Relation between boundary slip mechanisms and water-like fluid behavior

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Abstract

The slip of a fluid layer in contact with a solid confining surface is investigated for different temperatures and densities using molecular dynamic simulations. We show that for an anomalous water-like fluid the slip goes as follows: for low levels of shear, the defect slip appears and is related with the particle exchange between the fluid layers; at high levels of shear, the global slip occurs and is related to the homogeneous distribution of the fluid in the confining surfaces. The oscillations in the transition velocity from the defect to the global slip is shown to be associated with changes in the layering distribution in the anomalous fluid.
I. INTRODUCTION

The no-slip condition is the assumption that the fluid velocity is zero when in contact with the solid confined geometry. For a macroscopic flow this is a trustworthy boundary condition, and it is fundamental for the continuum theory validity. For confined geometries the hydrodynamic equations are no longer valid and, in this case, the use of the no-slip boundary condition is at least questionable. Many experimental [1–8], theoretical and computational results [9–15] report that there are several flow boundary conditions consistent with the fluid behavior and mobility [16–19] beyond the no-slip boundary condition. The amount of slip is usually measured through the magnitude of the slip length, defined as the ratio between the shear rate and the slip velocity [16–19]. For most liquids the slip length increases with the shear rate and stabilizes at $v_0$ [19]. Its value, however, depends on the thickness of the confining system in a non trivial way. For apolar materials, such as the hexane [20] and the n-decane [17, 19], the slip length increases with the film thickness. However, for the polyamide-6,6 [21] and for water [22] the slip length decreases with the increase of the film. Complementary the behavior of the shear viscosity gives the slip length. For the n-decane the viscosity increases with the increase of the film thickness [23] while for polyamide-6,6 [21] the viscosity decreases with the increase of the film.

For water the situation is even more complex. Confined water in microchannels presents a slip length in the order of nanometers [24–28] and therefore no-slip boundary conditions is no applicable. As the channel size decreases, water mobility increases [29–32]. The slip length for nanochannels becomes of the order of micrometers what implies that the use of no-slip boundary conditions could be problematic.

Even thought the qualitative behavior of the slip length is known, the specific value of the slip length is widely scattered. In the particular case of water, it depends on the surface energy and roughness, the fluid temperature and density [26, 33–42]. Then, a strategy to understand this qualitative behavior is to explore the mechanism behind the change of the slip with the shear rate, if the slip occurs through one single process or if it involves a number of steps which depend on the velocity. In the case of apolar Lennard-Jones fluids the slip changes through two mechanisms: the defect slip and the global slip [16–19]. The transition from the defect to the global slip occurs at a shear rate $v_0$. Therefore for a given fluid and wall, the slip length depends on the temperature and density from the behavior of
v₀. Unfortunately very little is known about the behavior of v₀.

Here we add another component to this already complex problem. We explore the mechanism behind the liquid slip in the case of anomalous water-like fluids. An anomalous fluid is characterized by having a maximum in the density versus temperature at fixed pressure and a maximum and a minimum in the diffusion coefficient versus pressure at constant temperature [43–48]. Under high confinement, these fluids exhibit additional anomalous behaviors and new phases [49, 50]. When an anomalous fluid is nanoconfined the thermodynamic and dynamic properties differ from the properties observed in the bulk [29–31, 51]. For instance, for the bulk system the fluid is described as homogeneously distributed. This is not the case for the confined systems. The water-like fluid forms layers which depend on the film thickness [49, 50, 52–55]. Due to the layering, particles have different behavior at different layers, what allow for the anomalous flux observed in confined water-like materials.

In this paper we investigate the slip mechanism of a water-like fluid. After testing the fluid for the defect slip and global slip transition at v₀, we study the connection between the behavior of v₀ at different temperatures and densities with the structure and dynamics of the layers.

The water-like fluids is modeled by an effective potential with two length scales separated by an energy barrier. The use of an effective potential allows us to explore a large range of the temperature versus density phase diagram. Molecular dynamics simulations of the planar Couette flow for this anomalous fluid test the presence of defect and global slip at different densities and temperatures. This paper goes as follows: section II presents the model and simulation details, section III shows the results and the section IV has the conclusions.

