ESRF	**Experiment title:** Surface X-ray diffraction study of the terminating layer and surface reconstruction of $Nd_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$ films	**Experiment number**: SI545
Beamline: ID 32	**Date of experiment**: from: 21 June 2000 to: 10 July 2000	**Date of report**: 28.02.2001
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Names and affiliations of applicants (* indicates experimentalists):

*Carmela Aruta,
*Fabrizio Ricci,
*Marco Salluzzo,
*Umberto Scotti di Uccio, INFM, Dip. di Scienze Fisiche Università di Napoli Federico II, P.le Tecchio 80, I-80125 Napoli, Italy
*Xavier TORRELLES Institut de Ciencia de Materials de Barcelona (C.S.I.C.) Campus de la U.A.B., 081893 Bellaterra, Barcelona, Spain
*Ivan Maggio-Aprile, Ø. Fischer, Département de Physique de la Matière Condensée, Université de Genève, CH-1211 Genève 4, Switzerland
Luc Ortega CNRS, Laboratoire de Cristallographie BP166, 38042 Grenoble

Report:

Structure and stability of the surfaces of high temperature superconductors (HTSC), as RBCO ($R_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$, R= rare earth or Y), are of basic interest concerning the heteroepitaxial growth processes of HTSC thin films. The surface properties of these type of films can be different from those of the bulk. These differences are usually manifested as surface reconstructions. For example, depending on the rare earth, oxygen content or cationic R/Ba ratio, a (2x2) or c(2x2) reconstruction can take place as observed for stoichiometric and Nd-rich $Nd_{1+x}Ba_{2-x}Cu_3O_{7-\delta}$ films, respectively.

The main objective of experiment SI545 carried out on ID32 beamline was the structural study of the $Nd_{1.1}Ba_{1.9}Cu_3O_{7-\delta}$ films.

These films exhibit a well defined c(2x2) surface reconstruction as observed films in situ by LEED on as grown. The same reconstruction is recovered on the same NBCO films exposed to air after a surface cleaning performed by an annealing at high temperature (500^o C) in an oxygen pressure of 1-10 mbar. This cleaning procedure was performed in situ during the experiment by using an additional UHV chamber specially conditioned for this purpose. Later, the sample was transferred to the diffraction chamber without breaking of the UHV conditions. The NBCO film was grown on a $SrTiO_3$(001) substrate and its thickness was of 60 nm as checked by x-ray diffraction.

The selected energy of the incident X-Ray beam was tuned to 13.9 KeV. In order to avoid contributions from the substrate, all measurements were performed at grazing incidence geometry. The angle of the incident beam was selected to a value of 0.35º which is slightly higher than the critical angle for this compound.

The analysis of the experimental data (CTR's) shows the presence of chemical disorder between Nd layers, where Ba and Cu layers are partially intermixed between them. The fit was performed considering 6 surface NBCO cells plus a bulk unit cell. The stoichiometry of this bulk unit cell was also adjusted. The c-parameter of the NBCO orthorhombic unit cell is 11.68 Å. All cationic positions are weakly relaxed along the normal surface direction.

Fractional order rods belonging to the c(2x2) surface reconstruction that was detected at the surface were also measured. As an example an L-scan for the (1/2 1/2) rod is shown in Fig. 1. The depth of this reconstruction is extended at least to 34 Å from the surface. This estimation was obtained after indexing the fractional order peaks. All fractional order rods show similar shapes with peak maximums located in the same positions. This is a characteristic behavior of centered unit cells. We used the fact that the L-spacing of the first peak is two times smaller than the separation L-distance between neighbour peaks in order to define the effective c-parameter of this c(2x2) reconstruction.

The final structure refinement is still in progress.

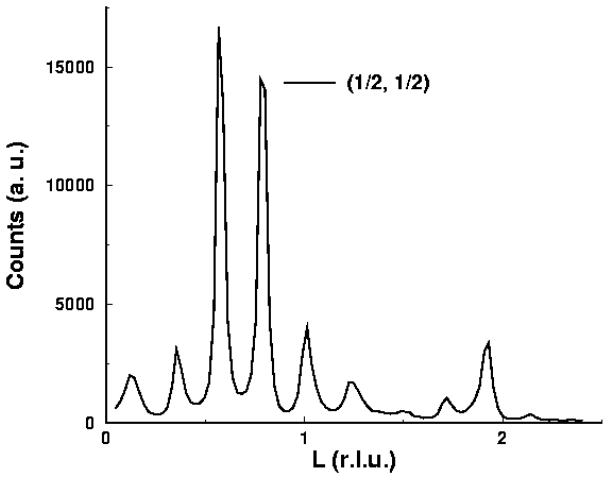

Fig. 2. L-scan of the (½, ½) fractional order rod measured on ID32 beamline for the c(2x2) reconstruction of a NdBaCuO film