Effect of Surface Roughness on Shear Rate Dependent Slip Flow of Simple Fluids: A Molecular Dynamics Study

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Movies @ http://www.egr.msu.edu/~priezjev

N. V. Priezjev, “Rate-dependent slip boundary conditions for simple fluids”, *Physical Review E* **75**, 051605 (2007); “Effect of surface roughness on rate-dependent slip in simple fluids”, *Journal of Chemical Physics* **127**, 144708 (2007).

Motivation for investigation of slip phenomena at liquid/solid interfaces

- What is *THE* boundary condition for liquid on solid flow in the presence of slip?

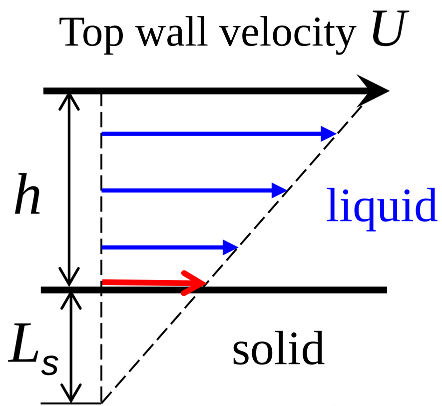
  Still no fundamental understanding of slip or what is proper BC for continuum studies. Issue very important to micro- and nanofluidics.

- Navier slip boundary condition (1827) assumes constant slip length. Is this always true? Does slip length depend on local shear rate?

- Combined effect of surface roughness, wettability and rate-dependency on the slip length L_s

  1) thermal surface roughness
  2) periodic and random wall corrugations

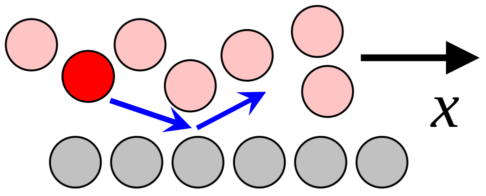
- Experimental studies indicate huge differences in the slip length. What is the fundamental cause of such variability?



Navier slip law

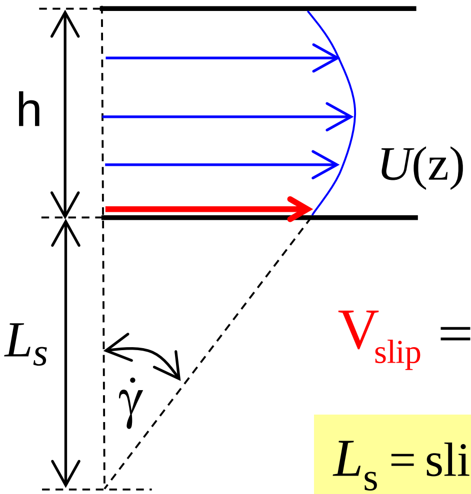
$$V_{slip} = L_s \, \dot{\gamma}$$

Molecular Dynamics simulations



atoms of FCC wall

Details of Molecular Dynamics (MD) simulations



Poiseuille
slip flow

$$V_{slip} = L_s(\dot{\gamma})\,\dot{\gamma}$$

L_s = slip length

$\dot{\gamma}$ = shear rate = $dU(z=0)/dz$

$$m\ddot{y}_i + m\Gamma\dot{y}_i = -\sum_{i\neq j}\frac{\partial V_{ij}}{\partial y_i} + f_i$$

$\Gamma = \tau^{-1}$ friction; f_i = random force

Langevin thermostat: $T = 1.1\ \varepsilon/k_B$

Thompson & Robbins, *PRA* (1990).

