

Abstract Submitted
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Friction at ice-I_h / water interfaces¹ PATRICK B. LOUDEN, J. DANIEL GEZELTER, University of Notre Dame — We present evidence that the prismatic and secondary prism facets of ice-I_h crystals possess structural features that alter the effective hydrophilicity of the ice / water interface. This is shown through molecular dynamics simulations of solid-liquid friction, where the prismatic {10 $\bar{1}$ 0}, secondary prism {11 $\bar{2}$ 0}, basal {0001}, and pyramidal {20 $\bar{2}$ 1} facets are drawn through liquid water. We find that the two prismatic facets exhibit differential solid-liquid friction coefficients when compared with the basal and pyramidal facets. These results are complemented by a model solid/liquid interface with tunable hydrophilicity. These simulations provide evidence that the two prismatic faces have a significantly smaller effective surface area in contact with the liquid water. The ice / water interfacial widths for all four crystal facets are similar (using both structural and dynamic measures), and were found to be independent of the shear rate. Additionally, decomposition of orientational time correlation functions show position-dependence for the short- and longer-time decay components close to the interface.

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