	Experiment title: **Study of the surface structure of (110) and (111) SrTiO3 single crystals hosting a 2D electron**	Experiment number: HC-900
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Report:

The recently-discovered two-dimensional electron gases (2DEGs) that can be induced at interfaces between the wide-gap band-insulator $SrTiO_3$ (STO) and other bulk insulators, like $LaAlO_3$, have renewed a widespread interest in the physical properties of STO surfaces [1-3]. The STO (001) surface alone, if properly prepared, show a 2DEG with properties similar to the one observed in the case of interfaces obtained by depositing a LAO film on a STO crystal [4, 5]. Remarkably, 2DEGs were recently observed also at the interfaces between (110) or (111) STO single crystals and LAO thin films [6] and at the bare surface (110) [7] and (111) surfaces [8]. In spite of detailed Angle resolved Photoemission Spectroscopy (ARPES) studies, the surface structure and chemical composition of (100), (110) and (111) STO surfaces hosting a 2DEG are unkown, and the mechanism leading to the formation of the 2DEG is debated. In particular, there is no consensus about the surface chemical termination, nature of structural reconstructions (if any), and on the rumpling of the ionic planes. Following on LAO/STO interfaces [3] and STO surfaces [4] (see experiment SI 2335 and SI2522), here we used Grazing Incidence X-ray Diffraction (GXID) to establish the nature of the surface of (110) and (111) STO crystals hosting 2D-states.

The (110) and (111) surfaces hosting a 2DEG were prepared just before the GXID experiment by long (14 h) in-situ ultra high vacuum annealing (P<10-10 mbar, T=300°C) of 5x10x1 mm3 (110) and (111) STO single crystals. Prior to the experiment, as received single crystals were first prepared to get single terminated surfaces composed by steps one unit cell high. Preliminary lab-based experiments performed at the CNR-SPIN laboratories, showed that after the in-situ vacuum annealing step, both (110) and (111) surfaces are conducting, as shown by scanning tunneling spectroscopy. Both surfaces show very clean terrace-structure. However, Spot profile Analysis LEED, show that (110) surfaces are 4x1 reconstructurd and (111) surfaces are 3x1 reconstructed.

The same reconstruction has been found by GXID and thoroughly characterized by acquiring fractional order rods as well crystal truncation rods data Large data sets were acquired thanks to the 2D Maxipix detector using a beam energy of 24 KeV. The large data sets were corrected and integrated using the recent data reduction and analysis software BINocular developed at ID03 of ESRF.

In Fig. 1 we show an example of CTRs and fractional order rods acquired at room temperature on a STO(111) 3x1 reconstructed surface, and corresponding data fitting using ROD [9]. The data analysis shows that the STO(111) surface is composed by two topmost Ti layers, thus it is not stoichiometric (see Fig.2) The surface reconstruction extends down to 2 unit cells (about 1.3 nm) and involves both Ti, oxygen and SrO layers (see Fig. 2). Moreover , the surface displacements along the surface normal were found to be very small. The STO(111) surface structure and composition is extremely different from that one reported for STO(111) single crystals at the interface with $LaAlO_3$ (111) films [7], which also host a 2DEG. Similar analysis have been performed on STO(110) surface.

