Omega$) of the system was $\rho^* \approx 0.8$, which corresponds to the liquid state of argon around 100 K [18]. We used the Lennard-Jones (LJ) potential as

$$V(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

where the mass of an argon molecule is $m = 6.63\times10^{-26}$ kg, the molecular diameter is $\sigma = 0.3405$ nm, and the depth of the potential well (ε) is $119.8\times k_b$ (1.6539×10^{-21} J). Intermolecular interaction forces were truncated and switched to zero at a cut-off distance of 1.08 nm (approximately 3σ). We used the velocity Verlet algorithm for time integration [19]. The characteristic time $\tau_c = \sigma\sqrt{m/\varepsilon}$ was 2.16×10^{-12} s, and the simulations used 4 fs ($\sim 0.002\tau$) time steps. The channel height corresponded to approximately 10σ, where both the interface phenomena and bulk fluid behavior are observable [24], and was extended to 40σ for the cases of large length compared to molecular diameter. The simulation domain has interactive thermal walls [17] with perfect FCC crystals with (001) surfaces on the fluid molecules. The top and bottom wall temperatures were set to 100K (isothermal walls), and no thermostat was applied to the liquid flow because the heat generated by viscous heating was dissipated through the interactive thermal walls. For the shear driven flow, the characteristic wall velocity (U^*) was set to $U^* = 0.5\sqrt{\varepsilon/m}$ (Approximately 79 m/s). For the given channel height, fluid density and wall velocity, our simulations were within the linear response regime [8]. Periodic boundary conditions were imposed in the x and z directions for both the solid walls and the liquid molecules. The velocity, shear rate, viscosity and heat dissipation ratio were obtained using 10 slab bins (Numbered 1~10 from bottom to top) positioned parallel to the walls. The 0th and 11th bins represented the bottom and top walls, respectively. Simulations were started from the Maxwell-Boltzmann velocity distribution for both the liquid and the walls, and 2×10^5 time steps (0.8 ns) were used to reach a steady state, after which another 4×10^5 time steps (1.6 ns) were performed for time averaging. Prior to data collection, a longer time averaging period was performed to confirm convergence of the statistical data profiles to the steady state.

The strong wetting wall surface case, where the ratio between wall/fluid interaction strength (ε_{wf}) and fluid/fluid interaction strength (ε_{ff}) is 4, exhibited significant variations in shear rate. These variations induce drastic increases in density and viscosity near the surfaces, which has previously been reported [9, 13, 20-23]. Fig. 1 is also a snapshot of the steady state of the shear-driven flow for the strong walls. There is strong evidence of dynamic structuring of the liquid molecules on the solid surface, and there is almost no flow in the two

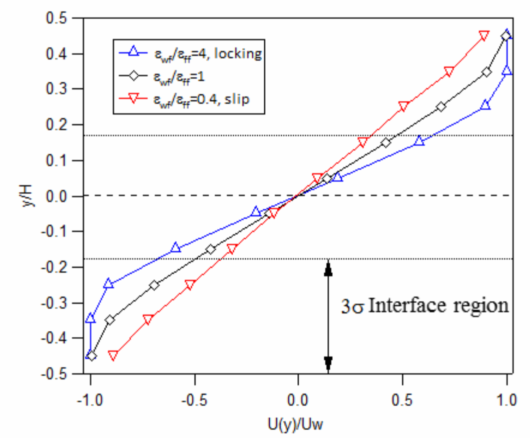


Fig. 2. Velocity profiles (H = 3.24 nm) using 10 slab bins with strong, normal or weak wetting solid/liquid interfaces showing shear locking and velocity slip at interface.

layers of liquid molecules where are defined as the interface region. FCC-like structured liquid molecules at the bottom of the liquid bulk is scrutinized by removing the bottom walls from the visualization. However, these structured layers are not observed for weak wetting walls. Therefore, it is necessary to separately define the interface region and flow boundary region for the strong wetting walls. Different surface wettability values at the wall/liquid interface results in velocity-slip or -stick on the boundary, which induces different shear rates in the middle of the fluid region, even under the same shearing velocity. Under such conditions, liquid molecules are dynamically structured, with a certain number of layers corresponding to the wall force penetration depth and interaction strength. Such behaviors have been shown previously [8]. However, this study demonstrates variations in fluid properties corresponding to gradual changes in strong surface wettability in the flow, which induces dynamic structuring of the liquid molecules on the interface.