Lennard-Jones (LJ) potential:

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6}\right]$$

σ – molecular length scale

ε – LJ energy scale

$\tau = (m\sigma^2/\varepsilon)^{1/2}$ – LJ time scale

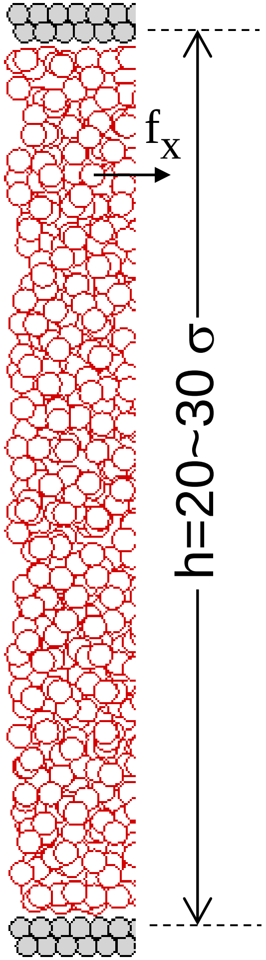
$N = 10^3 \sim 10^5$ fluid molecules

Fluid density: $\rho = 0.81\,\sigma^{-3}$

Weak wall–fluid interactions:

$0.3 \leq \varepsilon_{wf} \leq 1.1$

FCC solid walls: $\rho_w = 2.73\,\sigma^{-3}$

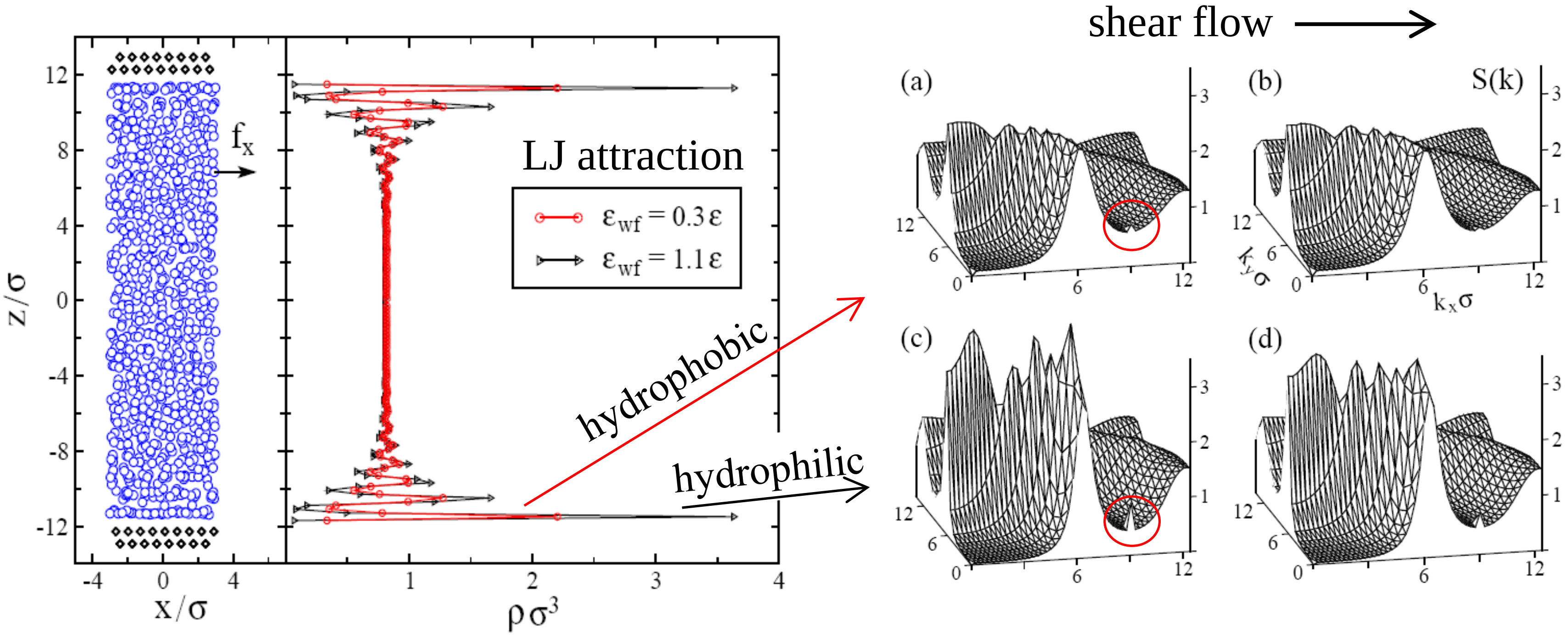


Fluid structure near fcc walls: layering and in-plane order

xz plane

Fluid density profiles

Structure factor in the first fluid layer



Incommensurate wall-fluid structures

Higher surface energy ε_{wf} results in:

