

MAR11-2010-004420

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Deciphering the morphology of ice films on metal surfaces¹

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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]. 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 ~ 160 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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¹Joint work with N.C. Bartelt and S. Nie, Sandia Natl. Labs, CA. This work was supported by the Office of Basic Energy Sciences, Division of Materials Sciences, U.S. DOE under Contracts No. DEAC04-94AL85000.