II. THE MODEL, SIMULATION AND METHODS

A. The model

The water-like fluid is confined in a planar Couette geometry shown in the figure 1. Each plate is formed by Nₚ = 676 spherical particles of diameter σₚ, organized in two planar layers, forming a face centered cubic lattice, with Lₓ = Lᵧ = 20.2σₚ and Lₜ = 0.7σₚ, as shown in the figure 1. The separation between the plates, or channel height, is d. The liquid is sheared by moving the bottom bounding wall (plate 1 in the figure 1) with the speed vₓ while the
The top bounding wall (plate 2 in the figure) is held fixed. The contact layer, is composed by fluid particles whose centers of mass lie between the plate 2 and the first minimum in the density profile.

![Diagram of water-like fluid confined within parallel plates](image)

**FIG. 1.** (Color online) Schematic representation of water-like fluid confined within parallel plates. The y-direction is omitted.

The particles at the plates are tethered to its lattice site by a linear spring with constant \( k^* = k [\sigma^2_{w}/(m\varepsilon)]^{1/2} = 50 \) and characteristic excursion \( \xi = \sqrt{k_B T/k} \) \[56\], where \( k_B \) is the Boltzmann constant, and \( T \) is the plate temperature. The particles at the plates also interact with each other via a standard Lennard-Jones (LJ) 12-6 potential with \( \varepsilon \) depth and \( \sigma_p \) \[54, 58\]. The fluid is modeled by \( N_w = 500 \) identical water-like particles with diameter \( \sigma_w = \sigma_p \). The fluid particles interact through a core-softened potential given by \[46, 47\]

\[
U_w (r_{ij}) = 4 \left[ \left( \frac{\sigma_w}{r_{ij}} \right)^{12} - \left( \frac{\sigma_w}{r_{ij}} \right)^6 \right] + u_0 \exp \left[ -\frac{1}{c_0^2} \left( \frac{r_{ij} - r_0}{\sigma_w} \right)^2 \right].
\]

This potential presents two length scales which consists of a standard Lennard-Jones 12-6 potential (LJ) plus a Gaussian centered at \( r_0 \), with width \( c_0 \) and depth \( u_0 \), where \( r_{ij} = |\vec{r}_i - \vec{r}_j| \) is the distance between fluid particles \( i \) and \( j \) \[46, 47\]. Varying the parameters \( u_0, c_0, r_0 \) and \( \sigma_w \) this potential can represent a whole family of intermolecular interactions. In this work the chosen parameters are \( u_0 = 5.0, c_0 = 1.0 \) and \( r_0 = 0.7\sigma_w \). For these parameters the potential presents one scale at \( r_{ij} \approx 1.2\sigma_w \) and other scale at \( r_{ij} \approx 2\sigma_w \), being each scale related to the interaction between two water tetramer clusters, as shown in the illustration of the force in the figure \[59, 60\]. The bulk system of spherical particles interacting through
FIG. 2. (Color online) Left axis: isotropic effective potential as a function of the particle separation (blue solid line). Right axis: force related to the effective potential as a function of the particle separation (orange dashed line).

this potential exhibits diffusion, structural and density anomalous behavior observed also in bulk water \[46, 47\].

The particles of this water-like fluid interact with the wall particles through the purely repulsive potential given by the Weeks-Chandler-Andersen Lennard-Jones (WCA) potential \[61, 62\]

\[
U_{wp}(r_{ij}) = \begin{cases} 
U_{LJ}(r_{ij}) - U_{LJ}(r_c) ; & r_{ij} \leq r_c \\
0 ; & r_{ij} > r_c 
\end{cases},
\]

where \(U_{LJ}\) is a standard 12-6 LJ and \(r_c\) is cutoff distance \((r_c = 2^{1/6}\sigma_{wp})\). The effect radius, \(\sigma_{wp}\), is determined through Lorentz-Berthelot mixing rule \((\sigma_{wp} = (\sigma_p + \sigma_w)/2)\) and is used when one fluid particle is interacting with one wall particle \[63\]. The repulsive fluid-plate interaction causes an excluded volume, therefore the fluid effective density will be \(\rho = N_w/[(d - \sigma_{wp})L_xL_y] \[64, 65\].