In this study, we kept the wall force penetration depth constant at σ but varied the strength of the wall force by varying the L-J potential depth ratio between the wall/fluid and fluid/fluid ($\varepsilon_{wf}/\varepsilon_{ff}$) from 0.4 to 4, where 0.4 is a weak wetting wall, 1 is normal and 4 is strong. For data collection based on molecular degrees of freedom, bin sizes smaller than the molecular diameter are questionable for comparisons to the continuum regime [3]. Therefore, we used bin sizes comparable to the molecular diameter and investigated the finest velocity profiles corresponding to the variation in wall/fluid interaction strength, as shown in Fig. 2. The first two bins represent the interface region, the next two bins correspond to the flow region, and the two middle bins are used for the middle of the flow region, where the wall forces have the least effect. With a strong wetting wall, the interface region shows similar velocities for fluid molecules and wall molecules, which mean that the fluid molecules are attached to the wall and travel with the wall molecules. As the fluid molecules behave like extended layers of the walls, the shear rate in the strong wall case is increased more than in the normal and weak wetting wall cases. For shear flows with nano-scale thin liquid films, the fluid molecules attached to the wall molecules are considered as an extended wall layer, which induces an increased shear rate in the middle of the fluid region by reducing the width of the flow for the shearing wall velocity. In nano-scale fluid flow, boundary variations of a few molecular diameter lengths significantly affect the characteristics of the flow region, as shown in Fig. 2. In particular, the shear rate in the flow region is increased because the layering induces an increased shear rate in the flow region (Middle of the fluid). For strong wetting walls with fluid layering, layered fluid molecules result in narrower channel width as they reduce the thickness of the flow region, and the narrower channel width together with the same shearing wall velocity induces an increased shear rate.

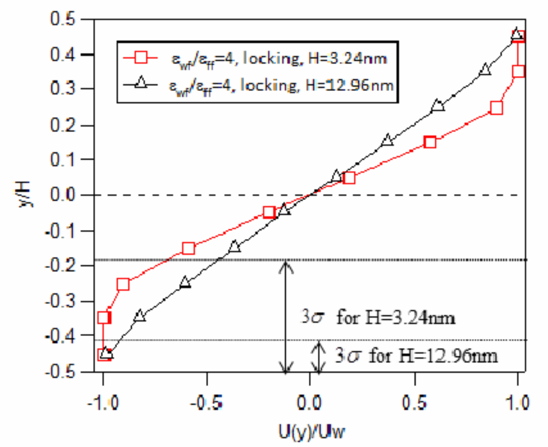
3. Results and discussion

3.1 Slip/shear locking at the interface

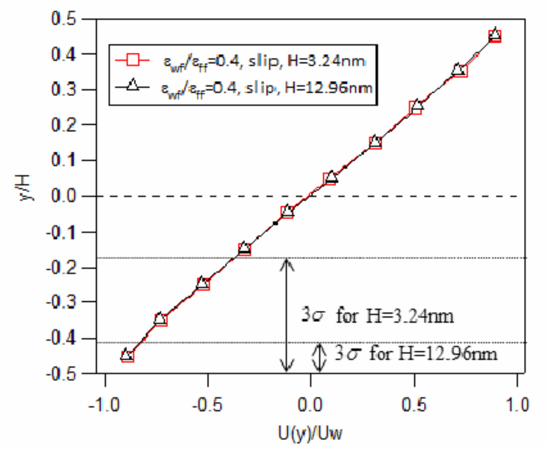
Many previous works [1, 5, 9, 11, 15] have shown that a no-slip boundary condition is not ideal in molecular flow. In our MD simulation results using 10 slab bins with either a strong, normal or weak wetting interface, as shown in Fig. 2, the boundary flow either locks or slips depending on the wall/fluid interaction strength. For weak wall/fluid interactions, the fluid molecules on the interface slip and form a slip length. However, in most cases, the wall force affects the fluid molecules in the region affected by the interaction strength. Therefore, the liquid layering significantly affects the flow boundary conditions. The strong wall/fluid interaction causes the fluid molecules near the wall to be captured on the interface and form liquid layers to a depth of two or three molecular diameter. This region has a higher fluid density and viscosity than other flow regions and shows different shear and heat dissipation rates. Therefore, an investigation of the variations in fluid properties over the different fluid regions (Interface, boundary and flow regions) caused by gradually varying the wall/fluid interaction strength is essential for understanding nano-scale fluid flow behavior.

