Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

The relationship between induced fluid structure and boundary slip in nanoscale polymer films: A molecular dynamics simulation study NIKOLAI PRIEZJEV, Michigan State University — The molecular mechanism of slip at the interface between polymer melts and weakly attractive smooth surfaces is investigated using MD simulations. In agreement with our previous studies, it is shown that the slip length passes through a local minimum at low shear rates and then increases rapidly at higher rates. We found that at sufficiently high shear rates, the slip flow over flat crystalline surfaces is anisotropic. It is demonstrated numerically that the friction coefficient (the ratio of viscosity and slip length) undergoes a transition from a constant value to the power-law decay as a function of the slip velocity. The characteristic velocity of the transition correlates well with the diffusion velocity of monomers in the first fluid layer. We also show that in the linear regime, the friction coefficient is well described by a function of a single variable, which is a product of the magnitude of surface-induced peak in the structure factor and the contact density of the adjacent fluid layer. The universal relationship between the friction coefficient and induced fluid structure holds for a number of material parameters of the interface: fluid density, chain length, wall-fluid interaction energy, wall density, lattice type and orientation, thermal or solid walls. Reference: cond-mat/1007.4534.

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Date submitted: 04 Aug 2010 Electronic form version 1.4