Effect of surface roughness on slip flows in nanoscale polymer films
Molecular dynamics simulations versus continuum predictions
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Motivation to investigate the slip phenomena at interfaces

- What is the boundary condition for liquid on solid flow in the presence of slip?
- Still no fundamental understanding of slip at or proper BC for continuum studies.
- Navier slip boundary condition (1827) assumes constant slip length. Is it always true?
- How does surface roughness affect slip flow and conformation of a polymer chain?
- How does molecular dynamics simulations compare with continuum results?

Rheology of a polymer melt near rough surfaces

- Fluid density profiles
- For a fixed wavelength, slip velocity $\gamma$ is reduced at larger amplitudes. $R_{s0}$ increases with shear rate.
- For a fixed amplitude, more slip at larger wavelength and smaller shear rate.
- The contact density inside the valley is larger than its value above the peak.

Rheology of a polymer melt near rough surfaces

- Fluid velocity profiles
- $\dot{\gamma}$ = 1.4 $\sigma$
- Continuum modeling of slip flow past a curved boundary
- Method of solution
- Finite element penalty function with bilinear rectangular grid
- 2D Stokes flow without body force
- $\mu \partial U / \partial y + \nabla p = 0$ $\nabla U = 0$

Boundary conditions
- Couette flow with constant slip length at the top wall.
- Either slip boundary conditions:
- $\dot{\gamma} = L_0 \dot{\gamma} = \frac{dU}{dz} = \frac{\partial U}{\partial y}$
- $\sigma$ normal vector to the surface

Velocity vanishes in valleys with increasing slip length

Pressure increases

Conclusions

- At small wavelengths $\lambda < R_{s0}$ polymer chain tend to stretch in the direction of the shear flow in the regions above peaks of sinusoidal corrugation and elongate inside valleys along the $y$ direction.
- Molecular dynamics results recover the continuum solutions in the Stokes regime in the limit of small surface roughness $R_{s0}$ and $\lambda < 66.6 \sigma$.
- Effective slip length is reduced at small wavelengths $\lambda$ and for large amplitude $a$ of the corrugated surface.

References