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Two-stage melting of the ice Ih (0001) surface by molecular dynamics: A molecular dynamics study MIZUKI KUGA, Graduate School of Science and Technology, Niigata University, HIROSHI IYETOMI, Department of Mathematics, Niigata University — We report a molecular dynamics simulation study of the structure and energetics of Ice Ih with a free basal (0001) surface. Especially we cast a new light on the formation of a quasi-liquid layer (QLL) at the surface prior to the melting of bulk ice. Detailed analysis of functional behavior of the total and potential energies with respect to temperature clearly separates the surface melting process into two stages. As temperature is increased, the outermost bilayer of the ideal surface first starts disordering in a progressive way with detachment of water molecules from the surface. During this first stage of surface melting, the energies show no discontinuous change as a function of temperature. Subsequently to fully developed disordering of the top layer, the surface shows stepwise melting in a narrow temperature range of around 10 K. This second stage of surface melting has first-order phase-transition-like characteristics as demonstrated by structural relaxation from an initial metastable (super-heating) state to the stable state during which the surface is liquefied layer by layer. Accordingly, it turns out that each of the stable QLL states designated by the number of liquefied bilayers has its own branch of the potential energy.

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