ESRF

SI1035

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## Report:

Oxide surfaces are important for applications in catalysis and thin film growth. Heteroepitaxial growth on oxide surfaces is strongly influenced by the exact surface composition and structure. However theoretical prediction of the surface structure of oxide surfaces is still a controversial issue. Among the perovskite $ABO_3$ compounds, $SrTiO_3$ is one of the most interesting examples because of its wide use as substrate for thin film growth [1] and for the potentiality in devices like Field effect Transistors (FET) [2]. The $SrTiO_3$ surface shows different kinds of reconstruction that depends not only on the treatment but also on the surface condition before the annealing procedure [3]. For example 1x1, 2x1, c(4x2) and c(6x2) reconstructions have been observed by LEED and STM. The major part of the experimental work has been performed on Ti-rich surfaces [3]-[5]. It turns out that the most stable surface termination is $TiO_2$, which can be obtained both by chemical etching [6] or by annealing in UHV at high temperature [3]. Recently SrO oxide terminated $SrTiO_3$ surfaces have attracted much interest because of the possible ferroelectricity predicted for this surface [7] and for thin film growth of HTS superconductors [8]. However to the best of our knowledge there is only one study on a presumed Sr-rich $SrTiO_3$ surface showing a $(\sqrt{5}\times\sqrt{5}) - R\ 26.6^\circ$ reconstruction [9].

In SI1035 experiment we have used Grazing incidence X-ray diffraction to study the surface structure of (100) $SrTiO_3$ substrates characterized by nominally Ti and Sr terminations. The single crystals have been

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| **T1** | $TiO_2$ | a) | 1x1 | 1.5 | 1.3 |
| **T2** | $TiO_2$ | b) | 1x1 | 1.5 | 1.3 |
| **T3** | $TiO_2$ | c) | 2x2 | 2.8 | 2.2 |
| **S1** | SrO | d) | 1x1 | 2.4 | 1.3 |
| **S2** | SrO | e) | 2x2 | 2.1 | 1.2 |

monolayer of SrO is deposited on a $TiO_2$ terminated $SrTiO_3$ substrate by Pulsed Laser Deposition. As reported in Ref. [10] the monolayer growth is obtained by the use of imposed layer-by-layer growth by pulsed laser interval deposition. The RHEED intensity oscillations are used to stop the deposition after one monolayer is deposited. In Fig. 1b the AFM image of a SrO terminated substrate is shown.

During SI1035 experiment we have used the new surface characterization laboratory (SCL) associated with ID32 that is equipped with STM, LEED, AES facilities, for preliminary characterization prior to the x-ray experiments at the beamline.

We studied five surfaces, three of them expected to be TiO2 terminated, and the other two expected to be SrO terminated [Table 1, 11]. Surfaces T3 and S2 were created by annealing T1 and S1 in 0.1 mbar of flowing O2 at 700 °C. These are typical conditions for the growth of oxides on STO single crystals. Only these surfaces are reconstructed and both of them exhibit a 2**x**2 lattice. After many attempts with a large number of possible structures, we have found that a surface composed of two different terminations is the only one able to reproduce the data. Starting from the interface with vacuum, we consider i) a 1x1 $TiO_2$ terminated STO unitcell covered by a disordered oxygen layer composed by two oxygen sublattices (O(0) and O'(0)) with equal population, and ii) a 1x1 STO $TiO_2$ surface having an additional SrO monolayer on the top. Both types of terraces are considered coherent, corresponding to a representation of a surface where both types of terminations are distributed without any particular order. The model is completed by the addition of one unit cell to the structure, common to the two surface terminations. The $TiO_2$ termination is composed of two layers, Ti(1) and Sr(1), while the SrO one consists of three, i.e. S(2), Ti(2) and Sr(3). The relative ratio between the two surfaces is a fitting parameter of the model, together with 19 parameters for the Z-displacements (cation and oxygen are considered separately), plus one Debye-Waller coefficient for each surface termination, a scaling factor and a roughness parameter. An average reduced $\chi^2$ for all data sets of about 2 (model I in Table I) is obtained, while single terminated models do not give a $\chi^2$ value lower than 4.

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