Polymer friction Molecular Dynamics

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We present molecular dynamics friction calculations for confined hydrocarbon solids with molecular lengths from 20 to 1400 carbon atoms. Two cases are considered: a) polymer sliding against a hard substrate, and b) polymer sliding on polymer. In the first setup the shear stresses are relatively independent of molecular length. For polymer sliding on polymer the friction is significantly larger, and dependent on the molecular chain length. In both cases, the shear stresses are proportional to the squeezing pressure and finite at zero load, indicating an adhesional contribution to the friction force. [Sivebaek, I.M., Samoilov, V.N., Persson, B.N.J. Eur. Phys. J. E 27, 37–46 (2008). and Persson, B.N.J., Sivebaek, I.M., Samoilov, V.N., Zhao Ke, Volokitin A.I., Zhenyu Zhang. J. Phys.: Condens. Matter 20, 395006 (2008).]

Concerning the effective viscosity of nanometer thin confined polymer films we find shear thinning effects similar to those seen in Surface Force Apparatus measurements [Yamada S. Tribology Letters, 13 (3), 167 (2002)]. We also find that the temperature alters these shear thinning effects going from solid like state at 0K to a Newtonian liquid at high temperatures [Sivebaek, I.M., Samoilov, V.N., Persson, B.N.J. In preparation].

log(viscosity) = c – nlog(shear_rate)