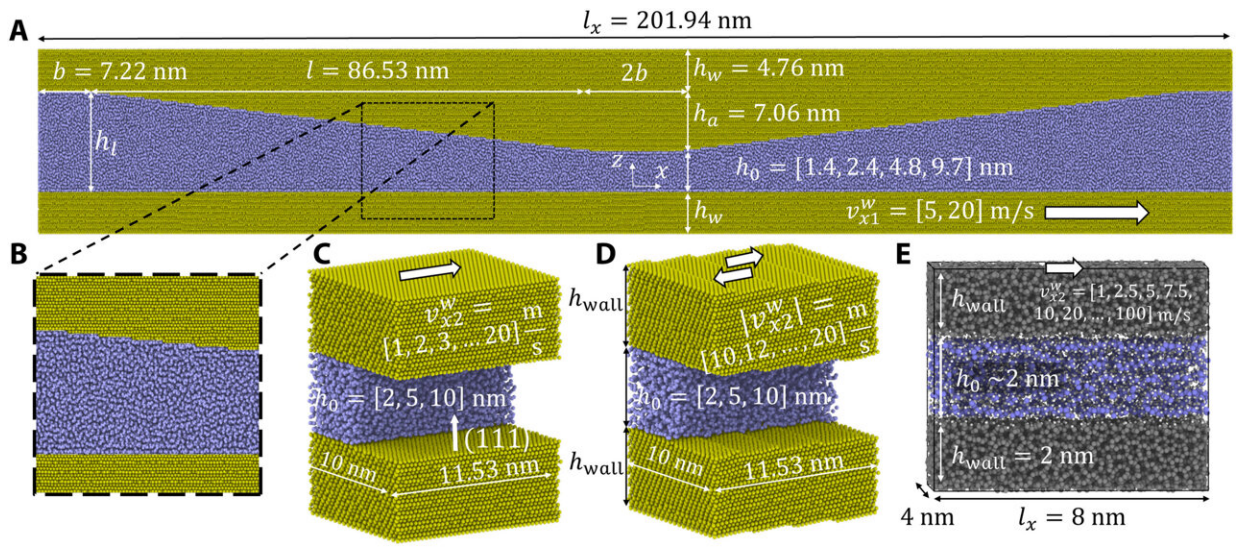
Making extremely thin lubricating films predictable: Extension of the Reynolds equation by a non-linear wall slip law

December 7 2023, by Anabel Thieme



Atomistic models used in the MD simulations.(**A**) Converging-diverging channel of gold filled with hexadecane. Gold atoms are depicted in yellow and hexadecane molecules are depicted in blue. The *z*/*x* aspect axis ratio is 2.5 to improve the readability of the plot. Periodic boundaries are applied in *x* and *y* directions. (**B**) Magnification of the dashed rectangle in (A) showing the atomic structure of the gold surfaces. (**C** and **D**) Parallel channels with Au surfaces having the same roughness characteristics as the bottom and top walls of the CDC, namely, atomically flat Au(111) and Au(111) terraces, respectively. Only half of the hexadecane molecules are shown. (**E**) Parallel channel formed by hydrogenated amorphous carbon surfaces (in black) and filled with 1-decene trimers (in blue). Because of the pressure equilibration in the hexadecane and the elasticity of the walls of the CDC, there are deviations from the target values h_0

= [2, 3, 5, 10] nm of the minimum gap height. Pressure equilibration was performed with p_n = [0.2, 0.4, 0.6, 0.8, 1] GPa in (A), p_n = [0.1, 0.4, 0.6, 0.8, 1] GPa in (C), p_n = [0.8, 1] GPa in (D), and p_n = [0.2, 0.5, 1, 1.5, 2] GPa in (E). During sliding with constant h_0, there are small deviations from the nominal values of the average pressure (