- more pronounced layering near walls
- larger surface induced fluid ordering

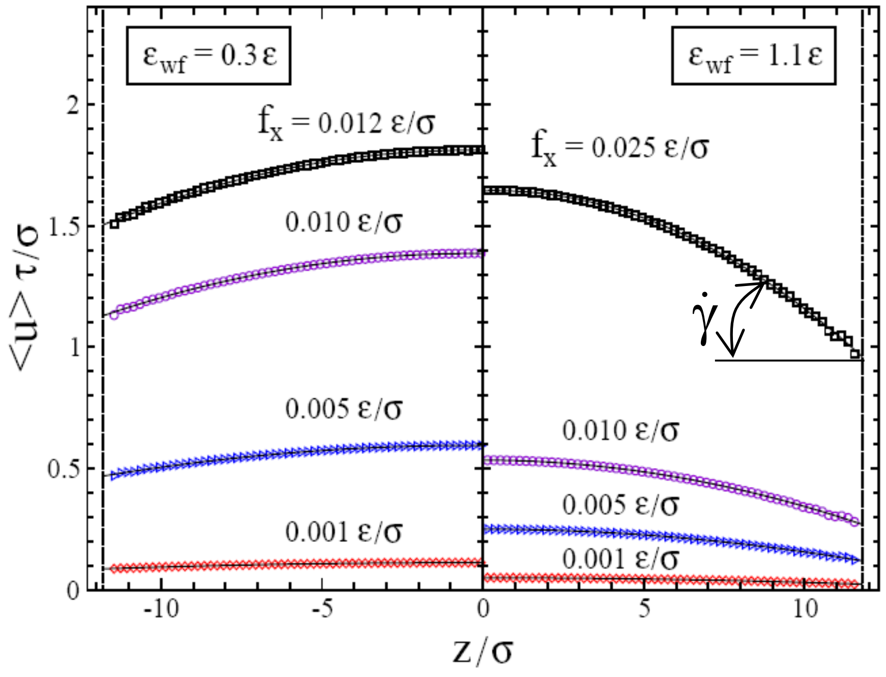
In-plane fluid structure factor:

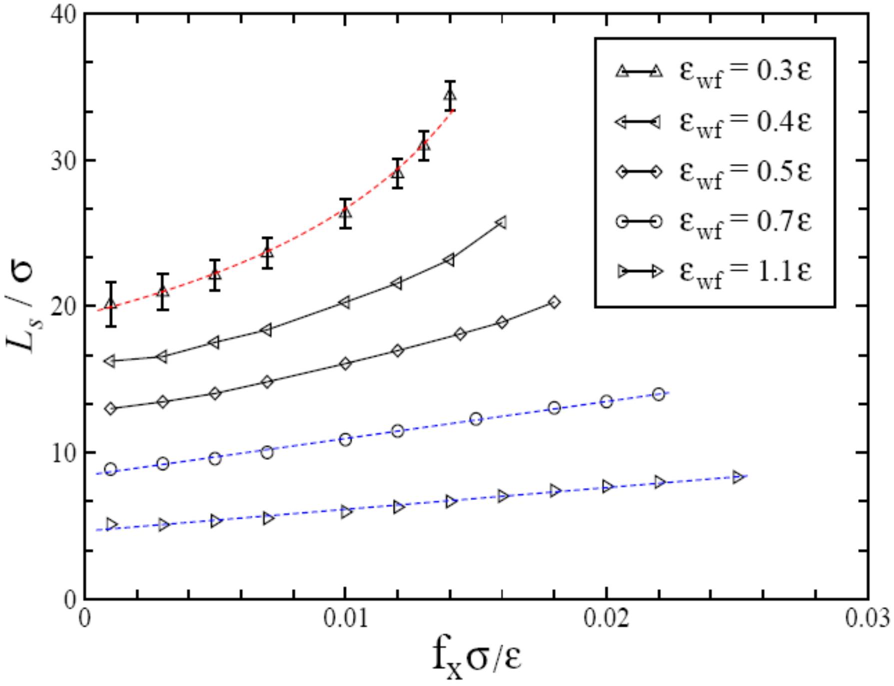
$$S(\mathbf{k}) = 1/N_\ell \,|\sum_j e^{i\,\mathbf{k}\cdot\mathbf{r}_j}|^2$$

