

ESRF

	Experiment title: Surface Relaxation of SrTiO ₃ (100)	Experiment number: SI 160
Beamline: ID3 BL7	Date of experiment: from: 03 Apr 1996 to: 09 Apr 1996	Date of report: 25 Feb 1997
Shifts: 18	Local contact(s) : Dr S Ferrer	<i>Received at ESRF:</i> 28 FEB. 1997

Names and affiliations of applicants (* indicates experimentalists):

G. Charlton *, C.A. Muryn *, R. McGrath, G. Thornton *, IRC in Surface Science, Manchester and Liverpool Universities, UK
S. Breman *, SSRL, Stanford, USA.
D. Norman, T.S. Turner, CCLRC, Daresbury Laboratory, UK.

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 SrTiO₃(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-T_c materials on SrTiO₃(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 SrTiO₃(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.

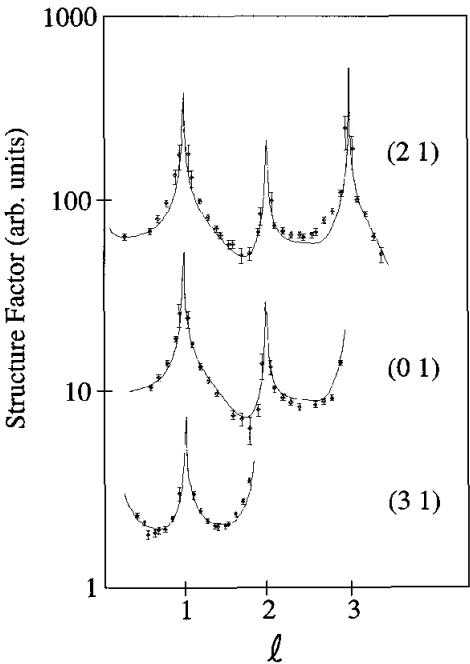


Figure 1: Selected rod profiles measured from $\text{SrTiO}_3(100)$.

SrO and TiO termination, as shown in Fig. 2. Included in the analysis was a variable concentration of the two terraces, the best fit giving a value of 25% SrO and 15% TiO .

Our experimental results for the atomic displacements are shown in the Table below, along with the relative displacements. The latter allow us to compare with theory [1].

DISPLACEMENTS (\AA)				RELATIVE DISPLACEMENTS (\AA)			
SXRD		TiO_2 Surface		SXRD		THEORY[1]	
SrO Surface	TiO ₂ Surface	SrO Surface	TiO ₂ Surface	SrO Surface	TiO ₂ Surface	SrO Surface	TiO ₂ Surface
Sr(1)	-0.24 ± 0.03	Ti(1)	0.00 ± 0.01	Sr(1)-O(1)	0.11 ± 0.20	Sr(1)-O(1)	0.18
O(1)	-0.35 ± 0.17	O(1)	-0.01 ± 0.13	Sr(1)-Ti(2)	0.00 ± 0.06	Sr(1)-Ti(2)	-0.19
Ti(2)	-0.24 ± 0.03	Sr(2)	-0.47 ± 0.01	Ti(2)-Sr(3)	-0.26 ± 0.05	Ti(2)-Sr(3)	0.06
O(2)	-0.42 ± 0.30	O(2)	0.23 ± 0.04	TiO ₂ Surface		TiO ₂ Surface	
Sr(3)	0.02 ± 0.02	Ti(1)-O(1)		Ti(1)-O(1)		Ti(1)-O(1)	
O(3)	0.14 ± 0.10	Ti(1)-Sr(2)		0.47 \pm 0.02		-0.15	
		Sr(2)-Ti(3)		*		Sr(2)-Ti(3)	

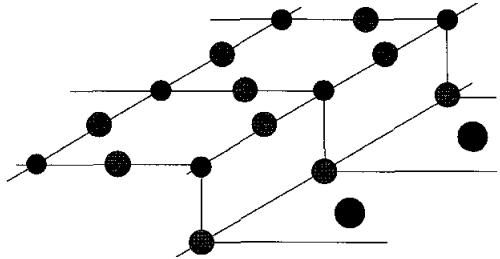


Figure 2: Schematic of the bulk-terminated $\text{SrTiO}_3(100)$ surface, showing the two types of termination. The upper terrace is TiO , the lower terrace is SrO .

The room temperature data has been **analysed** using the code of Vlieg et al [4]. The best fits to the three CTR's are shown in Fig. 1. In addition to these rod scans, in-plane intensities with symmetry equivalents were measured, giving rise to 12 inequivalent in-plane structure factors. The overall R-factor reduced to 2.4. Analysis is complicated by the fact that there are two terminations of a perovskite (100) surface. In this case there is a

References

1. J. Prade et al, J. Phys.: Condensed Matter 5 (1993) 13.
2. W.C. Macrodt, Phys. Chem Minerals 15 (1988) 228.
3. N. Bickel, G. Schmidt, K. Heinz and K. Muller, Phys. Rev. Lett. 62 (1989) 2009.
4. E. Vlieg et al. Surf. Sci. 209 (1989) 100.