In order to observe the behavior of layered liquid molecules in the vicinity of the wall markedly, we obtain normalized liquid density by using bins that are 10 times smaller than the molecular diameter [3]. Investigations of liquid density distributions along the channel have shown that the interface region has a higher fluid density than other fluid flow region [3, 9, 21], and the layering of fluid molecules varying in number density is a well-known effect of the neighboring wall molecules [24]. The other properties of nano-scale fluid flow with the variations of wall surface wettabilities such as shear rate, viscosity, and heat dissipation rate will be discussed in next section.

In nano-scale fluid flow, it is important to clarify the effects of channel widths greater than the molecular scale. The velocity profiles for shear driven flow with weak and strong wetting



(a) Strong wetting surfaces



(b) Weak wetting surfaces

Fig. 3. Velocity profiles for strong wetting surfaces for H=3.24 and 12.96 nm (a); and weak wetting surfaces for H=3.24 and 12.96 nm (b) at constant shear rate.

walls at a constant shear rate in a 12.96 nm channel are shown in Fig. 3. For the weak wetting interface with slip, shown in Fig. 3(b), velocity is the same for the four times thicker liquid film at the same shear rate. However, in the strong wetting case shown in Fig. 3(a), the shear rate decreases with increased channel height, where the interface region thickness is negligible compared to the liquid film thickness. On the other hand, velocity is significant at molecular flow scales, where the interface region and wall penetration depth are comparable to the flow width. Moreover, it should be noted that the thickness of interface region is independent to height of channels; increase in channel height does not increase the interface region thickness as showed in Fig. 3. Liquid molecules fluctuate and form dynamic structuring near the strong wetting surface due to the solid-liquid interaction and local liquid-liquid interaction. Moreover, the wall force penetration depth was kept at constant while the height of channel was increased. Therefore, variation of channel height has no effect on the thickness of interface region. We also gradually increased the interaction strength ($\varepsilon_{wf}/\varepsilon_{ff}$) from 0.4 to 4 and observed the velocity changes in both the interface and flow boundary regions. Fig. 4 shows the variations in the velocity profiles for different wall surface wettabilities in both the boundary/interface and flow regions. The figure shows the transition from locking to slipping as we decrease the surface wettability; even with slipping, there is slight evidence of a wall force in the 2nd bin. For cases of locking where the wettability is greater than 2, there is almost no flow in the 1st and 2nd bins, and the liquid molecules in the 3rd bin are still affected by the wall force fields, while a continuum analysis would predict a linear velocity profile.

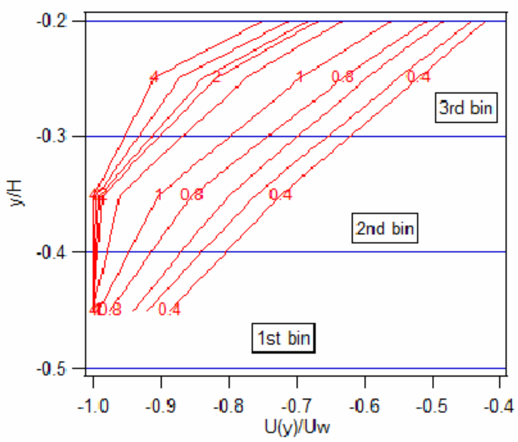


Fig. 4. Variations in shear rate according to wall surface wettability in both the boundary/interface and flow regions. In the transition from locking to slipping and in the slipping case, there is a slight evidence of the wall force in the 2nd bin.

