Fast increase of wall slip in supercooled water: the key role of dynamics

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Cooling down water in its supercooled regime has been widely considered to better understand the bulk transport properties of this ubiquitous liquid. Here we apply the same approach to investigate the wall slip induced by low interfacial friction, a key factor in the performance of nanofluidic systems. Specifically, we investigated the temperature dependence of friction and slip for water and methanol on model Lennard-Jones walls and on graphene. Surprisingly, although interfacial friction and viscosity in bulk follow the same fundamental laws and are proportional at high temperatures, the relation of proportionality breaks down in the supercooled regime. This implies that wall slip, controlled by the ratio between viscosity and friction, increases in the deep supercooled regime – by up to a factor of 5 for water on graphene. Whereas most previous studies have focused on the role of static features of the interface, here we focus on the intriguing role of dynamics. We find that the interfacial density relaxation of the fluid – and how it evolves with respect to the bulk one – governs the temperature dependence of wall slip. Overall, exploring the temperature dependence of water-wall slip provides new insight on its molecular mechanisms, and can also shed light on the bulk transport properties of water.

INTRODUCTION

Nanofluidics, i.e. the study of fluidic transport at nanometer scales, has emerged as a new and interesting field in the past few decades due to novel behaviors associated to this length scale [112] – e.g. dielectric anomalies of confined water [3] or exotic ionic transport [46], with promising applications related to new 2D materials such as the development of sustainable energies [7, 8]. As confinement increases, interfacial properties have an increasingly important role. An interfacial characteristic of special concern at the nanoscale is the existence of a velocity jump \( \Delta v \) (‘slippage’) at the liquid-solid interface [911]. The simplest approach to describe slip, initially proposed by Navier [12], is to consider that the viscous shear stress \( \tau \) in the liquid at the wall is proportional to the velocity jump, \( \tau = \lambda \Delta v \), where \( \lambda \) is the liquid-solid friction coefficient.

Several efforts have been pursued in order to understand the molecular mechanisms that control friction, with special interest on the discussion of the relation between the friction coefficient and the time autocorrelation of the force exerted by the liquid on the wall [1319]. Further work has been performed to study the impact on friction of different wall features such as wettability [20, 21], roughness [22], crystallographic orientation [23], electronic structure [24], or electrostatic interactions [25]. Yet a large number of questions with regard to the interface properties, such as its viscoelastic or purely viscous nature [20, 28] or the possible link with its interfacial thermal transport equivalents via wall’s wetting properties [29, 31], remain open nowadays, limiting the perspectives for a rational search of optimal interfaces.

Among all fluids, the study of water has always been of special concern for scientists from a broad variety of research fields [3254]. Its interest not only lies on its ubiquitous nature but also on its many thermodynamic and dynamic anomalies like, among others, the non-monotonous temperature dependence of its isothermal compressibility and density [35, 36]. These anomalies are enhanced when water is driven to its supercooled regime (i.e. the range of temperatures below the freezing point where water keeps its liquid state), making this regime ideal to test and refine our current understanding of water. In particular, the temperature dependence of the transport properties of bulk water has been thoroughly explored over the last decade [37, 38], considering especially the connection between viscosity and structural relaxation times [39, 43]. In contrast, the temperature evolution of water friction remains unclear nowadays. Several questions can be explored with that regard, such as the impact of different surfaces or liquids on \( \lambda \), or its relation with the corresponding bulk transport property, i.e. viscosity.

In that context, we report a study in which the temperature dependence of liquid-solid friction and of bulk liquid viscosity are examined in detail, in connection to the dynamical behavior of interfacial liquids in the supercooled regime. To this end we perform extensive molecular dynamics (MD) simulations of water and methanol on graphene and generic Lennard-Jones surfaces. We find that whilst the liquid-solid friction coefficient and the viscosity follow the same fundamental laws and are proportional to each other at room temperature and above, their behavior in the supercooled regime is strikingly different. For the widely studied system of water on graphene, this implies that the slip length is enhanced up to five times in the deep supercooling regime, reaching \( \sim 230 \) nm at 225 K. Our analysis reveals that the dynamics of inter-
facial water, specifically the time relaxation of the interfacial density fluctuations, is the most important factor governing the temperature behavior of liquid-solid friction and slip. This fundamental mechanistic insight sheds new light on the general molecular mechanisms underlying water slip.

