



	<b>Experiment title:</b> Surface Relaxation of SrTiO <sub>3</sub> (100)	<b>Experiment number:</b> SI 160
<b>Beamline:</b> ID3 BL7	<b>Date of experiment:</b> from: 03 Apr 1996                      to: 09 Apr 1996	<b>Date of report:</b> 25 Feb 1997
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Report: In this work we investigated the surface relaxation of the stoichiometric 1x1 surface 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.

The surface structure of SrTiO<sub>3</sub>(100)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. This work is motivated by recent theoretical work which has predicted significant rumpling and relaxation at room temperature [ 1,2]. It also allows us to investigate the claim that the surface phase undergoes the ferroelectric transition at a temperature 20 K higher than the bulk [3]. This is of potential importance in connection with the epitaxial growth of high-Tc materials on SrTiO<sub>3</sub>( 100).

The diffraction data were collected using conventional rocking scans which enabled in plane data and a set of CTRs to be compiled. Gaussian profiles were fitted to the scans recorded from SrTiO<sub>3</sub>(100). 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.