3.2 Liquid properties with a strong wetting wall

In MD simulations with a solid-liquid interface, the effects of interaction strength on the interface and the disorder of the lattice crystal surface with stationary liquids have been frequently investigated. We, on the other hand, studied the influence of the interface interaction strength under flow conditions. We varied ε_{wf} from $0.4\varepsilon_{ff}$ to $4\varepsilon_{ff}$ with the crystal bonding stiffness fixed at $K=3K_w$ [25]. This modification mainly affects the attractive portion of the L-J potentials. Fig. 5 shows the shear rate variations in the boundary/interface and flow regions in log scale. A rapid decrease of the shear rate in the interface region as the surface wettability increases was observed, with a shear rate of almost zero when the interaction strength ratio (surface wettability) is greater than 2. This means that the two layers of liquid molecules at the interface do not flow and behave like solid layers which form a distinctive flow boundary extended from the walls. Therefore, the shear rate increases with narrowing flow width in the flow region (with the shearing wall velocity kept constant). In our previous work, we found that a strongly attractive wall ($\varepsilon_{wf}>2\varepsilon_{ff}$) also enhances heat transfer at the interface, with the thermal resistance length (Kapitza length) reduced almost to zero [25]. Moreover, weakened at-

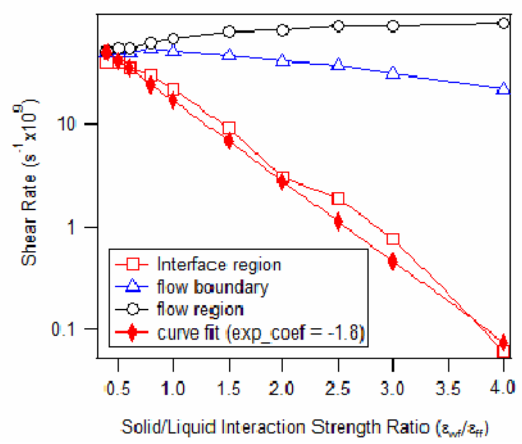


Fig. 5. Shear rate variations in both the boundary/interface and flow regions with log scale and fitted curve.

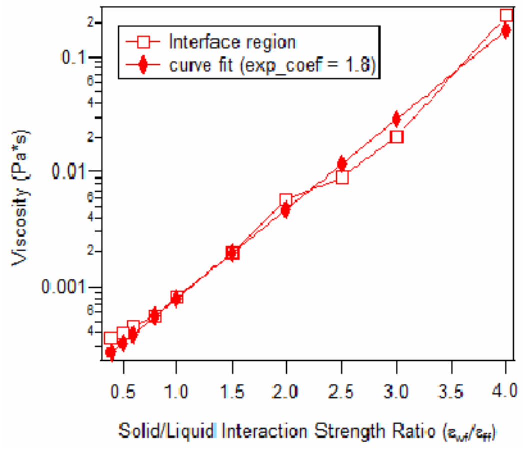


Fig. 6. Viscosity variations for different wall surface wettabilities in the interface region with log scale and fitted curve.

