



	Experiment title: The structure of the TiO ₂ (110)-H ₂ O interface	Experiment number: SI-1718				
Beamline: ID32	Date of experiment: from: 27/06/08 to: 08/07/08	Date of report: 14/08/08				
Shifts: 18	Local contact(s): Dr Blanka Detlefs and Dr. Jörg Zegenhagen	<i>Received at ESRF:</i>				
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Report:

In this experiment we performed a quantitative structural determination of the interface between TiO₂(110)1x1 and liquid water, employing surface X-ray diffraction (*SXRD*). *In situ* substrate preparation was carried out in *UHV* facilities located in the Surface Characterisation Laboratory (*SCL*) by repeated cycles of argon ion sputtering and annealing until a sharp 1x1 *LEED* pattern and characteristic STM images were obtained. The sample was then transferred under *UHV* to beam line *ID32*, using a *Baby* chamber configured for solid/liquid interface experiments [1]. *SXRD* measurements were performed on the diffractometer in *EHI*, employing a photon energy of 17.71 keV. Data were collected at room temperature using conventional rocking scans, in which the sample is rotated about its surface normal while scattered x-ray intensity is measured. For a given (*h,k*) these were performed at different *l*, enabling crystal truncation rods (*CTRs*) to be compiled. Prior to water exposure, 12 *CTRs* (550 reflections) were acquired from the TiO₂(110)1x1/*UHV* interface, both to ensure sample integrity and to easily identify structural changes due to the presence of liquid water. Water immersion was achieved using a capillary tube to deliver a water droplet onto the TiO₂(110)1x1 surface, which had previously been exposed to an atmospheric pressure of N₂. 30 *CTRs* (1450 reflections) were measured from the TiO₂(110)1x1/H₂O interface.

Representative *CTRs* from the $\text{TiO}_2(110)1\times 1/\text{UHV}$ and $\text{TiO}_2(110)1\times 1/\text{H}_2\text{O}$ interfaces are displayed in Fig. 1. Clear differences are observed, demonstrating that *SXRD* is sensitive to the geometric changes induced by liquid water. Detailed analysis of these results to elucidate the precise atomic scale structure is currently ongoing. We note that the data from $\text{TiO}_2(110)1\times 1/\text{UHV}$ replicated that collected previously [2], indicating the reliability of our present substrate preparation.

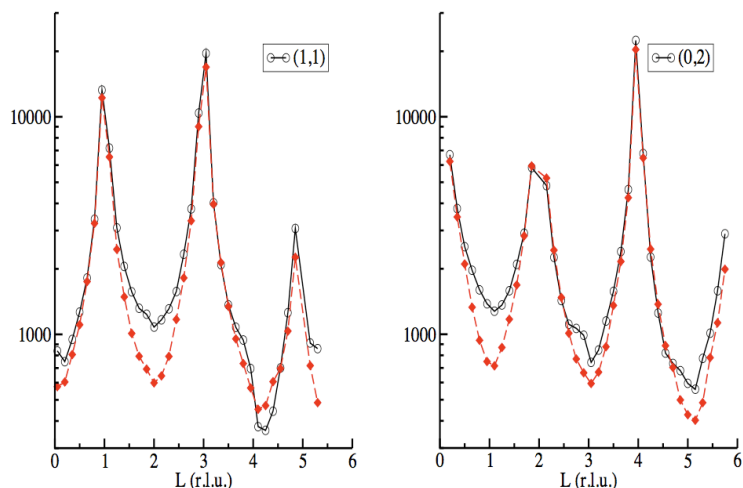


Fig. 1. *CTRs* from the $\text{TiO}_2(110)1\times 1/\text{UHV}$ interface (black: open circles) and $\text{TiO}_2(110)1\times 1/\text{H}_2\text{O}$ (red: filled circles)

References

- [1] www.esrf.fr/UsersAndScience/Experiments/SurfaceScience/ID32/SurfaceLab/
- [2] G. Cabailh, X. Torrelles, R. Lindsay, O. Bikondoa, I. Joumard, J. Zegenhagen and G. Thornton, Phys. Rev. B Rapid Comm. 75, 241403 (2007)