Velocity profiles and slip length L_s as a function of the force f_x

Velocity profiles are fitted by parabolas

For all curves: $L_{max} / L_s^* = 1.63 \pm 0.13$





$\dot{\gamma}$ = local shear rate $= du(z=h)/dz$

Fluid velocity in the channel and near the interfaces increases with the applied force

Gradual transition in $L_s(f_x)$ is observed by varying the strength of the wall-fluid interaction ε_{wf}

Dependence of slip length L_s on shear rate $\dot{\gamma}$ and surface energy ε_{wf}

Gradual transition in $L_s(\dot{\gamma})$ is observed by varying the strength of the wall-fluid interaction ε_{wf}

For weak surface energy:

$$\boxed{L_s/L_s^* = \left(1-\dot{\gamma}/\dot{\gamma}_c\right)^{-1/2}}$$

Fitting parameters:

$L_s^* = 19.5\,\sigma$ and $\dot{\gamma}_c = 0.093\,\tau^{-1}$

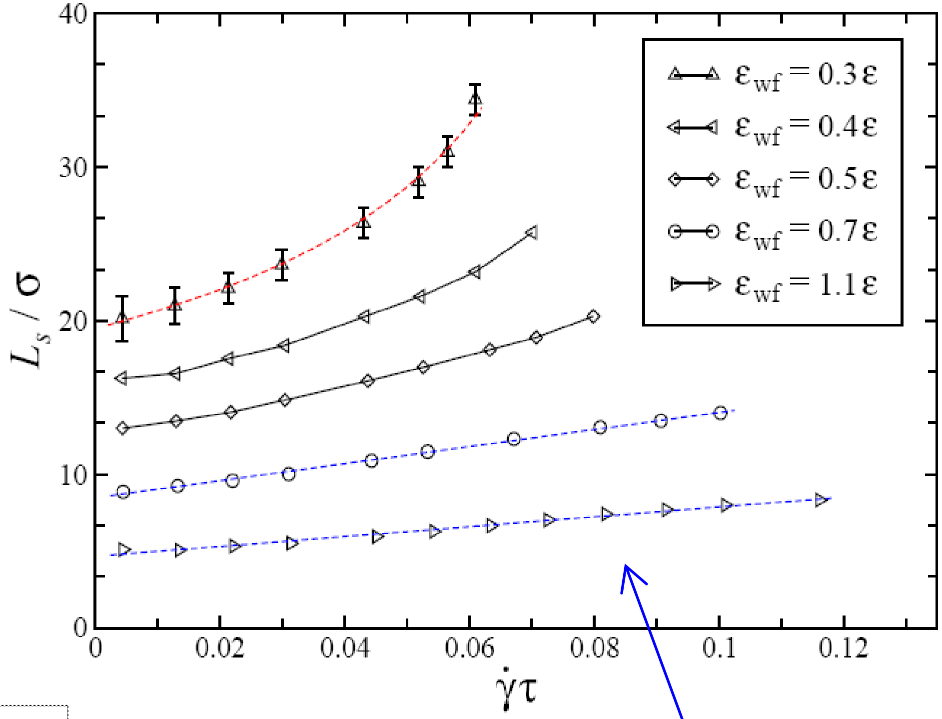
Thompson & Troian, Nature (1997)

