The Atomic Surface Structure of YBa$_2$Cu$_3$O$_{7-δ}$ Thin Films and its Relation to Electronic Properties

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Introduction
Despite much work on YBa$_2$Cu$_3$O$_{7-δ}$ (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$_2$ (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) [1]. 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.

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.

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References