**MD SIMULATIONS**

All the simulations were carried out with the LAMMPS package [44]. The confined system consists in a fluid – TIP4P/2005 water [15] or methanol (MeOH) [46, 47] – between two parallel walls – graphene, or a generic hydrophobic wall made of Lennard-Jones (LJ) particles – with periodic boundary conditions applied in the directions parallel to the walls (Fig. 1), see details in SI Appendix. The surfaces were characterized by contact angles of $\theta \sim 134^\circ$ for water-LJ walls, $\theta \sim 80^\circ$ for water-graphene, $\theta \sim 100^\circ$ for MeOH-LJ walls and $\theta \sim 0^\circ$ for MeOH-graphene.

The wall dimensions were $L_x = L_y = 58.92 \, \text{Å}$ for the LJ wall, and $L_x = 56.57 \, \text{Å}$, $L_y = 58.92 \, \text{Å}$ for graphene. The pressure was set to 1 atm by using the top wall as a piston during a preliminary run; the vertical height was then obtained by fixing the top wall at its equilibrium position for the given pressure and it corresponded to $H \sim 40 \, \text{Å}$ for water and $H \sim 90 \, \text{Å}$ for MeOH. The temperature $T$ was varied between 225 and 360 K, by applying a Nosé-Hoover thermostat to the liquid (only along the directions perpendicular to the flow for non-equilibrium simulations). Equivalent results were obtained for different damping times, and with a Berendsen thermostat.

To measure the hydrodynamic transport coefficients we performed non-equilibrium molecular dynamics (NEMD) simulations, applying a constant shear velocity $U$ to the walls in opposite $x$ directions for each wall (see Fig. 1), producing a linear velocity profile far from the wall. The friction coefficient was measured from the ratio between the shear stress $\tau$ and the velocity jump at the interface $\Delta v$ – defined at the effective wall position $z_s$ [15]: $\lambda = \tau/\Delta v$, and the viscosity was measured from the ratio between the shear stress and the bulk shear rate, $\eta = \tau/\langle \partial_z v_x \rangle$, see SI Appendix for details.

Both interfacial and bulk equations can be combined in the so-called partial slip boundary condition [49].

$$\Delta v = \frac{\eta}{\lambda} \partial_z v_x \big|_{z=z_s} = b \partial_z v_x \big|_{z=z_s},$$  

(1)

defining the slip length $b := \eta/\lambda$. Viscosity and friction have been measured for 3 different shear velocities for each temperature, $U \in [1, 70] \, \text{m/s}$ in order to verify that our measurements where performed in the linear response regime. For a given shear velocity, 3 independent simulations were run and we measured the shear stress at the top and bottom walls for each of them. Overall, 18 independent measurements were taken for a given $T$ and the error bars in this article correspond to the statistical error within 95% of confidence level.

**RESULTS**

We first computed the shear viscosity $\eta$ from NEMD with LJ walls to test the applicability of the different temperature dependence laws, Vogel-Tammann-Fulcher (VTF), Speedy-Angell (SA) and Bässler (B) laws, see SI Appendix. For TIP4P/2005 we find good agreement between our data and the experimental ones [37, 50], as well as previous MD simulations with the TIP4P/2005 and TIP4P/2005f water models [47, 51, 52]. Our viscosity measurements are best described by VTF law (see SI Appendix). For MeOH simulations viscosity’s temperature dependence is weaker than for water. The results are in good agreement with previous work [47] and they are well described by an Arrhenius law.

We then proceeded to explore temperature effects on friction. For each fluid, when varying the wall type, we already saw a difference at a given temperature in the absolute value of $\lambda$, being more than one order of magnitude smaller for graphene than for LJ walls (see SI Appendix). This effect has already been measured and discussed in previous work [24, 53, 54] and it is due to the extreme smoothness of graphene. Additionally, in Fig. 2 one can see that the temperature dependence changes with the fluid, but for a given fluid, depends weakly on the wall type. Interestingly, the temperature dependence of $\eta$ and $\lambda$ can be fitted by the same laws (VTF for TIP4P/2005 and Arrhenius for MeOH, corresponding to continuous lines in Fig. 2), although with different parameters.

