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Deciphering the morphology of ice films on metal surfaces

Although extensive research has been aimed at the structure of ice films [1], questions regarding basic processes that govern film evolution remain. Recently we discovered how ice films as many as 30 molecular layers thick can be imaged with STM [2]. The observed morphology yields new insights about water-solid interactions and how they affect the structure of ice films. This talk gives an overview of this progress for crystalline ice films on Pt(111) [2-5]. STM reveals a first molecular water layer very different from bulk ice: besides the usual hexagons it also contains pentagons and heptagons [3]. This structural motif also occurs on other metal substrates [6]. Slightly thicker films ($\sim 1\text{nm}$, at $T>120\text{K}$) are comprised of $\sim 3\text{nm}$ -high crystallites, surrounded by the one-molecule-thick wetting layer. These crystals dewet by nucleating layers on their top facets [4]. Measurements of the nucleation rate as a function of crystal height provide estimates of the energy of the ice-Pt interface. For $T>115\text{K}$ surface diffusion is fast enough that surface smoothing and 2D-island ripening is observable [5]. By quantifying the T -dependent ripening of island arrays we determined the activation energy for surface self-diffusion. The shape of these 2D islands varies strongly with film thickness. We attribute this to a transition from polarized ice at the substrate towards proton disorder at larger film thicknesses. Despite fast surface diffusion ice multilayers are often far from equilibrium. For example, ice grows between ~ 120 and $\sim 160\text{ K}$ in its cubic variant rather than in its equilibrium hexagonal form. We found this to be a consequence of the mismatch in the atomic Pt-step height and the ice-bilayer separation and propose a mechanism of cubic-ice formation via growth spirals around screw dislocations [2].

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