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Comparative molecular dynamics study of vapor-exposed basal, prismatic and pyramidal surfaces of ice

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We present the results of molecular dynamics simulations in which ice Ih slabs with free basal, prismatic, 28 degrees pyramidal, and 14 degrees pyramidal facets are exposed to vapor. All simulations were carried out at 250 K using a six-site intermolecular potential. Characteristics common to all facets include spontaneous development of a quasi-liquid layer (QLL) within ˜10 ns, and QLL stratification into outer and inner sublayers having on average two and three hydrogen bonds, respectively. Vapor pressure, based on the rate of sublimation of molecules from the ice surface to the vapor phase, is found to be greatest for the 14 degrees pyramidal and basal facets (˜230 Pa), while significantly lower values are obtained for the prismatic and 28 degrees pyramidal facets (˜200 Pa). E-folding lifetimes and layer-specific bulk ice accommodation coefficients indicate much more frequent exchange between the QLL and inner ice layers for pyramidal surfaces compared to basal and prismatic surfaces. The free prismatic facet and 28 degrees pyramidal facets exhibit significant anisotropic diffusivity, in-plane motion being faster in the trans-prismatic direction than in the basal-to-basal direction. Implications of these molecular-level findings for the growth of ice crystals by vapor deposition and for adsorption of gas phase species of atmospheric relevance onto ice will be discussed.

Please list some keywords

ice surface, vapor pressure, surface diffusivity, surface lifetime, basal, prismatic, pyramidal

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