An Investigation into the Structure of Water on an Open-Face of Ni(110)

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The rise of the ice bilayer model led to the assumption that a hexagonal, hydrogen bonded network of water molecules was the preferred arrangement, whether for an intact or (partially) dissociated water structure. It was only after recent investigations, on systems such as Cu(110) [1] and Pt(111) [2], that other cyclic arrangements were found, encouraging the consideration of other networks when investigating surface wetting.

Following the discovery of 1D pentagonal chains built exclusively from intact water molecules on Cu(110), Carrasco *et al*. studied the relationship between metal lattice parameter and water structure.[1,3] DFT calculations predict a strong correlation between the lattice parameter of open-faced metal surfaces and the relative stability of water pentamers versus hexamers. The results concluded metals with larger lattice parameters to have a preference for structures built from water hexamers, whilst those with lattice parameters smaller than Cu are expected to favour smaller pentagonal water units. With Ni having a lattice parameter 2.4% smaller than Cu, one would expect a pentagonal arrangement of water molecules to be even more favourable for the first wetting layer structure on Ni(110). Here we describe recent measurements of water adsorption on Ni(110) and compare the structures formed to those seen on Cu(110).

The 1D chains of pentagonal water rings observed on Cu(110) at low temperature [4] are not found on Ni(110). Water instead forms a 2D network growing along the close-packed Ni rows, built from hexamers and a larger doubled ring structure, quite different to that reported by Forster *et al*. on Cu(110). This abrupt change in binding geometry may either be due to the strong hydrogen-bonding network favouring the formation of an extended 2D overlayer rather than 1D chains along the close packed direction on Ni(110), or else the enhanced reactivity of this surface causing dissociation of the water molecules even at 77 K. When water is adsorbed at a higher temperature (180 K), two structures are observed; a 2D hexagonal network and 1D branched chains. Both of these have also been seen for water adsorption on Cu(110).[4][5] Annealing to 200 K desorbs water and eliminates the 2D hexagonal structure, replacing it with chains resembling the 1D branched structures previously reported on Cu(110). This overlayer exhibits two different arrangements, and is assigned to be the partially dissociated 1:1 H_2O:OH structure. Annealing above 210 K introduces another structure, coexisting with the partially dissociated 1D branched chains, associated with OH.

References:
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