B. The simulations

The system was studied by Molecular Dynamics (MD) simulations at constant \(NVT\) through a homemade program. Nosé-Hoover heat-bath with coupling parameter \(Q = 2\) was
applied at the plates particles in order to maintain the temperature fixed \[66, 67\]. The system was analyzed for different densities and heat-bath temperatures. The temperature varies from \(T^* = k_B T/\varepsilon = 0.025\) up to \(T^* = 0.650\), and \(\xi\), varies from 0.022 up to 0.110. \(N\) is fixed and the density decreases by increasing the distance between the plates from \(d^* = d/\sigma_w = 3.8\) to \(d^* = 9.8\). The initial configuration of the confined fluid is set on the solid state and, without shear (\(\vec{v}_x = 0\)), further equilibrated over \(5 \times 10^5\) steps. Then, in order to obtain the temperature versus density phase diagram of the confined system, \(2 \times 10^6\) steps were performed. The transversal pressure, \(P\), is computed analogously to bulk pressure \[68\]

\[
P = \rho k_B T + \frac{1}{V} \langle \nu_\perp \rangle ,
\]

where \(\nu_\perp\) is the transversal Virial expression,

\[
\nu_\perp = -\sum_i \sum_{j>i} \frac{z_{ij}^2}{r_{ij}} \left( \frac{\partial U_w(r_{ij})}{\partial r_{ij}} \right).
\]

Next, the bottom bounding wall moves with a constant speed \(\vec{v}_x\). For each density and temperature, several simulations with wall velocities varying from low shear levels, \(v^*_x = v_x (m/\varepsilon)^{1/2} = 0.001\), up to high shear levels, \(v^*_x = 15.0\) (where the bottom wall velocity is about five times greater than the fluid thermal velocity) were carried out. The fluid heats up due to shear and the system reaches a new equilibrium temperature after \(3 \times 10^5\) steps. Since the equilibrium temperature of the fluid depends on shear level, the temperature used in the graphs is the heat-bath obtained from the thermostat fixed at the wall. After the equilibration, additional \(8 \times 10^6\) steps were performed to store physical quantities for the system with shear. The structure of the water-like fluid in the contact layer was analyzed through the parallel radial distribution function, \(g_{\parallel}(r_{xy})\). This distribution function is defined as \[64\]

\[
g_{\parallel}(r_{xy}) \equiv \frac{1}{\rho^2 V} \sum_{i \neq j} \delta(r_{xy} - r_{ij}) \left[ \theta(|z_i - z_j|) - \theta(|z_i - z_j| - \delta z) \right],
\]

where \(r_{xy}\) is the parallel distance between particles, and \(\theta(z)\) is the Heaviside function which limits the particle sum in a layer of thickness \(\delta z\). The fluid structure was also analyzed through the translational order parameter, defined as \[69\]

\[
t \equiv \int_0^{\xi_c} |g_{\parallel}(\zeta) - 1| d\zeta,
\]
where $\zeta_c = 0.5 L_x \rho_l^{1/2}$ is the cutoff distance set to half of the simulation box times density of the contact layer, and $\zeta = r_{xy}(\rho_l)^{1/2}$ is the distance $r_{xy}$ in units of the mean interparticle separation in the parallel direction. The translational order parameter measure how structured is the system. For ideal gas, $t = 0$ and for more structured phases, $t$ increases.

The equations of motion were integrate with a time step $\delta t^* = \delta t [\varepsilon/(m \sigma^2 w)]^{1/2} = 0.0025$, and five independent runs were used to evaluate the confined anomalous fluid properties. All the quantities are given in Lennard-Jones units and, for simplicity, the symbol (*) employed in the dimensionless quantities is excluded.