We can go further in exploring the relation between $\eta$ and $\lambda$ by plotting the slip length $b$ given by the ratio between both transport coefficients, see (1). In Fig. 3 one can see that for a wide range of high temperatures (between 270 K and 360 K), $\eta$ and $\lambda$ vary together with $T$,
so their ratio (or equivalently the slip length) is roughly constant. However, \( \eta \) grows faster than \( \lambda \) when we lower the temperature further and the liquid enters in its supercooled regime, resulting in an abrupt increase of \( b \) at low \( T \). The biggest temperature effect on \( b \) is observed for water and graphene walls where it grows by a factor of 5 from the highest to the lowest temperature, reaching a maximum value of 230 nm. Although experimentally it is difficult to reach such low temperatures, some experiments have already managed to supercool water down to 230 K \([27]\). This high value of slip opens the door to new striking possibilities, with the performance of supercooled nano-(/micro-)fluidics among them. Two main questions remain then to be understood. First, what is the main physical parameter that controls the temperature evolution of the friction coefficient observed in Fig. 2? Second, why bulk and interface have a similar temperature dependence at high temperatures and why they don’t at the lower ones (Fig. 3)? Because the effect of temperature is larger for water, from now on we will focus on this liquid to address these questions.

**DISCUSSION**

In order to better understand the molecular mechanisms that control friction temperature dependence, \( \lambda \) can be related to the autocorrelation of the equilibrium force at the interface through a Green-Kubo formula \([13, 55]\):

\[
\lambda = \frac{1}{k_B T} \int_0^\infty \langle F(t) F(0) \rangle \, dt,
\]

where \( A \) is the surface area, \( k_B \) the Boltzmann’s constant, \( T \) the temperature and \( F \) the force applied by the fluid on the wall. This expression can be decomposed as a product of static (“\( \lambda_{\text{STAT}} \)”) and dynamical (“\( \lambda_{\text{DYN}} \)”) terms of the form – see Ref. \([20]\) and SI Appendix:

\[
\lambda = \lambda_{\text{STAT}} \cdot \lambda_{\text{DYN}}, \quad \text{with}
\]

\[
\lambda_{\text{STAT}} \approx S(q_\parallel) \int_0^\infty dz \rho(z) f_{q_\parallel}^2(z)
\]

\[
\lambda_{\text{DYN}} \approx \frac{\tau_z}{2k_B T}
\]

where \( S(q_\parallel) \) is the 2D structure factor in the contact layer, evaluated at the shortest wave vector of the solid surface \( q_\parallel \), \( \rho(z) \) is the fluid number density, \( f_{q_\parallel}(z) \) is the force corrugation and \( \tau_z \) is the density relaxation time defined as the integral of the intermediate scattering function in the contact layer taken at \( q_\parallel \): \( \tau_z = \int_0^\infty dt F(q_\parallel, t) \). The contact layer was defined as the liquid region between the wall and the first minimum of the liquid’s density profile. Note that we included the \( 1/(k_B T) \) term of the Green-Kubo integral in the dynamical part; we will come back to that choice later. Regarding the static terms in \([3]\), we found that \( S(q_\parallel) \) remained constant with temperature for both graphene and LJ walls (see SI Appendix). The main static contribution to friction \( T \) dependence comes from the integral in \([3]\). We used for \( f_{q_\parallel}(z) \) the analytical expression derived in \([50]\) for LJ walls and the measurements in \([53]\) for graphene (as detailed in SI Appendix). For both surfaces, the integral remains constant at low temperatures, and then increases by at most a factor of 2 at higher temperatures. Therefore, this temperature behavior does not explain the exponential decrease for increasing temperature observed for friction. It is only left to check the dynamical contribution from \([3]\), enclosed in \( \tau_z \). To measure this parameter we fitted the intermediate scattering function following Ref. \([57]\):

