ESRF

Experiment title:

The Structure of $SrTiO_3(100)$: The Effect of **O** Vacancies and the Ferroelectric Transition

Experiment number:

SI 160

Beamline:

ID3 BL7

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Local contact(s):

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Report: **In the** proposed experiment we had planned to investigate the surface relaxation of the stoichiometric 1x1 and reduced 2x2 phases of $SrTiO_3(100)$ 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.

While the main instrumentation worked very well, at the time of the allocated experimental period neither RHEED nor Auger equipment was available. For this reason we focussed on studies of the stoichiometric 1 xl surface of $SrTiO_3$(1 00), for which surface preparation is relatively straightforward. The additional time made available by the smaller programme on $SrTiO_3$(1 00) allowed us to make measurements of the surface relaxation of the 1x2 reconstructed surface of TiO_2(1 10) at room temperature by measuring partial order reflections and crystal truncation rods (CTR). The latter were selected on the basis of computer modelling using the code of Vlieg et al [1]. Because of the absence of Auger data to confirm that we had a nominally clean surface, it will be necessary to repeat a limited number of the diffraction measurements. For $SrTiO_3$(1 00), we have recently achieved this through an experiment at Daresbury. For TiO_2(1 10), we plan to repeat a few measurements during our future studies on ID3.

The surface structure of $SrTiO_3$(1 00)1x1 was investigated at three temperatures:

at room temperature and on either side of the cubic to tetragonal bulk ferroelectric phase transition at 100 K. The diffraction data were collected using conventional rocking scans which enabled a set of CTRS [3] to be compiled. Some rods measured from TiO_2(110)1x2 are shown in Fig. 1. Lorentzian profiles were fitted to the TiO_2(110)1x2 dataset whereas Gaussian profiles were fitted to the scans recorded from $SrTiO_3$(100). The diffraction profiles from a reconstructed surface are Lorentzian rather than Gaussian due to domain broadening effects. 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 $I_{hk} = |F_{hk}|^2$. Reference reflections were regularly measured throughout the data acquisition period as a method of monitoring surface contamination, none being apparent.

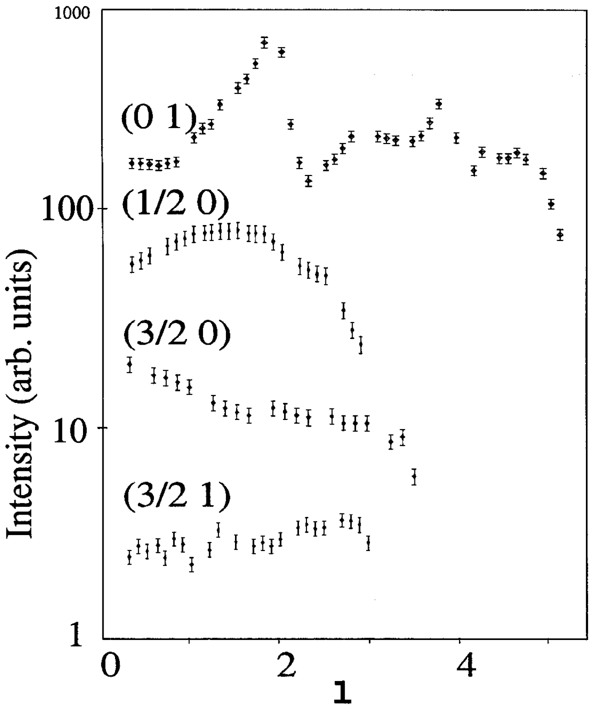

Figure 1: Selected rod profiles measured from TiO_2(110)1x2.

Full quantitative analysis of each dataset should yield a complete structural determination of the surface. In the case of $SrTiO_3$(100), this now in hand following the characterisation checks noted above. The measurements at 50 K and 110 K, in addition to the room temperature data will allow us to investigate the claim that the surface phase undergoes the ferroelectric transition at a temperature 20 K higher than the bulk [2]. This is of potential importance in conection with the epitaxial growth of high-Tc materials on $SrTiO_3$(1 00). The TiO_2(110)1x2 data will resolve a current discrepancy regarding the interpretation of STM data [4].

References

1. E. Vlieg et *al*, *Surf. Sci.* 209 (1989) 100.
2. N. Bickel, G. Schmidt, K. Heinz and K. Muller, Phys. Rev. Lett. 62 (1989) 2009.
3. R. Feidenhans'1, Surf. Sci. Rep. 10 (1989)105 .
4. U. Diebold *et al*, Phys.Rev.Lett. 77 (1996)1322.