C. The slip boundary conditions

Usually confined systems are analyzed employing no-slip boundary condition in which the mean velocity of the fluid particles in the contact layer is zero. Even though the no-slip boundary condition is good to describe confinement up to microchannels, this might not be the case for nanoconfined geometries. Different slip conditions mechanisms might occur as the relative velocity between the fluid and the wall is changed. For the planar Couette flow two boundary slip mechanisms are predicted for non-anomalous fluid: the defect slip and the global slip. The defect slip depends on the local and ordered hops of the fluid particles at the contact layer. These hops occur due to the presence of disorder in the ground state of the wall-fluid interaction which obeys an Arrhenius dynamics. The global slip occurs when all fluid particles of the contact layer are in movement detached from the wall.

It is possible to verify the occurrence of these boundary slip mechanisms by analyzing the average particle motion. In the no-slip condition the particles oscillate around the minimum of the ground state of the particle-wall interaction. In this case the fluid particles in the contact layer have no preferential direction of movement. For the slip condition the movement of fluid particles in the contact layer is in the driven direction. Then, to compute this move, we compute the probability of one particle moving in the driven direction, $P_{DD}$, defined as

$$P_{DD} = \frac{100}{S} \sum_{i=1}^{S} \left[ \frac{\sum_{j=1}^{N_{CL}} \left[ x_{j(i)} - x_{j(i-1)} \right] \sigma_{ij}}{\sum_{j=1}^{N_{CL}} \left| x_{j(i)} - x_{j(i-1)} \right|} \right],$$  

(7)

where $S$ is the number of simulation steps, $N_{CL}$ is the number of fluid particles in the contact
layer, \( x_j(i) - x_j(i-1) \) is the displacement of particle \( j \) between the steps \( i-1 \) and \( i \), and \( \sigma_{ij} \) is a piecewise function. If the displacement is in the driven direction \( (x_j(i) - x_j(i-1) \geq 0) \), then \( \sigma_{ij} = 1 \), and if the displacement is in opposite direction \( (x_j(i) - x_j(i-1) < 0) \), then \( \sigma_{ij} = 0 \). If \( P_{DD} \) is close to 50\% and the contact layer is stationary, the no-slip boundary condition are valid. As the fluid particles hop from one site to another, \( P_{DD} > 50\% \), the system is in the defect slip boundary condition and the particles move in one direction. For \( P_{DD} \) close to 100\% the particles at the contact layer move in the driven direction and the system is in the global slip boundary condition. Then the transition between the no-slip condition to the defect and global slip conditions is identified by the transition of the logistic function

\[
P_{DD} = 100 - \frac{50}{1 + (v_x/v_0)^\alpha},
\]

where \( \alpha \) is the steepness of the curve that is related with the necessary velocity increases to promote the transition between the defect slip to global slip, and \( v_0 \) is the logistic midpoint that is related with the bottom wall velocity that promote the global slip.

### III. RESULTS AND DISCUSSION

In order to understand the effect of different boundary conditions on the behavior of the water-like fluid, first we obtained the behavior of the system at no-slip boundary condition (without shear). For this system, the pressure versus density phase diagram presents isochores monotonic with the temperature above \( T^* = 0.400 \). Below \( T^* = 0.400 \) van der Waals loops indicate the presence of a coexistence between two phases. The coexistence densities were then obtained using the Maxwell construction, and the critical points are given by \( d^2P/d\rho^2 = 0 \). The temperature versus density phase diagram in the figure summarizes this information. The regions inside the curves in figure represent the coexistence between the various two-dimensional liquid, liquid crystal and crystal phases. The empty symbols in the figure are the critical points. For zero shear the phase diagrams obtained using the thermostat at the wall or at the fluid are equal.

The confined water-like system is characterized by the presence of planar layers. The number of layers dependents on the film thickness, as illustrated in figure. Since in our system the number of particles is kept fixed, the change of the film thickness is equal to the change of density. For temperatures from \( T = 0.025 \) to 0.65 and for the density \( \rho_I = 0.14 \)
FIG. 3. (Color online) Temperature versus density phase diagram without shear. The black solid lines represents the regions of first order phase transitions that ends in three critical points (empty symbols). The temperatures $T_I$, $T_{II}$ and $T_{III}$, and the densities $\rho_I$, $\rho_{II}$ and $\rho_{III}$, indicate values used in next results.