\[
F(q, t) = \left[ 1 - A(q) \right] e^{-t/\tau_z}^2 + A(q) e^{-(t/\tau_z)^\gamma},
\]
considering two characteristic time-scales: at short times with \( \tau_s = \tau_s \Gamma(1/2)/2 \) and at long times with \( \tau_\alpha = \tau_\alpha \Gamma(1/\gamma)/\gamma \), where \( \Gamma(x) \) is the Euler function. \( \tau_\beta \) was found to be constant with \( T \), while \( \tau_\alpha \) exponentially decreases with \( T \) (see SI Appendix). \( \tau_p \) is then defined as the integral of \( \frac{1}{\tau_s} \), i.e. \( \tau_p = (1 - A(q)) \tau_\beta + A(q) \tau_\alpha \). \( \tau_p \) data are well described by a VTF law, analogous to friction, showing that the density relaxation is the main interfacial molecular mechanism that controls friction’s temperature evolution. With that regard, in previous work on bulk supercooled liquids [39, 41–43, 58–60], it is not obvious what time should the viscosity be related to; usually, only \( \tau_\alpha \) is considered, and often an effective \( \tau_\alpha \) is defined as the time for which the self or coherent intermediate scattering function equals \( 1/e \). For friction however, it is clear in the derivation of (3) that the total relaxation time \( \tau_p \) should be used [22], and indeed, [3] predicted correctly the relative temperature evolution of \( \lambda \) only when using \( \tau_p \) (see SI Appendix, where large differences between the different relaxation times are reported). Note finally that [3] failed to reproduce \( \Lambda \) quantitatively: this is reminiscent of similar quantitative discrepancies reported in previous work using analogous approximations of the full Green-Kubo expression of \( \lambda \) [53, 61].

To then understand the temperature dependence of the slip length \( b = \eta/\lambda \), we will decompose the viscosity into a static and a dynamical part in the same manner as for the friction coefficient: \( \eta = \eta_{\text{STAT}} \times \eta_{\text{DYN}} \), with \( \eta_{\text{DYN}} = \tau_p^{\text{bulk}}/(2k_BT) \) – in analogy with the definition of \( \lambda_{\text{DYN}} \), and with \( \eta_{\text{STAT}} = \eta/\eta_{\text{DYN}} \). The slip length can then be decomposed as follows:

\[
b = \frac{\eta}{\lambda} = \eta_{\text{STAT}} \frac{\eta_{\text{DYN}}}{\lambda_{\text{DYN}}} \cdot \frac{1}{\lambda_{\text{STAT}}}. \tag{5}
\]

Figure 4 illustrates the temperature evolution of the three contributions to \( \lambda \) for water on LJ walls and graphene. In this figure, the lines are obtained from the ratios between VTF fits of the simulation results for \( \eta, \lambda, \tau_\rho \) and \( \tau_p^B \); specifically, \( \eta_{\text{STAT}} \propto T \eta/\tau_p^B \), \( \eta_{\text{DYN}}/\lambda_{\text{DYN}} = \tau_p^B/\tau_p^B \), and \( \lambda_{\text{STAT}} \propto T \lambda/\tau_p^B \). One can observe in Fig. 4 that \( 1/\lambda_{\text{STAT}} \) increases when decreasing \( T \) for both interfaces. As detailed in SI Appendix, the stronger temperature variation of \( \lambda_{\text{STAT}} \) for the LJ walls can be related to the larger extension of the density profiles toward the wall at high temperatures. In bulk, \( \eta_{\text{STAT}} \) remains constant at high \( T \), but it increases significantly when water enters its supercooled regime, for \( T \lesssim 273 \, \text{K} \), becoming the main contribution to \( b \) significant increase in the same \( T \) region. As a side note, following our choice to include \( 1/(k_BT) \) in \( \eta_{\text{DYN}} \), the fact that \( \eta_{\text{STAT}} \) is constant in the liquid state corresponds to \( \eta \propto \tau_p^B/T \); we suggest this correlation could replace more traditional ones used when studying supercooled liquids, \( \eta \propto \tau_\alpha \) or \( \eta \propto T \tau_\alpha \) [39, 41, 43, 58, 59].

Finally, to understand the relative increase of \( b \) by \( \sim 2 \) times for the LJ wall and by \( \sim 5 \) times for graphene, we looked at the dynamic ratio \( \eta_{\text{DYN}}/\lambda_{\text{DYN}} \). In Fig. 4(right), one can see that for LJ walls the interface relaxation time increases more when decreasing \( T \) than the bulk one, compensating the static contribution and resulting in a smaller \( b \) variation. In contrast, for graphene, due to the surface smoothness, there is no contribution from the wall to the slowing down of the interface dynamics with \( T \) when compared to the bulk dynamics. Therefore, as for the temperature dependence of \( \lambda \), we conclude that also with regard to \( b \) it is not the different interfacial structures which contribute to its \( T \) evolution but the different dynamics.

