Wetting and ice growth on a stepped surface

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Abstract

Despite the importance of heterogeneous ice nucleation in many areas of science, ranging from aviation through biology to metrology, no simple molecular picture is available to explain why some surfaces are good ice nucleation agents and others are not. The simple idea that close packed, hexagonal metal surfaces with the correct lattice parameter would act as good templates for ice growth has proven ill founded [1]. Rather than forming an ice structure, commensurate with the surface, water often forms complex networks with water bound flat or H-down towards the surface. Typically these first layer structures do not have either the correct topological network, the correct corrugation, nor the correct proton orientation to permit multilayer growth without completely restructuring to match the ice film [2] , inhibiting multilayer ice growth. Recent simulations suggest that having the correct corrugation to match bulk ice enhances nucleation [3], and may direct the structure formed. From a molecular perspective, little is known experimentally about ice nucleation and growth on such surfaces.

Here we explore water adsorption and the transition from monolayer to multilayer ice growth on a highly corrugated, stepped surface, Cu(511). Water prefers to bind at low coordinate step sites in preference to the terrace [4], so this surface presents regular 1D arrays of binding sites, creating a complex, heterogeneous environment to water. Rather than simply decorating the hydrophilic step sites to form 1D chains, water on stepped Cu(511) forms an extended, 2D hydrogen-bonded network that binds strongly to the steps but bridges across the intervening hydrophobic Cu(100) terraces [5]. The network contains pentamer, hexamer, and octomer water rings that leave a third of the stable Cu step sites unoccupied in order to complete a 2D H-bonding network. The (31,−31) network is stabilized by binding 40% of the water flat on the step sites, and 30% of the water H down immediately below the step with the water dipole aligned in opposition to the step dipole [5]. DFT calculations show several different detailed proton arrangements have identical binding energies and these are imaged by STM.

The wetting layer is corrugated, but does not match the structure of bulk ice. Continued adsorption causes the first layer water to compress into a hexagonal (30,-11) network. This network is highly corrugated and contains H atoms pointing towards and away from the surface, allowing it to bind directly to second layer water. The hexagonal layer has a density very close to that of bulk ice and multilayer ice grows freely on this template. Based on STM, LEED, HAS and DFT simulations we discuss ice growth on this highly corrugated template [6].

References

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