Flow rate $Q(L_s)$ increases due to $L_s(\dot{\gamma})$

$Q(L_{max})/Q(L_s^*) = 1.59 \pm 0.08$ for $\varepsilon_{wf} = 0.3$

$Q(L_{max})/Q(L_s^*) = 1.36 \pm 0.08$ for $\varepsilon_{wf} = 1.1$

For all curves: $L_{max}/L_s^* = 1.63 \pm 0.13$

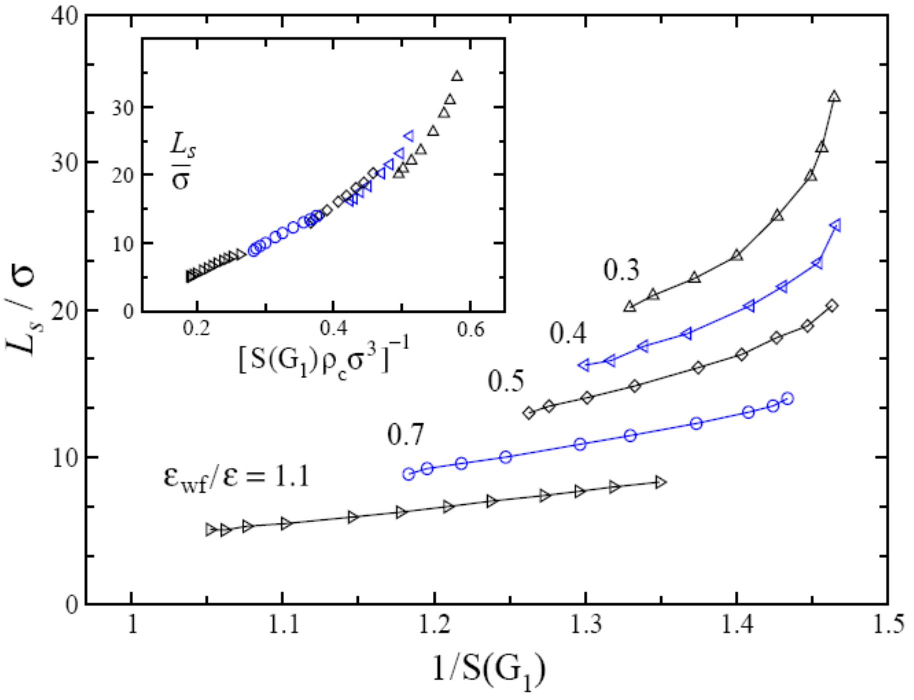


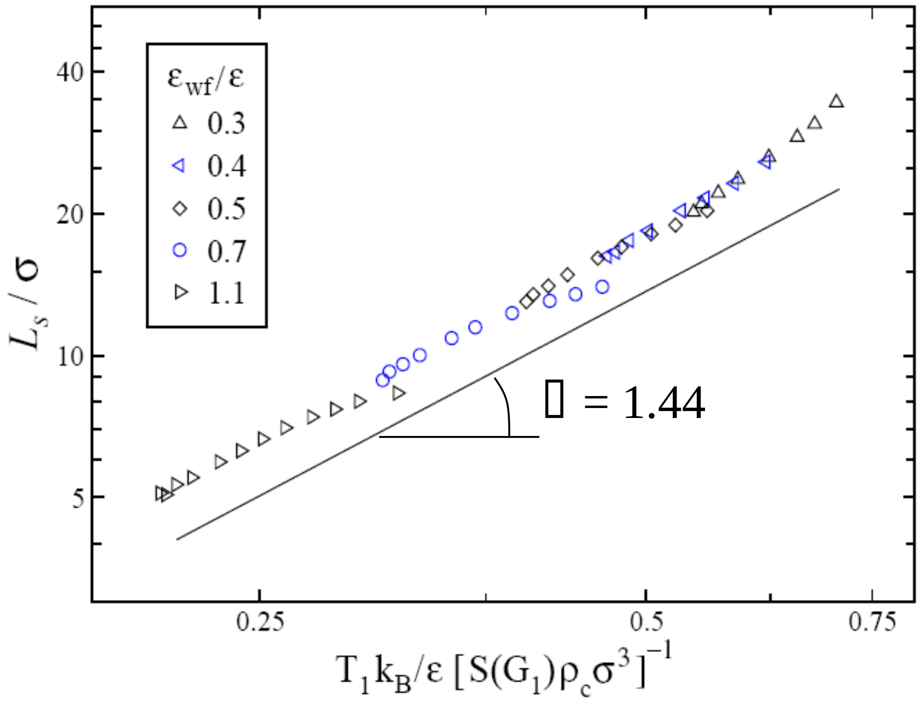
Strong wall-fluid interaction potential:

