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ABSTRACTS OF PAPERS ACCEPTED FOR THE SYMPOSIUM BUT NOT PRESENTED

ENTHALPY RELAXATION PHENOMENON IN A HEAVY ICE CRYSTAL

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Abstract. The heat capacities of quenched and annealed heavy ice Ih were measured in the temperature range 14 to 300 K by an adiabatic calorimeter. A relaxational thermal anomaly was found at around 115 K and this phenomenon was ascribed to the onset of deuteron ordering in the crystal. The average activation enthalpy of the relaxational process was determined to be (26 ± 5) kJ mol^{-1}. Residual entropies of the crystal were recalculated on the basis of the present heat-capacity data combined with the revised values for enthalpy of vaporization, saturated vapour pressure, and spectroscopic entropy. They are $(3.47\pm0.41$ J K^{-1} mol^{-1} for the quenched crystal and (3.44 ± 0.41) J K^{-1} mol^{-1} for a crystal annealed at 102–106 K for 264 h. The characteristics and the origin of the anomaly are discussed in comparison with that of ordinary ice.

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RECONSTRUCTED LEDGES: ICE CRYSTAL GROWTH WITHOUT DISLOCATIONS

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Abstract. We give a simple explanation of recent experimental evidence that ice crystals may grow in water vapor at low supersaturation (i.e. under atmospheric conditions) without screw dislocations. Examination of the intermolecular potential shows that by assuming non-bulk-like orientations, dangling molecules at surface-cluster edges may form strong hydrogen bonds with substrate molecules. This leads to a study of ice surfaces within the framework of an Ising-like model in which molecules with nearest neighbor vacancies which can provide vertical bonding are allowed *two* distinct states, yielding *bulk-like* as well as *reconstructed* monolayer ledges. The surface roughening transition is examined for this model by means of (i) a Monte Carlo determination of critical points and (ii) an analytical treatment of nucleation clusters. It is found that rough surfaces and, correspondingly, (dislocation-less) surface nucleation growth, prevail at temperatures below the bulk melting point over a wide range of feasible binding energies.

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