Surface X-ray Diffraction on Magnetite (001)

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Magnetite (Fe_3O_4) raises interest due to its ability to catalyse the water-gas shift reaction, its potential use in spintronics, and as a building block in organically linked magnetite nanoparticle supercrystals with exceptional mechanic properties. Since these applications depend on the surface properties of magnetite, it is important to understand the structure of the surface exposed to the different molecules used in these applications.

The (001)-surface of magnetite is of particular interest because it is present as a facet on nanoparticles and could be used as a template to study single-atom catalysis. Upon preparation in ultra-high vacuum, it forms a $(\sqrt{2}\times\sqrt{2})R45°$ surface reconstruction. It was reported that this reconstruction gets lifted upon the adsorption of formic acid as well as atomic hydrogen and water vapor. The mechanisms of the lifting, however, remained unknown, especially since the previously established model for the structure of the reconstructed surface was recently shown to be incorrect, leading to the introduction of a new, significantly different structural model with a different stoichiometry[1,2] and thereby invalidating the previous interpretations of the lifting process.

Formic acid is known to dissociate into formate and hydrogen upon adsorption on the surface of magnetite from XPS, IR and STM measurements [3], with the formate binding in a bidentate configuration. The structure of the surface, however, remained unsolved. Water vapor is known to partially dissociate upon adsorption, hydroxylating the surface, and was proposed to show ordered mixed adsorption [4].

To get insights into the lifting process as well as the structure upon both adsorption of formic acid and water, we studied the surface structure of a Fe_3O_4 (001) single crystal by surface x-ray diffraction upon adsorption of formic acid at the ID03 beamline of the ESRF. We will present results on the lifting mechanism of the surface reconstruction with formic acid as well as the structure of the unreconstructed surface.

In addition, we studied the surface structure upon adsorption of water and atomic hydrogen by surface x-ray diffraction at the SixS beamline at the SOLEIL-synchrotron as well as at the MPG diffraction beamline at ANKA. We will briefly discuss the results of the structural analysis for the structure during and after water vapor dosing.

References:

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