Abstract Submitted
for the DFD13 Meeting of
The American Physical Society

Effect of chain stiffness on interfacial slip in nanoscale polymer films NIKOLAI PRIEZJEV, Wright State University — The results obtained from molecular dynamics simulations of the friction at an interface between polymer melts and weakly attractive crystalline surfaces are reported. We consider a coarse-grained bead-spring model of linear chains with adjustable intrinsic stiffness. The structure and relaxation dynamics of polymer chains near interfaces are quantified by the radius of gyration and decay of the time autocorrelation function of the first normal mode. We found that the friction coefficient at small slip velocities exhibits a distinct maximum which appears due to shear-induced alignment of semiflexible chain segments in contact with solid walls. At large slip velocities, the friction coefficient is independent of the chain stiffness. The data for the friction coefficient and shear viscosity are used to elucidate main trends in the nonlinear shear rate dependence of the slip length. The influence of chain stiffness on the relationship between the friction coefficient and the structure factor in the first fluid layer is discussed. Financial support from the National Science Foundation (CBET-1033662) is gratefully acknowledged.

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Date submitted: 01 Aug 2013 Electronic form version 1.4