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Slip Behavior in Liquid Nanoscale Films: Influence of Molecular Ordering, Wall Roughness and Patterned Surface Energy[1]

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The development of micro- and nanofluidic devices for actuation of liquid films, drops and bubbles requires detailed knowledge of the interfacial forces affecting transport. The small dimension size guarantees that all tranport properties are strongly dominated by boundary effects. The large surface to volume ratios, however, also cause significant frictional losses which can be reduced by generating slippage at the liquid-solid interface. Slippage can be enhanced by surface chemical treatments, textured substrates and nucleation of nanobubbles. High molecular weight polymers also generate large slip lengths, defined as the distance within the solid phase where the extrapolated flow velocity vanishes. While hydrodynamic analyses are useful in providing a continuum description of fluidic response at the microscale, molecular dynamics (MD) simulations offer detailed resolution of the molecular behavior near chemically or topologically modified surfaces, a necessity in constructing nanofluidic devices. In this talk we show how the slip length in nanoscale liquid films is affected by the amplitude and wavelength of surface roughness. We also consider periodic variations in the liquid-solid interaction potential mimicking regions of no-shear and no-slip, as with surfaces covered by nanobubbles. A detailed comparison between hydrodynamic predictions and MD simulations elucidates what geometric and molecular parameters govern the slip length at different length scales. Excellent agreement is obtained when the system size is about an order of magnitude larger than the molecular size. We end this talk with discussion of a simplified model for predicting the dynamic exponent observed in the MD simulations for the power law increase in slip length with shear rate. These studies clearly pinpoint the molecular origin of the dynamic exponent and help explain the different slip laws expected for liquid versus gas flow.

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