(dashed line in the figure 3), the fluid forms five layers; for the density $\rho_{II} = 0.18$ (dotted line in the figure 3), the fluid is structured in four layers; and for the density $\rho_{III} = 0.25$ (dot-dashed line in the figure 3), the fluid forms three layers.

FIG. 4. (Color online) Snapshots of water-like fluid confined between parallel plates, without shear, at $T_I = 0.025$. To simplify viewing, the y-direction is omitted.
We also explored the effect of different boundary conditions. In particular, we studied the behavior of the fluid as the bottom wall moves for systems with different fluid densities and several thermal bath temperatures. The figure illustrates the probability of particle move in the driven direction as a function of the bottom wall speed. We identified three characteristic regions. The no-slip condition is valid for small velocities of the bottom wall, 50% of the particles move in driven direction while the another 50% move in the opposite direction. For the temperatures of $T_I = 0.025$ and $\rho_I = 0.14$, the condition of no-slip is valid for velocities up to $v_x < 2$. As the bottom wall velocity increases, $P_{DD}$ increases leading to defect slip condition in which a few more particles move in the same direction of the bottom wall. As $v_x$ increases even further, the system reaches the global slip condition when $v_x > v_0$, which implies that most fluid particles in contact layer move in the same direction as the bottom wall. The transition between the boundary conditions is characterized by the logistic equation (eq. 8) illustrated by the solid line in the figure. For $T_I$ and $\rho_I$, the logistic fit is given by $v_0^I = 7.15(4)$ and $\alpha^I = 3.39(7)$. A similar graph is also observed for higher densities and temperatures. This behavior was also observed for a Lennard-Jones-like fluid for one specific temperature and density [19].

![Graph showing probability of particle movement](image)

**FIG. 5.** (Color online) Left axis: Probability of the particles at the contact layer to move in the driven direction as a function of the bottom wall velocity. The blue circles are results from simulations for thermal bath temperature, $T_I = 0.025$, and density of the fluid, $\rho_I = 0.14$. The blue solid line is a logistic fit. Right axis: translational order parameter as a function of bottom wall velocity for $\rho_I$ at $T_I$. 

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In order to understand how the slip condition is affected by the thermodynamic state of the anomalous fluid, the behavior of \( v_0 \) and \( \alpha \) are analyzed for different temperatures and densities (in our system this implies thickness of the film). The figure 6 shows the behavior of the logistic midpoint, \( v_0 \), defined by the equation as a function of the density for distinct temperatures indicated in the figure (\( T_I, T_{II} \) and \( T_{III} \)). This result shows that \( v_0 \) increases with the density at a fixed temperature.

At low temperatures the particles at constant density are more structured and higher kinetic energy, larger \( v_0 \), from the moving wall would be needed for the transition to the global slip. Similarly, at constant temperature, as the system becomes more dense, it is also more structured, therefore, would require higher value of \( v_0 \) for the transition to the global slip. The logistic steepness, \( \alpha \), defined by equation \ref{eq:alpha} versus \( \rho \) for the temperatures \( T = 0.025, 0.15, 0.3 \) is shown in the figure 7. For low densities the value is almost constant, and for high values of the densities the \( \alpha \) value increases in a power law behavior.

An oscillatory behavior around a line is observed for both \( v_0 \) and \( \alpha \) as a function of density. The oscillatory behavior presented in the figures 6 and 7 occurs for the same densities in both figures. The oscillations occur for densities from 0.25 to 0.20 and from 0.17 to 0.16, where the number of layers shown in the figure change from three to four, and four to five layers, respectively. So, even though the qualitative behavior of \( P_{DD} \) (fig. 5) is also observed for
Lennard-Jones-like fluids, the small oscillations in \( v_0 \) and \( \alpha \) versus density indicate that the values assumed by \( v_0 \) and \( \alpha \) are related with the unusual structures assumed by water-like fluid under confinement.

