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Understanding the nanoscale liquid-solid interfacial phenomena in a Couette flow XIN YONG, LUCY ZHANG, Rensselaer Polytechnic Institute — Molecular dynamics simulations are used to study a nanoscale Couette flow and investigate the slip behavior at liquid-solid interfaces. We model liquid argon confined between two smooth rigid copper walls and the upper wall velocity is imposed to shear the fluid slab. The velocity fields, density distributions, flow boundary conditions and liquid structures/orderings are studied for walls ranging from hydrophobic to hydrophilic. We observe various flow boundary conditions ranging from pure slip to multi-layer locking in the simulations. The results show that, temperature, liquid-solid interaction parameter and shear rate are the major factor influencing the fluid structures at liquid-solid interfaces, thus determine the flow boundary condition. Different liquid states are named which are characterized by different liquid structures. Continuous transitions between states are also found. Furthermore, the positive correlation between shear rate and slip length is established and the temperature shift of the shear rate-slip length curve is observed. We confirm the unbounded slip length at high shear rates and correlates it to momentum transfer mechanism between liquid and solid atoms. In transient simulations, liquid may transit from several metastable states to a ground state under certain conditions.

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