$$\boxed{L_s = L_s^* + A\,\dot{\gamma}}$$

Choi, Westin & Breuer, *Phys. Fluids* (2003).

A correlation between L_s and structure factor $S(\mathbf{G}_1)$ in the first fluid layer





ρ_c = contact density of the first fluid layer

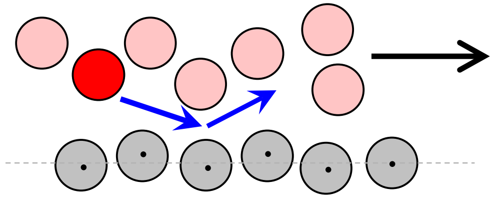
Slip length $L_s(\dot{\gamma})$ strongly correlates with the surface induced fluid order $S(\mathbf{G}_1)$ in a *rate-dependent* regime.

Master curve in a wide range ε_{wf} and $\dot{\gamma}$

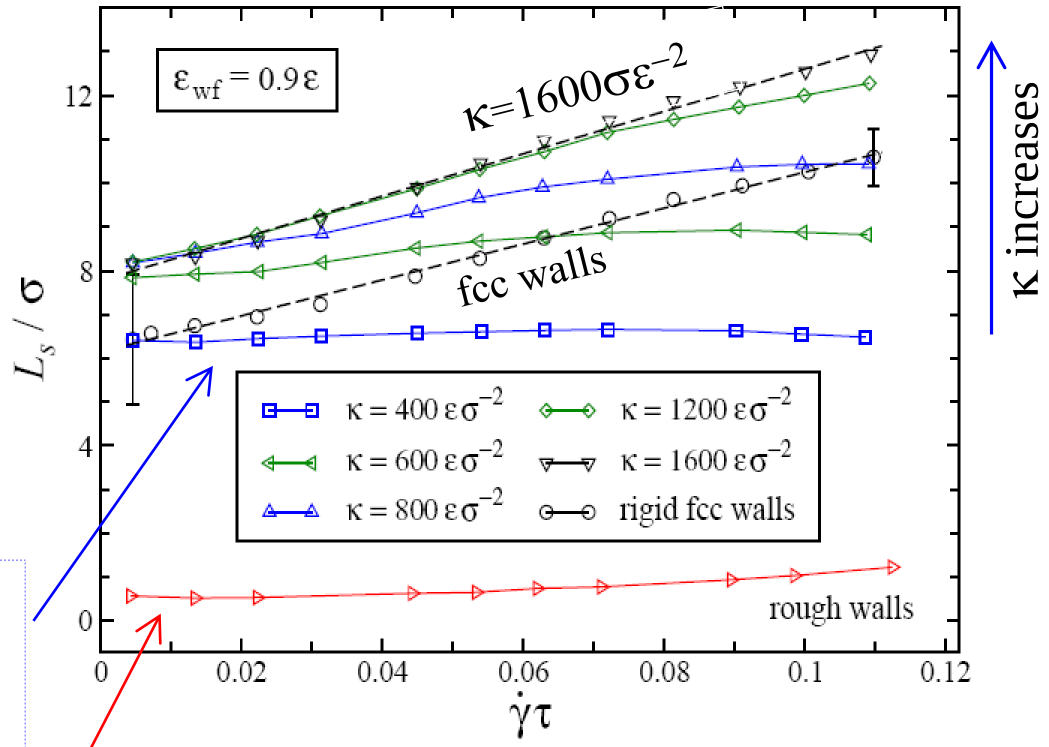
$$L_s \sim (T_1/S(\mathbf{G}_1)\,\rho_c)^{\alpha}$$

