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ESRF	**Experiment title:** Determining the structure of TiO_2(110)(2x1)-HCOO using surface x-ray diffraction	**Experiment number:** SI-313
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Report:

In the proposed experiment we had planned to investigate the structure of a 2x1 overlayer of formate on TiO_2(110)1x1 using surface X-ray diffraction (SXRD). This work forms part of a larger research programme of the applicants which studies the structure/property relations of well-defined metal oxide surfaces. This is a frontier area of surface science which has enormous fundamental and technological potential.

On the basis of STM [l], NEXAFS [2] and photoelectron diffraction [3], formate adopts the geometry shown below. Modelling of the surface x-ray diffraction from the 2x1 formate overlayer indicated that the fractional order reflections should easily have been visible. In the event, we could not detect fractional order reflections. This could arise because of a problem with sample preparation exacerbated by the lack of LEED optics on the end station. However, this is unlikely because the method of formation of the ordered overlayer is well established, and the research group has considerable experience in the methodology. It seems more likely that x-ray beam

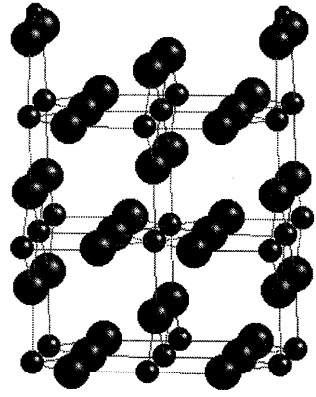

Figure 1: The current model for TiO_2(110) (2x 1)-formate. The formate molecules at the top right and left of the model are bonded in a bidentate fashion to two Ti atoms.

damage caused the overlayer to dissociate. Desorption of C-containing species did not occur, as evidenced by Auger measurements before and after exposure of the overlayer to the beam.

Two crystal truncation rods, the 0,l and 2,1, were measured to gather more information about the state of the surface. The diffraction data were collected using conventional rocking scans, After subtracting the background intensity, the diffraction peaks were corrected for effective sample area, polarisation of the X-ray beam and Lorentz factor, such that $I_{hk} = |F_{hk}|^2$.

Data were analysed from a starting point of the clean surface structure [4] and the formate geometry calculated by the Hartree-Fock method [3]. Only the height of the molecule above the surface was allowed to vary in the fit along with the bridging 0 and the top layer Ti atom positions, the formate occupancy and a Debye-Waller factor. In addition, the scale factor, surface fraction and roughness parameter were varied. The best fit is shown in Fig. 2. It corresponds to an R factor of 7.2. The principle feature of the fit parameters is the very high roughness parameter (0.22). This is not inconsistent with x-ray induced dissociation of formate.

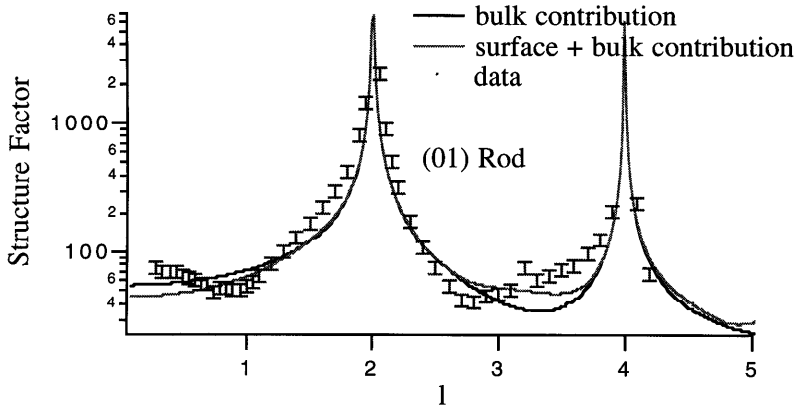

Figure 2: The 0,1 rod profile recorded from TiO_2(110)/formate at room temperature.

References

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