

High-Resolution XPS and NEXAFS Experiments on Water and Formic Acid on Si(111)7 \times 7

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Water is known to adsorb dissociatively at room temperature on the Si(111)7 \times 7 surface, through a process in which one molecular O-H bond is broken, and the two resulting fragments bond to a rest atom (the OH group) and an adatom (the hydrogen) respectively. Together with dissociative adsorption, as the exposure level is increased surface oxydation takes place, where the oxygen atoms bond to Si atoms first and eventually insert in the Si-Si backbonds. This oxydation process has been followed in previous experiments by monitoring the XPS peak related to the Si 2p core level and observing the increase of new features on the high binding energy side of the peak which were attributed to Si atoms in different oxydation stages (Si⁺ up to Si⁴⁺). The measurements have been taken at MAX-Lab synchrotron on beamline I511. We were able to follow this oxydation process by monitoring for the first time the relative intensity and peak shape of the XPS spectral features related to the O 1s core level. This feature is rather weak, due to the low saturation coverage for this system, but the XPS measurements as a function of coverage clearly reveal the presence of two different components, one of them relatively growing as the exposure is increased. This multiple spectral feature is relatively structureless, without resolved vibrational components. Since the total instrumental resolution available at beam line I511 would be more than sufficient to detect high-frequency vibrational modes such as O-H stretching modes, it is evident that the core-hole lifetime broadening prevents such fine structure to be observed.

Formic acid is known to adsorb dissociatively on the Si(111)7 \times 7 surface via a chemical reaction in which a O-H molecular bond is broken and the formate fragment then bonds to the surface, although some doubts remained on whether the two O atoms are equivalent. We obtained XPS spectra for the O1s core line which clearly show two different components, therefore implying that the two O atoms are unequivalent and then formate adsorbed species form a single O-Si s bond and not a Si-O-O-C ring with partly delocalized bonds.

The analysis of the NEXAFS spectra obtained for both systems is not yet completed. While in the water spectra there seem to be some background problems, possibly due to the oxide formation, the NEXAFS spectra for formic acid show two sharp features around the C K-edge, the lowest-lying one with no strong angular dependence and the second one with a pronounced polarization dependence. Around the O K-edge, only the lowest-lying feature is evident

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