Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Molecular Dynamics Simulations of Fractionation of Molecular Brushes During Spreading on Substrates JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Polymer Program, Institute of Materials Science, University of Connecticut, SERGEI SHEIKO, Department of Chemistry, University of North Carolina — We have performed coarse-grained molecular dynamics simulations of motion of brush-like molecules in a matrix of linear chains in contact with a substrate under Poiseuille flow conditions. Our simulations show that short brush molecules move faster than the long ones resulting in fractionation of the brush molecules according to their molecular weight in the spreading polymeric films. The simulation data are in a good qualitative agreement with the predictions of the theoretical model which relates the brush velocity with the ratio of the friction coefficients between brush and substrate and between substrate and linear chains and brush geometric characteristics (length of the brush molecule and its width). Computer simulations and theoretical model provide an explanation of the brush fractionation observed during spreading of the mixtures of brush-like and linear macromolecules on a solid substrate.

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Date submitted: 20 Nov 2009 Electronic form version 1.4