Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular dynamics simulations of a polymer brush-melt interface under shear CLAUDIO PASTORINO, Institüt für Physik, Johannes Gutenberg-Universität, Mainz, Germany, MARCUS MLLER, Department of Physics, University of Wisconsin-Madison, USA, KURT BINDER, Institüt für Physik, Johannes Gutenberg-Universität, Mainz, Germany — Molecular dynamics simulations of a polymer melt between two brush-covered surfaces under shear have been performed. The end-grafted polymers and the free chains of the melt have identical properties. The grafting density of the brush-layer provides a way of changing the surface behavior without altering the molecular interactions. The deformability and wettability of the brush layer, including the dewetting of a melt on the top of a dense brush of identical chains (autophobicity), are studied as functions of the grafting density. The chains are described by a coarse-grained bead spring model. We perform equilibrium and non-equilibrium simulations at constant temperature and volume using the Dissipative Particle Dynamics thermostat to duly account for hydrodynamic correlations. The equilibrium properties and behavior under shear are studied, as well as, the interdigitation of the melt into the brush, the polymer orientation on different length scales (bond vectors, radius of gyration, and end-to-end vector) of free and grafted chains, and velocity profiles. The viscosity and slippage at the interface are also calculated as functions of the grafting density and shear velocities. This work is a first step towards studying droplet spreading on top of a brush.

Claudio Pastorino
Institüt für Physik, Johannes Gutenberg-Universität, Mainz, Germany

Date submitted: 22 Mar 2013 Electronic form version 1.4