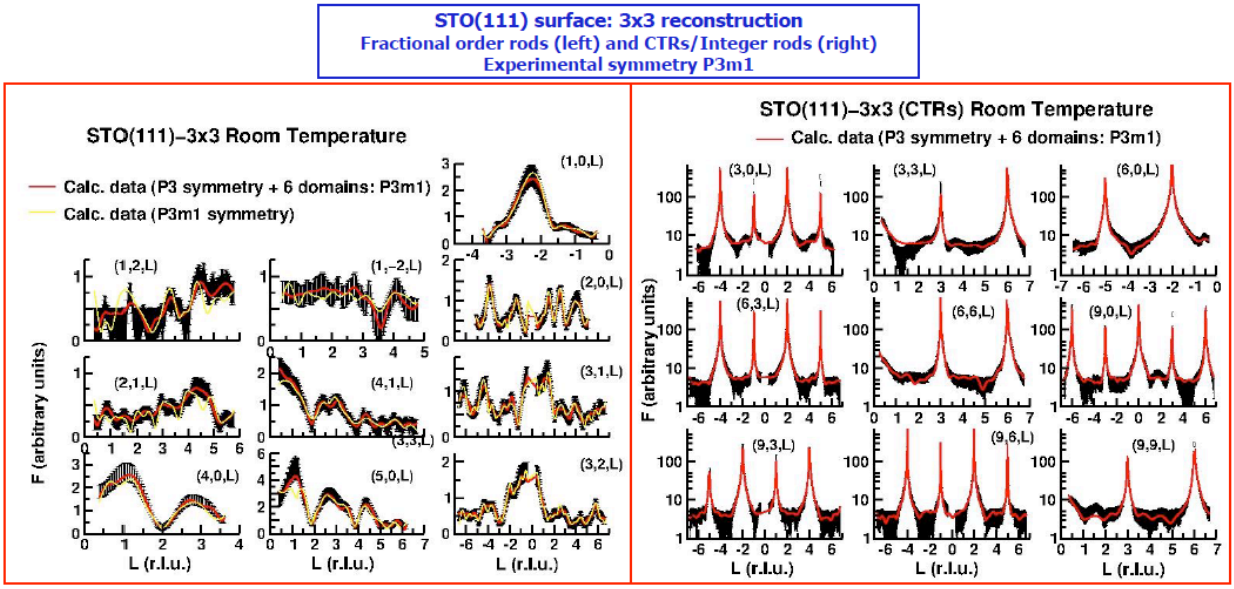

Fig.1: (a) Examples of fractional order rods (left) and CTR's (right) of 3x1 reconstructed STO(111) surface obtained from integration of 2D-Maxipix using BINocular. The data fitting have been performed using ROD-program and the model shown in Fig. 2.

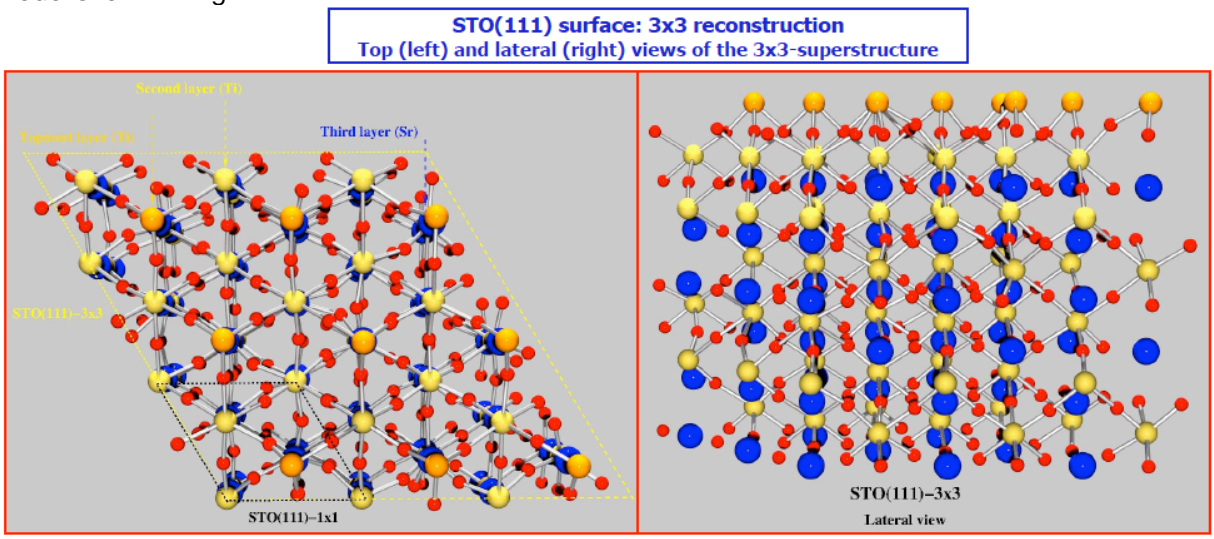

Fig. 2: Topmost (left) and later view of the reconstructed (111) STO surface. Yellow and orange ions are Ti-ions with different coordinations.

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