Slip behavior of the confined polymer melt near periodically roughened surface: comparison between molecular dynamics and continuum simulations ANOOSHEH NIAVARANI, NIKOLAI PRIEZJEV, Michigan State University — Molecular dynamics (MD) simulations are used to investigate the behavior of the slip length in the Couette flow of a polymer melt. For atomically smooth surfaces and weak wall-fluid interactions, the shear rate dependence of the slip length is a non-monotonic function, with a distinct local minimum. For corrugation wavelengths larger than the radius of gyration of polymers, the decay of the slip length with corrugation amplitude obtained from MD simulations agrees well with the continuum predictions for the following cases: (1) Stokes solution with constant local slip length, (2) Stokes solution with local shear-rate-dependent slip length, and (3) Navier- Stokes solution with local rate-dependent slip length. If the corrugation wavelength is less than or on the order of the radius of gyration, the continuum predictions (the Stokes solution) overestimate the values of the slip length extracted from MD simulations. The analysis of the conformational properties of the polymer melt indicates that polymer chains tend to stretch in the direction of shear at the peaks of the sinusoidal wave and align themselves along the bottom of the grooves.

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