Abstract Submitted for the DFD09 Meeting of The American Physical Society

Shear rate threshold for the boundary slip in dense polymer films¹ NIKOLAI PRIEZJEV, Michigan State University — The shear rate dependence of the slip length in thin polymer films confined between atomically flat surfaces is investigated by molecular dynamics simulations. The polymer melt is described by the 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. 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 faster relaxation of the polymer chains near the wall evaluated from decay of the time autocorrelation function of the first normal mode. We also show that at high melt densities the friction coefficient at the interface between the polymer melt and the solid wall follows power law decay as a function of the slip velocity. At large slip velocities the friction coefficient is determined by the product of the surface induced peak in the structure factor, temperature and the contact density of the first fluid layer near the solid wall. (Reference cond-mat/0906.2771).

¹ACS Petroleum Research Fund

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Date submitted: 05 Aug 2009

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