Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Explicit Solvent Simulations of Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules[1] J.-M.Y. CARRILLO, University of Connecticut, W.M. BROWN, Oak Ridge National Laboratories, A.V. DOBRYNIN, University of Connecticut — We study friction between charged and neutral brush layers of bottle-brush macromolecules using molecular dynamics simulations. The deformation of the bottle-brush macromolecules under the shear were studied as a function of the substrate separation and shear stress. For charged bottle-brush layers we study effect of the added salt on the brush lubricating properties to elucidate factors responsible for energy dissipation in charged and neutral brush systems. Our simulations have shown that for both charged and neutral brush systems the main deformation mode of the bottle-brush macromolecule is associated with the backbone deformation. This deformation mode manifests itself in the backbone deformation ratio, α, and shear viscosity, η, to be universal functions of the Weissenberg number W. The value of the friction coefficient, μ, and viscosity, η, are larger for the charged bottle-brush coatings in comparison with those for neutral brushes at the same separation distance, D, between substrates. The additional energy dissipation generated by brush sliding in charged bottle-brush systems is due to electrostatic coupling between bottle-brush and counterion motion. This coupling weakens as salt concentration, c_s, increases resulting in values of the viscosity, η, and friction coefficient, μ, approaching corresponding values obtained for neutral brush systems.

[1]NSF DMR-1004576

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Date submitted: 27 Dec 2012 Electronic form version 1.4