XMaS the UK-CRG	**Experiment title: The phase transition of $SrTiO_3$ doped with Calcium**	**Experiment number:** 28-01-62
Beamline: **BM 28**	**Date of experiment:** from: 26/01/00 to: 1/02/00	**Date of report:** 1/04/00
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Report:

The structural phase transition of $SrTiO_3$ has been exhaustively studied but is still not understood. In particular, the origin of the two divergent length scales close to the phase transition and the extent to which the long length scale is associated with defects are unresolved puzzles.

FIG. 1: FWHM vs T(K) for scans along [100] (H-scans) and [011] (K-scans)

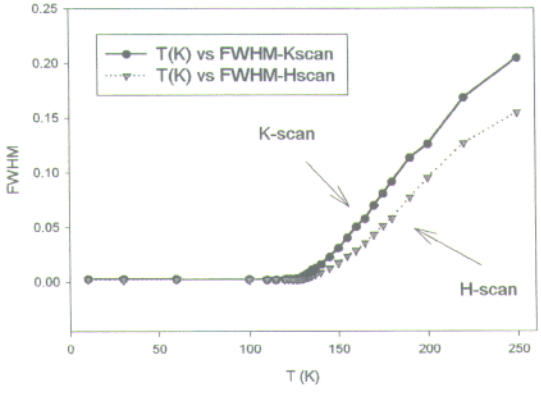
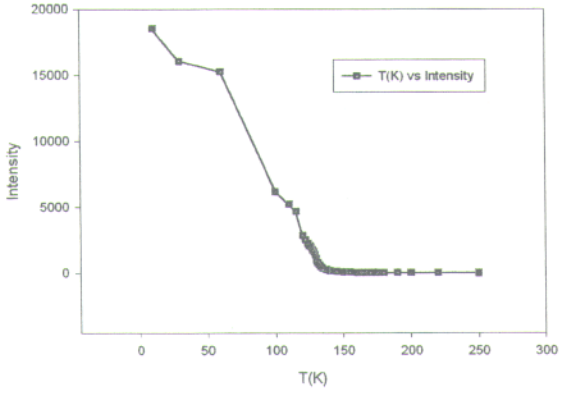


FIG. 2: Variation of the Intensity of a (3.5 0.5 0.5) satellite with a Temperature



We have studied a crystal of $SrTiO_3$ doped with 1% of Ca using x-ray scattering techniques and the XmaS diffractometer at the ESRF. The effect of only 1 % of Ca is to raise the structural phase transition by about 25K showing that in the neighbourhood of the Ca atoms the structure will be preferentially distorted.

We have measured the x-ray scattering close to the satellite vector (3.5 0.5 0.5) * $2\pi/a$ between 250K and 8K. The width of the scattering is shown in Fig. 1 as a function of temperature and it decreases with decreasing temperature until about 130K it is resolution limited. The intensity of the scattering is shown in Fig. 2 and it decreases with increasing temperature particularly abruptly near 130K. In more detail the widths are expected to have an exponent of about 0.7 whereas the data 130K and 180K suggest an exponent of larger than one. This suggests that the Ca has not only raised the transition temperature but has also given rise to a more rounded transition.

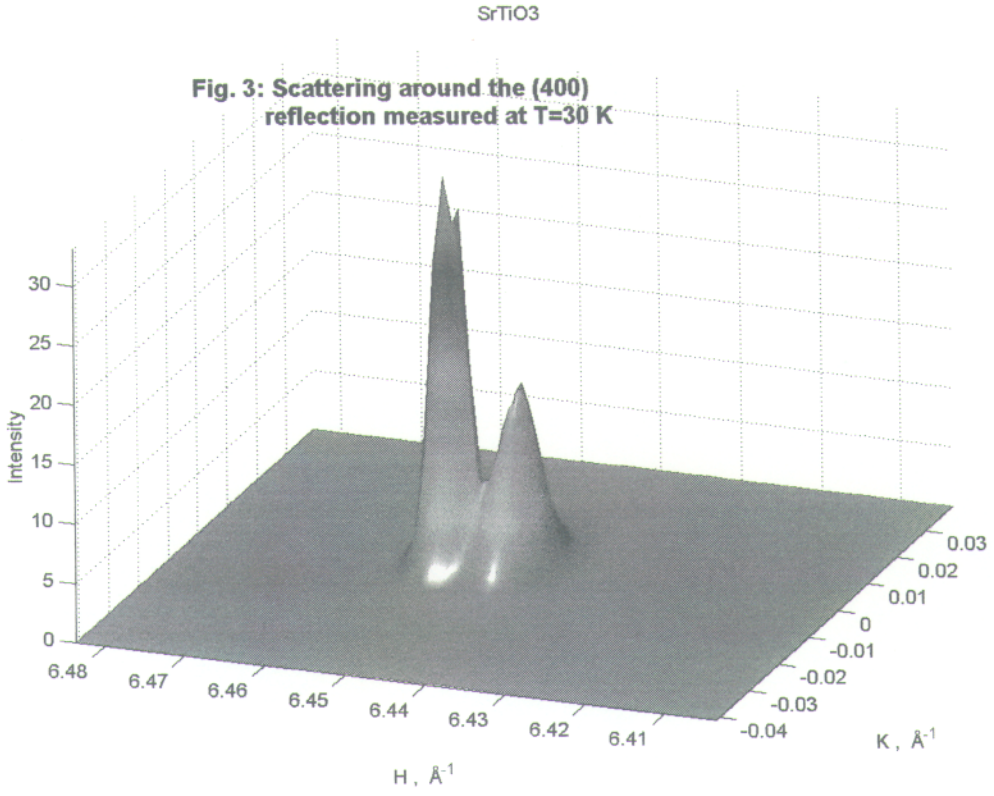


Fig. 3: Scattering around the (400) reflection measured at T=30 K

A more detailed analysis of the line-shape of the scattering is needed to determine whether there are two length scale components. In Figs. 3 and 4 we show three-dimensional plots of the scattering near the (400) and (3.5 0.5 0.5) satellite reflection at 30K. Near (400) two types of tetragonal domains are visible corresponding to domains with their long axis along or perpendicular to the [100] direction. Only one peak is visible for the satellite because the domains with rotations of the oxygen about (100) have zero structure factors. Combining these results we can deduce the properties of both domains.

Fig. 4: Scattering from the satellite peak at T= 30 K