MAR12-2011-006120

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Effect of electrostatic interactions on lubrication in polymeric and biological systems[1]

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Many connective tissues, such as cartilage demonstrate excellent lubrication and wear characteristics. Cartilages in mammalian joints can withstand pressures of the order of ten atmospheres and have remarkably low friction coefficient in the range of 0.001-0.03. The surface of the cartilage is covered with bottle-brush-like polyelectrolyte layer consisting of glycoproteins. This brush layer, which faces a similar layer on the opposing cartilage, is sheared as two surfaces slide passing each other during joint motion. We have performed molecular dynamics simulations of charged and neutral bottle-brush macromolecules tethered to substrates to understand the role of the electrostatic and hydrodynamic coupling between brush layers on the lubricating properties in biological and polymeric systems. Glycoprotein layers were modeled as two opposing layers of highly charged bottle-brush macromolecules composed of Lennard-Jones particles grafted to a substrate. Simulations have shown that charged bottle-brush systems have lower friction under shear and weaker dependence of the disjoining pressure on substrate separation than neutral bottle-brush systems. This was explained by formation of lubricating layer with excess of counterions located in the middle between brush-bearing surfaces. In overlapping brush layers the disjoining pressure between brush-bearing surfaces is controlled by the bottle-brush bending rigidity. Under shear, the main deformation mode of the charged bottle-brush layers is associated with the bottle-brush backbone deformation resulting in backbone deformation ratio and shear viscosity being universal functions of the Weissenberg number. In the case of neutral bottle-brush systems there is coupling between backbone and side chain deformation. This violates universality in backbone deformation ratio and manifests itself in shear viscosity dependence on the shear rate. The shear viscosity as a function of the shear rate for the neutral bottle-brush systems has two plateaus and two shear thinning regimes.

[1]NSF # DMR-1004576