

Inverse problem for slip boundary conditions in nanoscale polymer films: A molecular dynamics simulation approach

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The rheology of complex fluids in thin films is important for theoretical and experimental studies of such common phenomena as friction, lubrication and wear. Experimental measurements of the flow profiles and shear stresses on submicron scales might be subject to errors due to the possibility of liquid slip at the solid wall. An accurate prediction of flow, therefore, requires specification of a proper boundary condition. An inverse problem is to determine boundary conditions from the prescribed material properties of the substrate and liquid structure. In this presentation we describe our recent results on the shear rate dependence of the slip length in thin polymer films confined between atomically smooth surfaces using molecular dynamics simulations. The unentangled polymer melt is described by the coarse-grained bead-spring model of linear flexible chains.

We found that at low shear rates the velocity profiles acquire a pronounced curvature near the wall and the absolute value of the negative slip length is approximately equal to thickness of the viscous interfacial layer. In this regime the slip length is nearly rate-independent. At higher shear rates, the velocity profiles become linear and the slip length increases rapidly as a function of shear rate. The gradual transition from no-slip to steady-state slip flow is associated with "shear-melting" of the interfacial layer. The relaxation dynamics of polymer chains in shear flow is analyzed by evaluating the decay of time autocorrelation function of the first normal mode in the vorticity direction. We found that the rate behavior of the slip length correlates well with the inverse relaxation time of the polymer chains in the interfacial layer.

The rate-dependent slip boundary conditions can also be reformulated in terms of the friction coefficient at the polymer/wall interface and slip velocity of the first fluid layer. In agreement with the results of the previous study [Niavarani and Priezjev, *Phys. Rev. E* **77**, 041606 (2008)], we found that the friction coefficient at lower melt densities undergoes a transition from a constant value to the power law decay as a function of the slip velocity. At higher melt densities the friction coefficient decays as a power law function in a wide range of slip velocities. When the magnitude of the surface induced peak in the fluid structure factor is below a certain value, the friction coefficient is determined by the structure factor and contact density of the first fluid layer near the solid wall [Priezjev, *Phys. Rev. E* **80**, 031608 (2009)].