269c Viscosity of Hydration Water under Subnanometer Confinement between Mica Surfaces

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We have performed additional molecular dynamics simulations to investigate the shear dynamics of hydration water confined between two mica surfaces to subnanometer thickness at 1bar pressure and 298K to extend our previous work [1]. While Newtonian plateau of shear viscosity has been found around two orders of magnitude larger than the bulk value for D=0.92nm (three-layer water film), significant shear-thinning occurs in the whole MD regime (shear rate $\gamma \sim 10^8 - 10^{11}\ s^{-1}$) for D=0.62nm (two-layer water film). In the latter case, freezing of water film in confined geometry has been observed, similar to the first-order liquid to solid transition. We estimate that the longest rotational relaxation time of water molecules is at least in the order of µs, and extrapolate the shear viscosity of the ultrathin water film to Newtonian regime. It turns out that the Newtonian plateau is at least five orders of magnitude larger than the bulk value. Under shearing, very viscous behavior of water films is observed. The structure factor fluctuates between 0.4 (a comparably ordered structure) and 0.02 (a very fluidic structure).

[1] Leng, Y. S. and Cummings, P. T., "Fluidity of Hydration Layers Nanoconfined between Mica Surfaces," Phys. Rev. Letts., 94, Art. no. 026101 (2005).