# The Atomic Surface Structure of $YBa_2Cu_3O_{7-\delta}$ Thin Films and its Relation to Electronic Properties

C.M. Schlepütz, [1] P.R. Willmott, [1] R. Herger, [1] B.D. Patterson [1]

[1]*Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*

## Introduction

Despite much work on $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films, it remains an important open question how the film surface differs from the bulk structure and what consequences there might be for surface-sensitive measurements of electronic properties.

Here, we present a brief progress report of our attempt to answer some of these questions.

## Methods and Materials

High-quality flat YBCO thin films suitable for surface x-ray diffraction (SXRD) and angle resolved photo-emission spectroscopy (ARPES) are grown by a variant of conventional pulsed laser deposition (PLD), where a synchronized reactive gas pulse crosses the ablation plume, producing a highly-oxidizing plasma [1].

The UHV *in-situ* PLD growth chamber [2], in combination with a PILATUS II 2D X-ray pixel detector [3] at the Materials Science Beamline at the Swiss Light Source [4] is ideally suited to perform comprehensive SXRD studies. Using substrate materials with different lattice mismatches [i.e., $NdGaO_3$(110) (NGO), $YAlO_3$(001), and $SrTiO_3$(001) (STO)], strain effects on the film morphology can be investigated.

## Results

In order to monitor the evolution of the film structure, a precise knowledge of the underlying substrate structure is required. The (001) surface of STO has been investigated previously [5], and a comprehensive data set of more than 8000 structure factors has been collected for NGO(110). Figure 1 shows raw data of three representative scans: a) crystal truncation rod (CTR) for the quasi-cubic superstructure of NGO, b) nearly-forbidden CTR caused by the rhombohedral distortion, and c) fractional order rod (FOR) due to surface reconstructions.

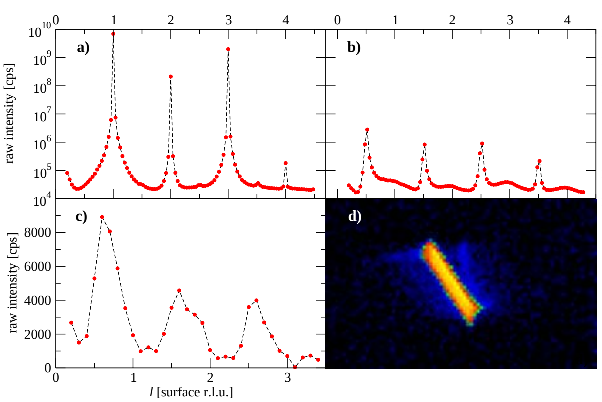


*Fig. 1: Diffraction data for the NGO(110) surface: a) and b) CTRs, c) FOR due to reconstructions, d) typical diffraction signal between Bragg peaks, collected with the PILATUS II pixel detector.*

YBCO films grown on NGO or STO are highly crystalline and very flat. Figure 2a) shows a x-ray reflectivity curve of a 74 nm thick film with a roughness of 1.34 nm, i.e., slightly more than one unit cell of YBCO, confirming 2D growth. Panel b) shows the four-point resistivity curve of a quenched (no post-growth-annealing in $O_2$) YBCO film. The transition is split (see arrows in figure) and quite broad, but indicates a very high degree of oxidation during film growth alone.

First SXRD measurements have been successfully performed on a 17.5 nm thick YBCO film grown on NGO and will allow for a complete structural determination.

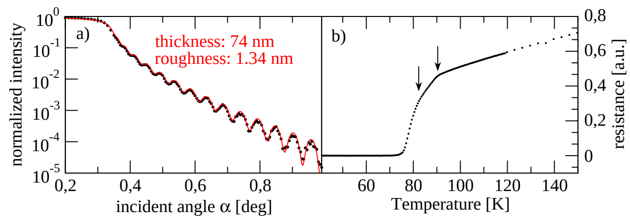


*Fig. 2: a) X-ray reflectivity curve of a 74 nm thick YBCO film. b) Four-point resistivity measurement of a quenched YBCO film showing a broad superconducting transition.*

## Discussion

The feasibility of our approach has been demonstrated. Film growth needs to be optimized with respect to the superconducting properties and crystalline perfection in a next step. The evolution of film morphology will then be monitored by growing monolayer-by-monolayer and performing SXRD for every growth step.

Ultimately, films will be grown in a second *in-situ* PLD growth chamber at the ARPES endstation of the Surface and Interface Spectroscopy Beamline, enabling us to measure their electronic structure, and can then be transferred in UHV to perform SXRD measurements on the same sample. This will hopefully allow us to directly relate the atomic surface structure with the ARPES bandstructure.

## Acknowledgments

The authors thank D. Martoccia and S.A. Pauli for their assistance during experiments and are grateful for the fruitful collaboration with the Surface and Interface Spectroscopy Beamline group.

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