tractive interactions exponentially increase the Kapitza length (L_K). A previous study [25] approximated that $L_K \propto \exp(-1.85\varepsilon_{wf}/\varepsilon_{ff})$ for $0.4 \le \varepsilon_{wf}/\varepsilon_{ff} \le 3$, which corresponds to ranges between extremely weak and strong interactions. This range was chosen so that there was a finite limit for the interface thermal resistance, even if the attractive interaction was reduced to zero. Even with the weakest interaction, the thermal resistance should persist under strong repulsive forces that prevent the overlap of molecules [26]. In addition, a strong liquid/solid interaction results in layering of the fluid molecules, which may change the thermal conductance [27]. Similar exponential behavior is shown in the shear rate, which deceases with surface wettability. The exponential decrease of the shear rate at the interface region was found significantly in Fig. 5. The fitted curve has an exponential coefficient of -1.8, where the exponential coefficient for the Kapitza length is -1.85 [25]. Another work modeled the Kapitza length with various solid/liquid interaction strengths and found an exponential coefficient of about -1.9 [26]. In a recent study, the interaction strength between solid and liquid molecules was shown to affect equally all components of the interfacial thermal resistance acting on each degree of freedom. However, the kinetic energy transfer due to molecular motion in the direction perpendicular to the surface is a major component of thermal transport at the interface [28]. In the case of interface thermal resistance on the solid-liquid interface, the wall-fluid interaction strength ($\varepsilon_{wf}/\varepsilon_{ff}$) for the intermolecular stiffness related to the virial calculation [3] becomes the sole parameter representing the interfacial thermal resistance. Therefore, under the identical FCC crystal wall configurations, we investigated whether other liquid properties (Shear rate and viscosity) show similar behaviors, which would mean that the modeling coefficient is a wall property which is not limited to thermal analysis.

The viscosity of a stationary liquid on the solid-liquid interface has been previously investigated by several researchers [3, 14, 20]. With a strong wetting wall, the layered fluid molecules caused by the dynamic structuring affect the fluid's viscosity and increase the local shear stress on the wall surface. However, a layered structure is not caused by the liquid molecule interaction strength but by the wall force. Therefore, the increased viscosity of a liquid in the interface region due to the wall force under flow conditions is an interesting observation. Fig. 6 shows changes in local viscosity calculated using Eq. (7) from Ref. [3] at the interface region for different wall-fluid interaction strengths. A log-scale increase in viscosity corresponding to the increased wall-fluid interaction strength with an exponential coefficient of 1.8 was obtained. Both viscosity and shear rate variations affect the local shear stress acting on the solid surface and are crucial in the spread and flow of thin liquid films on solid substrates. Interestingly, the shear rate, viscosity and interface thermal resistance all show a similar exponential dependence on surface wettability. Therefore, this exponential behavior is a characteristic of wall crystal structure type and density and can be considered a characteristic property that affects liquid behavior.

Increased surface wettability also enhances the heat transmission ratio at the solid-liquid interface [29]. For strong attractive walls, MD studies have shown that the layering effects of the liquid molecules next to the surface and the layered structure go through a transition as the interaction strength changes when the liquid is in a stationary state [30]. In addition, the structural changes of the layered molecules also change the thermal conductance at the interface [27]. For heat dissipation, the shear flow generates viscous heating, and the heat generated dissipates through the wall boundary. Heat dissipation is an important physical phenomenon on the interface. When there are no electronic contributions or net flow in the system, thermal motion becomes the sole contributor to thermal conductivity [31]. Fig. 7 shows a log scale curve fit with an exponential coefficient of -1.8 of heat dissipation rate [3] in the interface region for different wall surface wettabilities. Meanwhile, Fig. 8 shows the corresponding temperature profiles. The changes are less significant in the middle of the fluid region, but the interface region shows a logarithmically