Effect of thermal surface roughness on slip length $L_s(\dot{\gamma})$

Spring potential: $V_{sp} = 1/2\ \kappa\ r^2$



thermal atoms of FCC wall



Small spring stiffness $\kappa=400\sigma\varepsilon^{-2}$
Dynamically rough soft walls
$L_s \approx$ constant

Large spring stiffness $\kappa=1600\sigma\varepsilon^{-2}$
Effectively smooth flat walls

$$L_s = L_s^* + A\,\dot{\gamma}$$

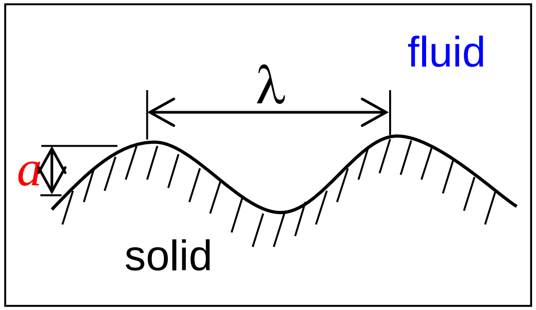
“Frozen” random roughness with $|\Delta u| \approx 0.07\sigma$ reduces slip length

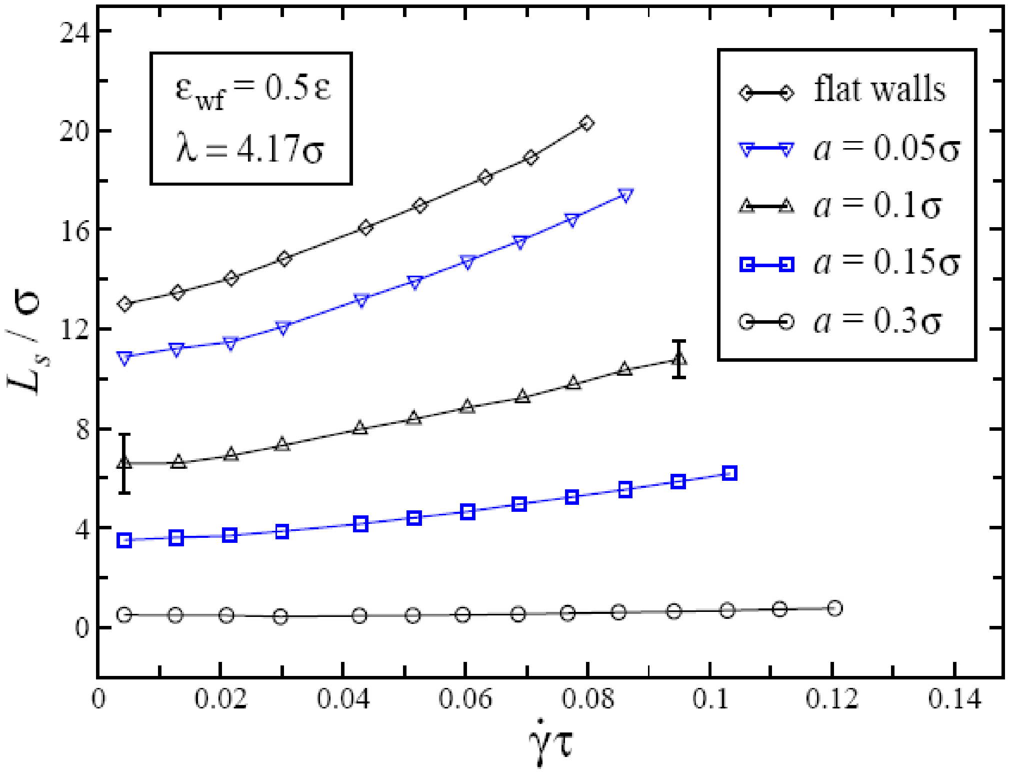
Slip length L_s rate dependence on periodic surface roughness *ka*