Next, we test if the behavior of \( v_0 \) with the temperature, for fixed density, is also affected by the number of layers. The figure illustrates the behavior of the density versus temperature. Three different density regions are identified in this figure. At the region I, \( \rho = 0.14, 0.15, \) and \( 0.16 \), the fluid forms five layers. At the region II, \( \rho = 0.18, \) and \( 0.19 \), the system is accommodated in four layers. At the region III, \( \rho = 0.25, 0.26, 0.27, \) and \( 0.28 \), three layers are formed. The figure shows the behavior of the logistic midpoint as a function of the temperature for densities in the regions I (circles), II (squares) and III (diamonds) identified in the figure. The transition velocity decreases linearly with temperature for all densities analyzed. Densities in the same region (equal number of layers) have the same slope in the \( v_0 \) versus temperature graph. For the region I in the figure the slope is \( b_I = -3.09(2) \), for the region II, \( b_{II} = -2.92(6) \), and for the region III, \( b_{III} = -2.4(2) \).

The figure shows the logistic steepness as a function of the temperature for densities in regions I (circles), II (squares) and III (diamonds). It decreases exponentially with temperature, with an exponential fit \( (\alpha = \alpha_0 \exp(-\lambda T)) \). In the region I the mean exponential decay coefficient is \( \lambda_I = 0.84(2) \), in the region II, is \( \lambda_{II} = 1.008(6) \), and in the region III,
is $\lambda_{III} = 1.62(7)$. Differently from the logistic midpoint, for high temperatures all curves collapse. In this case the $\alpha$ value is almost the same for all densities.

FIG. 8. (Color online) Logistic midpoint in function of temperature for several densities, where the lines are linear fits. The blue circles are systems with five layers, magenta squares are systems with four layers, and turquoise diamonds are systems with three layers.

FIG. 9. (Color online) Logistic steepness in function of temperature for several densities, where the curves are exponential fits. The blue circles are systems with five layers, magenta squares are systems with four layers, and turquoise diamonds are systems with three layers.
In order to understand how the transition to the global slip depends on the number of layers, the density profile of the system is analyzed for different global densities and temperatures. For $\rho_I = 0.14$ at $T_I = 0.025$, as shown in the figure 5, the no-slip condition is valid for velocities below 2, the defect slip is valid for $2 < v_x < v_0^I$, and the global slip is valid for $v_x > v_0^I$, where $v_0^I = 7.15(4)$. The figure 10 shows the dependence of the transversal density profile with $z$ for one bottom wall velocity in each boundary condition for $\rho_I$ and $T_I$ (see figure 3 for the location of this point in the density versus temperature phase diagram). The layering structure for different velocities in the no-slip condition ($v_x < 2$) is very similar to the $v_x = 0$ case, and exhibits layers without exchange of particles between them (solid line in figure 10). For velocities in the defect slip condition the layers are present, but particles move between the layers (dashed line in figure 10). For the global slip condition, at $v_x > v_0^I$, the central layers are not present, a uniform profile between the contact layers (dotted line in figure 10) is formed. For all densities studied at $T_I = 0.025$ we observe the same behavior seen in the figure 10. Figure 10 also shows a fluid velocity profile for $\rho_I = 0.14$ at $T_I = 0.025$ when the plate velocity is $v_x = 8.0$ (circles). Even when the system is in the global slip regime, the velocity profile is not linear. This behavior is due to the structure in layers and indicates the difficulty of an accurate determination for the slip length.

![Graph showing density and velocity profiles](image)

**FIG. 10.** (Color online) Left axis: transversal density profile for $\rho_I = 0.14$ at $T_I = 0.025$ for one bottom wall velocities in each boundary condition. Right axis: fluid velocity profile at the bottom wall velocity $v_x = 8.0$. 

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For the temperatures above the critical points in the figure 3 the scenario is slightly different. In this range of temperatures no transition is present even in the \( v_x = 0 \) case, and the increase of \( v_x \) promotes a smooth change in \( P_{DD} \) as show in figure 11 (A). In this case the increase in temperature promotes exchange of particles between the layers even for the no-slip case, as can be seen for \( v_x = 0.003 \) (solid line) in figure 11 (B). Consequently, the defect slip appears for very small bottom wall velocities (figure 11 (A)) with no significant change in the transversal density profile (dashed line, \( v_x = 3.0 \), in figure 11 (B)). At the global slip the central layers are destroyed, and the system presents a bulk profile between the contact layers (dotted line in figure 11 (B)). The velocity profile for high temperature continues to show the nonlinear behavior observed at low temperature (see fig. 11 (B)).