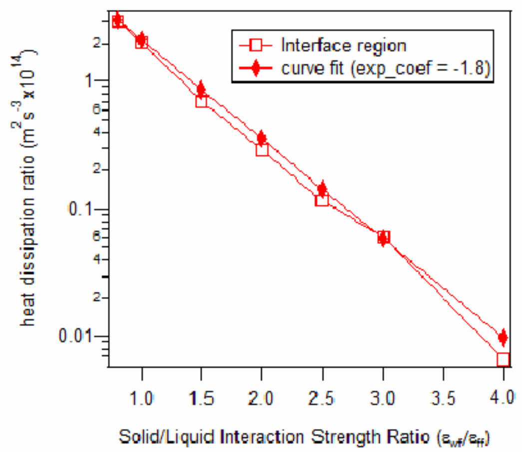
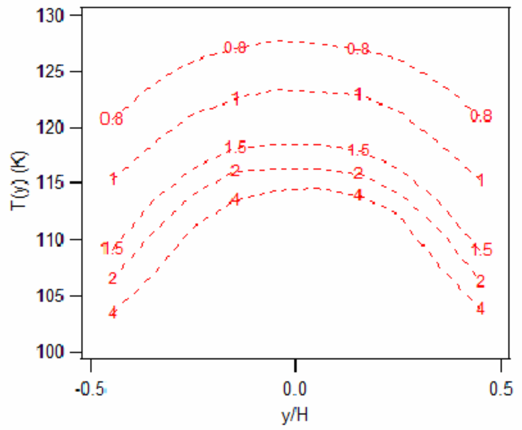
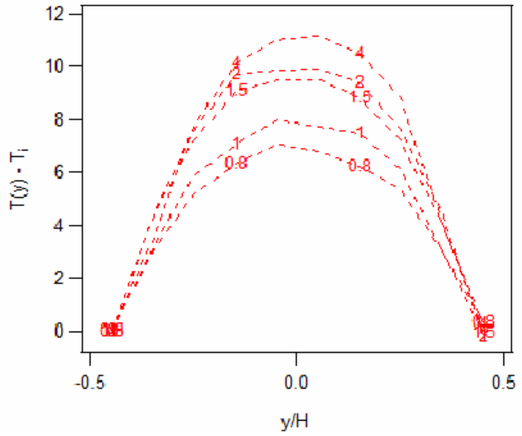


Fig. 7. Heat dissipation rate for different wall surface wettabilities in the interface region with log scale and fitted curve.



(a) Temperature profiles for different $\varepsilon_{wf}/\varepsilon_{ff}$



(b) Temperature profiles showing T(y)-$T_{interface}$

Fig. 8. Temperature profiles due to viscous heating and heat dissipation through the walls for different wall surface wettabilities (a); and temperature profiles showing T(y)-$T_{interface}$ for temperature gradient comparisons on the flow boundary (b).

decreasing heat dissipation ratio. As shown in Fig. 8(a), there are various parabolic temperature profiles which include temperature jumps at the interface, even under the same sharing wall conditions. Fig. 7 shows that the heat dissipation ratio decreases as the surface wettability increases, and Fig. 8(b) shows the temperature difference from the interface temperature for each temperature profile, so that the thermal gradient can be compared under different surface wettabilities. We found that the thermal gradient was steeper in the interface/boundary region with increased surface wettability.

4. Conclusions

Our MD simulation results show that both strong and weak wetting solid/liquid interfaces induce boundary flows that either lock or slip, depending on the wall/fluid interaction strength. Shear locking on strong wetting surfaces caused by the dynamic structuring of fluid molecules (Fluid molecule layering due to the wall force) induces increased density and viscosity and decreased shear rate and heat dissipation ratio, which are critical in nano-scale fluid flow analysis. The velocity of interface region shows almost same to wall velocity, which means the fluid layers behave as an additional wall layer. Boundary length variations of a few molecular diameters significantly affect the characteristics of nano-scale fluids in the flow region, where the decreased shear rate in the interface region due to layering induces increased shear rate in the flow region (The middle of the fluid). The result for viscosity, shear rate and heat dissipation ratio shows log-scale increase corresponding to the increased wall/fluid interaction strength. The variations in viscosity and shear rate affect the local shear stress acting on the solid surface and are crucial in the spread of the thin films. We also found significant changes in the heat dissipation rate in the middle of the fluid region, while the heat dissipation rate in the interface region decreased logarithmically with wall/fluid interaction strength. Interestingly, the shear rate, viscosity and interface thermal resistance all showed a similar exponential dependence on surface wettability. Thus, this exponential behavior is a characteristic of wall crystal structure type and density and can be used to model liquid behavior in the interface region.

Acknowledgment

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Nomenclature

H : Channel height
W : Channel width
L : Channel length
k_b : Boltzmann constant
ρ* : Number density ($\rho^* = N\sigma^3/\Omega$)
V : Interaction potential function
σ : Diameter of molecules (zero potential distance)

ε : Depth of LJ potential
r_{ij} : Distance between ith and jth molecules
τ : Characteristic time
m : Mass of molecules
K : Crystal bonding stiffness
L_K : Kapitza length
U^* : Characteristic wall velocity
U_w : Velocity of the wall

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