Before concluding, we would like to comment on a prediction for the temperature dependence of \( b \) introduced by Bouquet and Barrat [11], who wrote that \( b \) should be proportional to \( (k_BT)^2/\lambda_{\text{STAT}} \), in contrast with our results. This formula can be derived from (3) by relating the density relaxation time \( \tau_p \) to the collective diffusion coefficient \( D_{\eta_l} \): \( \tau_p = 1/(\eta_l^2 D_{\eta_l}) \), and by identifying \( D_{\eta_l} \) with the self-diffusion coefficient \( D_0 \), itself related to the viscosity through the Stokes-Einstein relation: \( D_0 \propto k_BT/\eta \). However, while we found that indeed \( D_{\eta_l} \approx D_0 \) at room temperature, their temperature evolution is quite different, specially in the supercooled regime (see SI Appendix). Indeed, both diffusion coefficients arise from processes that happen at different scales and their relation is non-trivial: while \( D_{\eta_l} \) is related to collective diffusion in the sense that it comes from the density Fourier transform integration to all atoms positions, \( D_0 \) is referred to the diffusion of one molecule of \( \sigma_l \) size.

CONCLUSIONS

In this work we investigated the temperature evolution of bulk and interfacial hydrodynamic transport coefficients for water and MeOH confined between LJ walls and graphene. For a given liquid, the temperature evol-
tion of viscosity and friction were described by the same laws, although with different parameters. The temperature evolution of interfacial friction was weakly affected by the wall type, but changed significantly with the liquid type. We then compared the temperature evolution of viscosity \( \eta \) and friction coefficient \( \lambda \) by considering their ratio, defined as the slip length \( b = \eta / \lambda \). We observed, from higher to lower \( T \), that both transport coefficients evolved together in the high temperature region but that viscosity increased faster than friction at low \( T \), implying a growing slip length in the supercooled regime, by up to a factor of 5 for water on graphene. At 225 K we reported a giant slip length of 230 nm for water on graphene; although we are aware of the experimental difficulties to supercool water at such low temperatures, successful experiments have been reported down to 230 K \[37\], and we suggest that beyond liquid-solid slip, many other exotic behaviors could arise in the future field of supercooled nanofluidics.

In order to understand the molecular mechanisms that control friction, we decomposed the friction coefficient \( \lambda \) into the product of a static contribution \( \lambda_{\text{STAT}} \) and a dynamical one \( \lambda_{\text{DYN}} \), in the form of an interface density relaxation time \( \tau_\rho \). We observed a small variation of the static part with \( T \), but the main contribution to the temperature dependence of friction came from the dynamical term. Finally, in order to explain the temperature dependence of the slip length \( b = \eta / \lambda \), we also decomposed the viscosity \( \eta \) into a static term \( \eta_{\text{STAT}} \) and a dynamical term \( \eta_{\text{DYN}} \), controlled by the bulk density relaxation time \( \tau_B \). The slip length could then be decomposed into three contributions: first, the interfacial static contribution \( 1/\lambda_{\text{STAT}} \); second, the bulk static contribution, \( \eta_{\text{STAT}} \); and third, the relation between the bulk and interfacial dynamical terms \( \eta_{\text{DYN}}/\lambda_{\text{DYN}} = \tau_B/\tau_\rho \). We observed that the viscosity static part, while it remained constant at high temperature, increased significantly in the supercooled regime, representing a major contribution to the slip length temperature evolution. We could finally relate the different slip length temperature dependence on LJ walls and graphene to the difference in interfacial dynamics on these two surfaces. Interestingly, for water, two decay times are necessary to describe the decay of the intermediate scattering function (a short time, \( \tau_B \), and a long time, \( \tau_\alpha \)). While previous work on bulk supercooled water explored correlations between viscosity and \( \tau_\alpha \) only, we showed that friction should be correlated to the total relaxation time \( \tau_\rho \); coming back to the bulk, we observed in the liquid state a correlation \( \eta \propto \tau_B^B/T \) differing from the ones usually considered in previous work, \( \eta \propto \tau_\alpha \) or \( \eta \propto T \tau_\alpha \) \[39, 43, 58, 59\].

Overall we hope the findings obtained here by investigating water friction at extreme temperatures will help understanding generally the molecular mechanisms underlying both interfacial and bulk hydrodynamic transport in this fascinating liquid.

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