![Graphs](A) and (B)

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**FIG. 11.** (Color online) (A) Left axis: particles probability moving in the driven direction in function of bottom wall velocities. The blue circles are results from simulations for \( \rho_I = 0.14 \) at \( T = 0.650 \). The blue solid line is a logistic fit according eq. 8 with \( v_0^I = 5.2(1) \) and \( \alpha^I = 1.97(9) \). Right axis: translational order parameter as a function of bottom wall velocity for \( \rho_I \) at \( T = 0.600 \). (B) Left axis: transversal density profile for \( \rho_I = 0.14 \) at \( T = 0.650 \) for one bottom wall velocities in each boundary condition. Right axis: fluid velocity profile at the bottom wall velocity \( v_x = 6.0 \).

Since the behavior of the number of layers is affected by \( v_x \) quite differently when the system is the coexistence region when compared with the supercritical region in the figure 3, the response of the structure to the change in the velocity rate is analyzed in detail for both regions. The figures 5 and 11 (A) shows the translational order parameter (squares)
as a function of bottom wall velocity for $\rho_I = 0.14$. The translational order parameter, $t$, decreases with increasing $v_x$, that is, the system becomes less structured with increasing shear level. In the coexistence region (fig. 5), the decrease in $t$ value is much more pronounced than in the supercritical region (fig. 11 (A)). The difference between the structures at low and high shear level is evidenced in the parallel radial distribution function. The figure 12 shows the parallel radial distribution function of contact layer for $\rho_I = 0.14$ at $T_I = 0.025$ (coexistence region)(A) and $T = 0.650$ (supercritical region)(B), for a low and a high wall velocities. For low temperature case (coexistence region), the wall velocity leads to a transition from an amorphous phase to a liquid phase at $v_x > v'_0$ (figure 12 (A)). This behavior also was observed for $\rho_{II} = 0.18$ and $\rho_{III} = 0.25$ at $T_I$ (coexistence region in the figure 3). For the temperatures above the critical points, the fluid is in the liquid phase independent of the bottom wall velocities (figure 12 (B)) and the $\alpha$ value is independent of the number of layers. This behavior also was observed for $\rho_{II}$ and $\rho_{III}$ at $T = 0.650$.

**FIG. 12.** (Color online) (A) Parallel radial distribution function of the contact layer for $\rho_I = 0.14$ at $T_I = 0.025$ and (B) $T = 0.650$.

**IV. CONCLUSIONS**

In this work, we studied the dynamical behavior of an water-like fluid under shear. As the wall speed increases a transition from the defect to the global slip conditions was observed.
We showed that the defect slip appears due to an exchange of particles between the different fluid layers present in the confined water-like fluid.

The dynamics of this exchange is defined by the bottom wall velocity and the temperature. For low temperatures, the velocity of the bottom wall required for the defect slip to occur is large while for high temperatures, this velocity is low.

The bottom wall velocity necessary to promote the global slip condition depends on density, temperature and number of fluid layers. For a fixed density, the velocity of the bottom wall required for the global slip to occur decreases linearly with increasing temperature, with a slope which depends on the number of fluid layers.

We also found that the transition between the no-slip to the global slip is more smooth for high temperatures where no phase transition is observed in contact layer. In this situation the parameter $\alpha$ is independent of density. For low temperatures the water-like fluid present different crystal-liquid phases, the parameter $\alpha$ present high values dependent of the number of fluid layers, and the the transition from no-slip to global slip is less smooth.

Our findings are consistent with the hypothesis that slip is dependent on temperature, density and shear rate. However, our work shows that although the slip is a dynamic phenomenon directly related to the contact layer, the behavior of the fluid between these layers is determinant for the occurrence or not of the slip. Therefore, the anomalous dynamics of confined water-like fluid can be understood through the relation of the occurrence of the slip at liquid-solid interface and the anomalous thermodynamic and structure that water assumes under confinement.

V. ACKNOWLEDGMENTS

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