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Effective Viscosity of Confined Hydrocarbons

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Surface Force Apparatus measurements at ambient temperature have shown that the logarithm of the effective viscosity depends linearly on the logarithm of the shear rate:

 $log(effective_viscosity) = C - n * log(shear_rate)$

With n=0.9 and C=4.9 for a large number of liquids and polymers: [Yamada S. Tribology Letters, 13 (3), 167 (2002)].

We present Molecular Dynamics (MD) friction calculations for confined hydrocarbon films with molecular lengths from 20 to 1400 carbon atoms. We find the same relation between the logarithm of the effective viscosity and the logarithm of the shear rate as in the Surface Force measurements. Also the same constants n and C were found by our calculations at ambient temperature (300K).

By heating and cooling of the hydrocarbons we have been able to establish that n varies from 1 (solid-like friction) at very low temperatures to 0 (Newtonian liquid) at very high temperatures, following an inverse sigmoidal curve. Only the shortest chain molecules melt, whereas the longer ones only show a softening in the studied temperature interval 0 < T < 900 K. The results are important for the frictional properties of very thin (nanometer) films and to estimate their thermal durability: [Sivebaek, I.M., Samoilov, V.N., Persson, B.N.J. Physical Review Letters, 108 (3), 036102 (2012)].

n and C factors

