	Experiment title: TiO2(110)1x2: Determining the structure of a reconstructed metal oxide surface	**Experiment number**: SI-1199
Beamline: ID32	**Date of experiment**: from: 06/07/05 to: 11/07/05	**Date of report**: 14/09/05
Shifts: 18	**Local contact(s)**: Dr Isabelle Joumard	*Received at ESRF:*

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Preliminary report:

In this experiment we performed a quantitative structure determination of the x-linked (1x2) reconstructed phase of clean TiO_2(110), employing surface x-ray diffraction (*SXRD*) and scanning tunnelling microscopy (*STM*).

Sample preparation, which involved repeated cycles of argon sputtering and annealing, was carried out using the *UHV* facilities located in the Surface Characterisation Laboratory (*SCL*) associated with ID32. Phase integrity, that is the presence of the *x-linked* (1x2) structure over the entire surface, was ascertained by *STM* (see Fig. 1), before transferring the sample to the beam line under *UHV*, using a *Baby* chamber [1]. Access to the *STM* proved to be invaluable, as it allowed us to determine that the first sample prepared was not of sufficient quality for SXRD (*N.B. LEED* pattern was sharp and bright). Images evidenced a high density of shear planes, which are characteristic of an over reduced sample, and limited terrace sizes. Both of these features would lead to the collection of significantly poorer *SXRD* data. The second sample prepared was satisfactory.

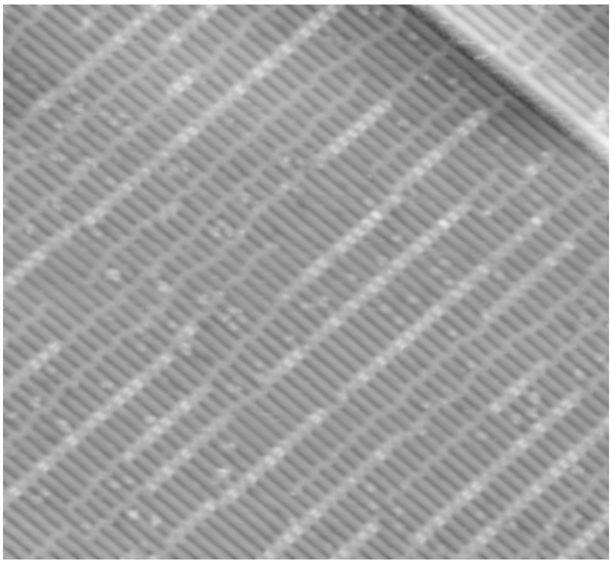

Figure 1: STM image of the TiO_2-(1x2) surface (1.26V, 0.36nA)

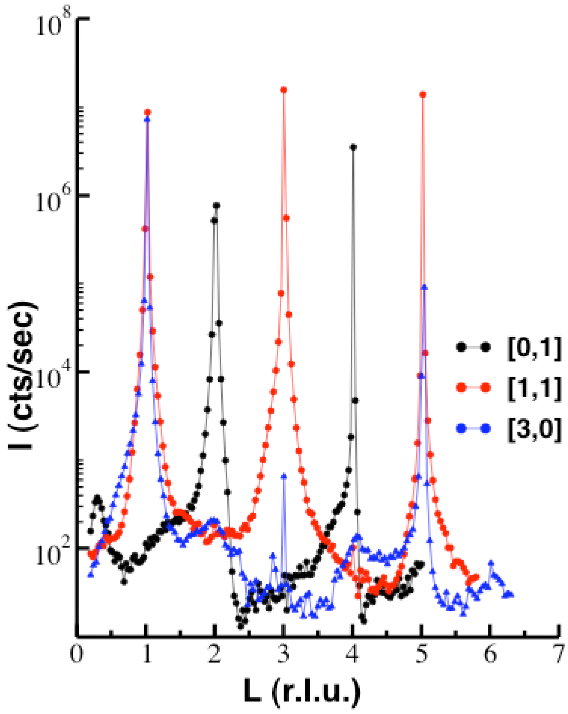

Figure 2: Experimental L-scans displayed on a Logarithmic scale

For the *SXRD* measurements an X-ray energy of 15.7 keV was utilised. Diffraction data were collected at room temperature using either conventional rocking scans, or so called L-scans. Using the former approach we acquired a large data set of fractional order rods that only contain information arising from the superstructure (approximately 1000 reflections). A number of crystal truncation rods (CTR's) were obtained using the L-scans approach. These contain information from both the substrate and the superstructure (approximately 400 reflections); several examples are depicted Fig 2.

Analysis is not yet complete, but given the extent and quality of the data we expect to be able to clearly identify the nature of the x-linked (1x2) reconstruction, discriminating between the various models presently circulating in the literature [2-5].

References:

[1] www.esrf.fr/UsersAndScience/Experiments/SurfaceScience/ID32/SurfaceLab/
[2] H. Onishi and Y. Iwasawa, Surf. Sci. 313, L783 (1994).
[3] C.L. Pang *et al*, Phys. Rev. B 58, 1586 (1998).
[4] R.A. Bennett *et al*, Phys. Rev. Lett. 82, 3831 (1999).
[5] S. Takakusagi *et al*, Surf. Sci. 523, L41 (2003).