

Abstract Submitted
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Shear and normal forces in charged polymer brushes QI LIAO, Chinese Academy of Sci (CAS), MICHAEL RUBINSTEIN, Department of Chemistry, University of North Carolina, Chapele Hill, 27599 NC, USA — We present the results of molecular dynamics simulations of steady shear between a pair of opposing charged polymer brushes in the osmotic-brush regime and compare the results with predictions of scaling models. Using the monomer and counterion density profiles, we have verified different regimes in the diagram of states of compressed polyelectrolyte brushes predicted by the scaling model of Zhulina *et al* [Macromolecules, 2014]. Our simulation results for the normal forces of compressed polyelectrolyte brushes are in excellent agreement with predictions of the scaling model. However, our results for the dependence of the shear forces on the separation between brushes are only in qualitative agreement with the predictions of the scaling model. The dependence of the interpenetration length on the separation of polyelectrolyte brushes exhibits a maximum instead of the plateau predicted by the scaling model for the partially interpenetrated brushes. Our simulation results confirm that our implicit solvent simulations of polyelectrolyte brushes that ignore hydrodynamics interaction are in agreement with the scaling predictions that include hydrodynamic interaction because of screening of hydrodynamic interaction and long range electrostatic interactions on the correlation length scale.

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