ESRF	**Experiment title: Structural study by grazing incidence high-resolution X-ray diffraction of epitaxial $SrTiO_3$ films grown by injection MOCVD on differents substrates – role of strain**	**Experiment number**: SI-1111
Beamline: ID32	**Date of experiment**: from: 08/09/2004 to: 14/09/2004	**Date of report**: 08/02/2005
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Report:

High dielectric permittivity (high K) oxides are extensively studied worldwide for the replacement of the SiO_2 gate oxide in CMOS and future advanced capacitors. Among the possible suitable candidates are the crystalline oxides such as the perovskite $SrTiO_3$ compound. The Laboratoire des Matériaux et du Génie Physique (LMGP) has developed a liquid injection source for Chemical Vapor Deposition reactor [1], now implemented on industrial equipment, allowing the control of the epitaxial growth of oxides with thickness on a nanometer scale (~ 0.4 nm, i.e. one monolayer) on monocrystalline iso-structural substrates [2]. The epitaxial growth of $SrTiO_3$ on silicon has not been successful yet by this technique. However, the first step is to generally understand the epitaxial growth of thin layers of STO on different substrates by this industrial CVD technique. Beside the fundamental interest of studying the growth of a ternary oxide by CVD, we believe that a better understanding of the initial growth stages will help us, in the future, to succeed in achieving epitaxial growth of $SrTiO_3$ on silicon by MOCVD by devising a proper strategy for the initial growth .

A first GIXRD study at 11keV has been performed at ID32 on two homoepitaxial $SrTiO_3$ thin films prepared by injection MOCVD (with thicknesses of 2.8 nm - 7 unit cells and 7.9 nm - 20 unit cells). The films exhibited excellent homoepitaxial quality and in plane measurements revealed a clear (2x2) surface reconstruction as shown on the Fig.1.

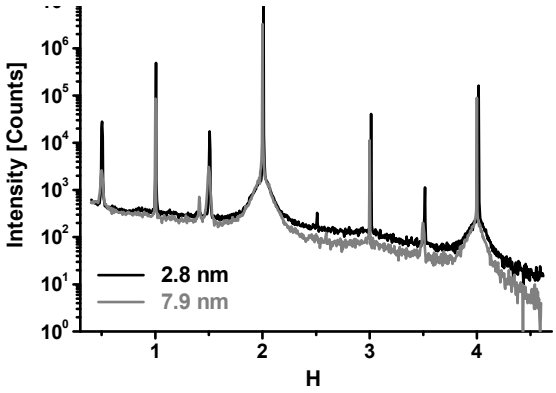

Fig. 1 H in-plane scans (K=0, L=0.1) of the homoepitaxial $SrTiO_3$ thin films with 2.8nm of thickness (dark line) and 7.9nm of thickness (grey line).

The fisrt step, in order to determine the atomic structure of this (2x2) reconstruction, was to determine its symmetry by recording and evaluating fractional order rods for different H and K values. We observed that the surface atomic structure has a P4mm symmetry and that the depth of the reconstruction extends over the last 1.5 unit cells (0.6 nm).
The reconstruction of the surface of a ternary compound can be very complicated. Thus, we chose to use direct method [3] to solve the structure. The P4mm symmetry allow us to limit the measurement of the fractional order rods to only 1/8 of the reciprocal space. Using an X-ray energy of 15keV, we measured 31 fractionnal order rods. The data were analysed by X. Torrelles from the Institut de la Cienca de Materials de Barcelona (Spain) using direct method. This method determine the electronic density at different depths below the surface. Figure 2 shows the resulting in-plane projection of the electronic density of a 2x2x4 supercell.

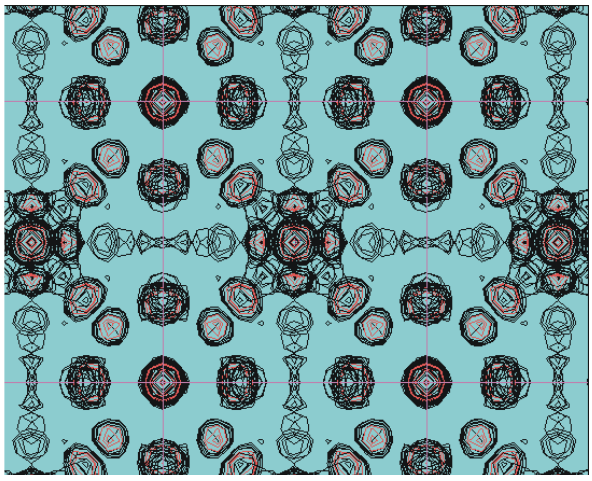

Fig. 2 Projection of the electronic density of a 2x2x4 supercell .

The position of the atoms in the supercell can be determined from the electronic density but a priori without discrimination between Sr, Ti or O. Refinement calculations are currently in progress to derive an atomic model for this 2x2 reconstruction.

[1] J.P. Sénateur, R. Madar, F. Weiss, O. Thomas, A. Abrutis, European patent 730671 (1994), US patent (2001)
[2] O.I. Lebedev, J. Verbeeck, G. Van Tendeloo, C. Dubourdieu, M. Rosina, P. Chaudouët, J. Appl. Phys. 94, 7646 (2003)
[3] J. Rius, C.Miravitlles, R. Allmann, Acta Cristallogr. A 52, 634 (1996)