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Friction between Brush Layers of Charged and Neutral Bottle-Brush Macromolecules. Molecular Dynamics Simulations[1] DANIEL RUSSANO, Boston University, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — We used MD simulations to study lubricating properties of neutral and charged bottle-brush coatings as a function of the compression and shear stresses, and brush grafting density. Our simulations have shown that in charged systems under shear there is a layer with excess of counterions found in between brush bearing surfaces. The main deformation mode of the charged layers is associated with the backbone deformation resulting in the backbone deformation ratio, α, and shear viscosity,η, being universal functions of the Weissenberg number, W. In the case of neutral systems in addition to the backbone deformation there is also side chain deformation. The coupling between backbone and side chain deformation violates universality in α dependence on $W$and results in scaling exponents varying with compression stress and brush grafting density. Existence of different length scales controlling deformation of neutral bottle–brushes manifests itself in shear viscosity,η, dependence on the shear rate, $\dot{\gamma}$. Shear viscosity,η, as a function of the shear rate, $\dot{\gamma}$, has two plateaus and shear thinning regimes. The low shear rate plateau and shear thinning regime correspond to the backbone deformation while the second plateau and shear thinning regime at moderate shear rates is due to side chain deformation. For both systems the value of the friction coefficient increases with increasing the shear rate.

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