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Report:

$SrTiO_3$ is one of the most widely studied perovskite oxide materials and it is characterized by a number of interesting electronic properties, including superconductivity, ferroelectricity under strain, or even exotic magnetism when combined with $LaAlO_3$ layers [1, 2]. After the discovery of a 2D Electron Gas (2DEG) at the (001) surface of cleaved $SrTiO_3$ (STO) single crystals [1], the physical properties of STO surfaces are deserving a renewed interest. Angle-resolved photoemission spectroscopy (ARPES) showed that the (001) $SrTiO_3$ surface hosts metallic 2D-electronic states independent of the bulk doping [1]. Following this finding, we performed a series of STM/STS (scanning tunnelling microscopy/spectroscopy) and ARPES experiments at the CNR-SPIN (Italy, Naples) and at the SIS beamline of PSI-SLS (Villigen, Switzerland), respectively, to investigate the nature of the 2DEG realized [3, 4]. One of the specific features of the electronic properties of the STO surface hosting a 2DEG is a splitting of the $3d_{xy}$ and $3d_{xz,yz}$ bands [1]. However, the structural and chemical nature of the (001) $SrTiO_3$ surface hosting a 2DEG remains unknown. This is particularly important, considering our recent finding of a correlation between the orbital reconstruction of the LAO/STO interface and the structural relaxation and rumpling of the $SrTiO_3$ layers close to the interface itself. In particular we have found that the simultaneous structural and electronic reconstructions precede the formation of the 2DEG, thus excluding the possibility that the phenomena is only driven by the electron doping of the

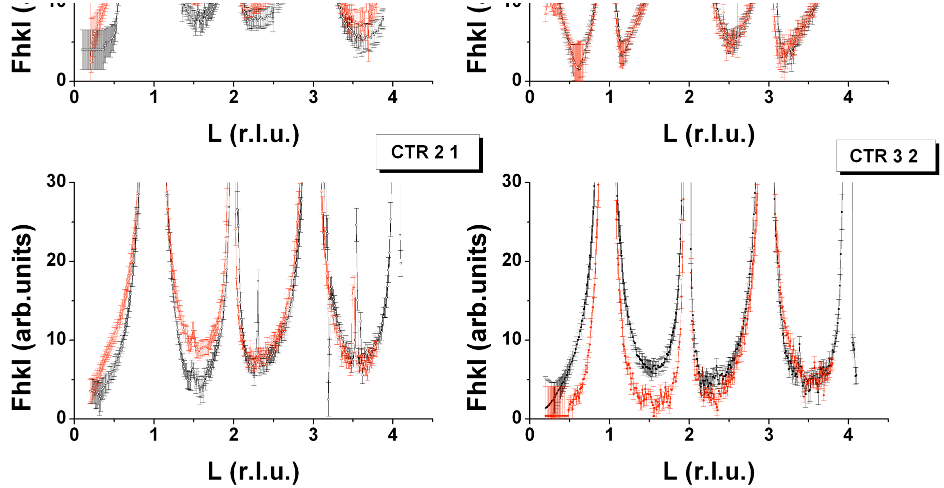

Fig.1: (a) Examples of CTR's obtained from integration of 2D-Maxipix data on high -mobility LAO/STO interfaces

used the 2D Maxipix detector and beam energy of 24 KeV. An example of CTR's are shown in Fig. 1, where we compare data at room temperature and at 30 K on an STO sample after annealing in vacuum at 250 °C. As shown in Tab. 1, some CTR's have been acquired as function of temperature during the annealing process and upon cooling. Finally, we have also studied the effect of oxygen adsorption at 30 K, to verify the role of oxygen overlayer on the structural properties of the sample.

The analysis of the experimental data is under-way. We are using both direct methods and standard fitting procedures (using ROD) to get a complete refinement of the structures of these samples to obtain information about intermixing and rumpling of the planes. In particular we have acquired up to 15 inequivalent (H, K) crystal truncation rods (CTR's) for each data set.

Sample	Data set	TEMPERATURE	TREATMENT
SURFACE NET #9	Complete set of CTRs	300 K	As received (etched)
SURFACE NET #8	Complete set of CTRs	30 K	UHV annealing 300°C
SURFACE NET#8	Partial set of CTRs	300K	UHV annealing 300 °C
SURFACE NET#8	Partial set of CTRs	30K	UHV annealing 300 °C and introduction of O2 10^{-6}mbar
SURFACE NET#9	Complete set of CTRs	30 K	UHV annealing 300 °C
SURFACE NET#9	Complete set of CTRs	300 K	UHV annealing 300°C
SURFACE NET PSI	Partial set of CTRs	300 K	UHV annealing 300°C

[1] A. Ohtomo and H. Y. Hwang, A high-mobility electron gas at the $LaAlO_3/SrTiO_3$ heterointerface, Nature

[4] Caviglia, A. D., Gariglio, S., Cancellieri, C., Sacépé, B., Fête, A., Reyren, N., et al. Two-Dimensional Quantum Oscillations of the Conductance at $LaAlO_3$/ $SrTiO_3$ Interfaces. Phys. Rev. Lett., 105, 236802 (2010).