Vertical offset of Lennard-Jones atoms of lower and upper walls:

$$\Delta z(x) = a \sin(2\pi x/\lambda)$$

Wavenumber: $k = 2\pi / \lambda$





Molecular dynamics and continuum analysis at low shear rates:

N.V. Priezjev and S.M. Troian, *J. Fluid Mech.*, **554,** 25 (2006).

Surface roughness *ka* reduces slip length L_s and its rate-dependence

Conclusions

- Molecular dynamics simulations predict a gradual transition in the functional dependence of the slip length on shear rate for simple fluids by varying surface energy.

Strong surface potential: Weak surface energy:

$$\boxed{L_s = L_s^* + \mathrm{A}\,\dot{\gamma}} \quad \xrightarrow{\varepsilon_{wf}} \quad \boxed{L_s/L_s^* = (1-\dot{\gamma}/\dot{\gamma}_c)^{-1/2}}$$

- A strong correlation between the slip length L_s and structure factor $S(\mathbf{G}_1)$ in the first fluid layer in a *rate-dependent* regime.

- Master curve in a wide range ε_{wf} and $\dot{\gamma}$:

$$\boxed{L_s \sim (T_1/S(\mathbf{G}_1)\,\rho_c)^{\alpha}}$$

N. V. Priezjev, “Rate-dependent slip boundary conditions for simple fluids”, *Physical Review E* **75**, 051605 (2007); “Effect of surface roughness on rate-dependent slip in simple fluids”, *Journal of Chemical Physics* **127**, 144708 (2007).

Experimental measurements of slip length

Reference	Slip length	Method	Liquid	Surface	Size	Shear rate	Roughness
Schnell (1956)	1 – 10 μm	Flow rate	Water	Glass + DDS	<800μm	$10^{2\sim3}$ sec^{-1}	——
Churaev, Sobolev Somov (1984)	30 –70 nm	Flow rate–press. drop	Water and mercury	Quartz	< 7.2μm	$10^{1\sim4}$ sec^{-1}	——
Watanabe, Udagawa (1999)	~ 100 μm	Flow rate–press. drop	Water, Glycerin	Acrylic resin, hydrophobic	6-12mm	——	——
Migler, Hervet & Leger (1993)	0.1–300μm	EWIF	PDMS	Quartz + OTS	——	0.1 –1 sec^{-1}	2 – 3 Å
Horn, Vinogradova *et al*. (00)	30 – 50 nm	SFA + drainage	Boger fluid	Mica	50-900nm	——	——
Zhu & Granick PRL (2001)	0 – 2 μm	SFA + drainage	Tetradecane and water	Mica + OTE	~100 nm	$10^{1\sim5}$ sec^{-1}	~ 1 Å
Zhu & Granick PRL (2002)	0 – 40 nm	SFA + drainage	Tetradecane and water	Mica + OTE	~100 nm	$10^{1\sim5}$ sec^{-1}	0.2 – 6 nm
Tretheway and Meinhart (2002)	~ 1 μm	μ–PIV	Water	Glass + OTS hydrophobic	30μm	10^{2} sec^{-1}	2 – 3 Å
Choi, Westen & Breuer (2003)	~ 30 nm	Flow rate–press. drop	Water	Glass + OTS hydrophobic	21μm	10^{5} sec^{-1}	2 – 3 Å
Charlaix group PRL (2005)	~ 20 nm	SFA + drainage	Dodecane and water	Glass + OTS hydrophobic	<200 nm	$< 5\cdot10^{3}$ sec^{-1}	~ 1 nm