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Studying nanoscale slip mechanisms of simple fluids at low and high shearing velocities by molecular dynamics XIN YONG, LUCY ZHANG, Rensselaer Polytechnic Institute — Understanding slip is of great importance, especially in the emerging research topics and applications of nanofluidics. In this study, we reveal the nanoscale slip mechanisms in different flow regimes that are characterized by shearing velocities. They are modeled using direct molecular dynamics simulation of a nanoscale Couette flow system. An isothermal fluid system is built by the Dissipative Particle Dynamics thermostat, with either rigid or thermal walls. The purpose of using isothermal simulation is to simplify the discussion by excluding the significant influence on the slip from dramatic viscous heating at high shear rates. Our results show an abrupt jump of slip length when the shearing velocity is increased to a critical value, implying a transition in the slip mechanisms. The transition is followed by a linear increase in slip length, with a slope that is dependent on the characteristic of the walls and wall models. Increasing the rigidity of the thermal walls results in slip behaviors that asymptotically approach the one of a rigid wall. The slip behavior supports the two mechanism hypothesis shown in Martini et al.,[1] but with a different interpretation for the slip mechanism at high shearing velocities.

[1]A. Martini, H.-Y. Hsu, N. A. Patankar, and S. Lichter, Phys. Rev. Lett. 100, 206001 (2008).

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