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**Investigation of Flow Boundary Conditions and Diffusion in Nanochannels using Molecular Dynamics Simulations** ALI KHARAZMI, NIKOLAI PRIEZJEV, Michigan State University — The influence of nano-confinement and slip boundary conditions on the thermal motion of fluid molecules is investigated using the LAMMPS molecular dynamics program. We consider a neutral Lennard-Jones fluid confined by crystalline walls with weak surface energy. Particular attention was paid to the implementation of a wall model that allows fine adjustment of the slip length without changing the interfacial fluid structure. We used the original Steele's surface energy decomposition, i.e., that the interaction potential between a fluid molecule and a solid substrate can be expressed as a Fourier expansion in the reciprocal-lattice vectors of the substrate surface. The local diffusion coefficients in the directions parallel and perpendicular to confining walls were estimated as a function of a distance from the walls and then correlated with the slip length. The results of this numerical study are important for interpretation of nano-PIV (Particle Image Velocimetry) measurements of interfacial shear flows and boundary slippage. Financial support from the National Science Foundation (CBET-1033662) is gratefully acknowledged.

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