Surface structure and growth of perovskites

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Introduction

Subtle structural differences in complex metal oxides (CMOs) lead to fundamentally different physical properties, due to the strong coupling of the valence electrons. On the one hand, this suggests that surface effects (e.g., relaxations and/or reconstructions) can set a lower limit to downsizing of devices that exploit bulk effects, while on the other, unexpected new phenomena (e.g., surface ferroelectricity) may occur in the surface region of such materials. There is therefore a need to obtain exact atomic surface coordinates to better understand such phenomena. In addition, interpretation of the electronic properties of such strongly correlated systems investigated with ARPES strongly depends on a reliable knowledge of the atomic structure down to the electron escape depth, which in many cases is presently missing.

Methods and Materials

The heart of the surface x-ray diffraction (SXRD) station at the Swiss Light Source are a large (2+3) circle diffractometer [1] and a fast, zero-noise, single x-ray photon-counting, area pixel detector [2]. These, in combination with a pulsed laser deposition chamber (Fig. 1) mounted on the diffractometer, have enabled us to study both the surface structure as a function of film thickness and the growth kinetics of perovskites [3, 4].

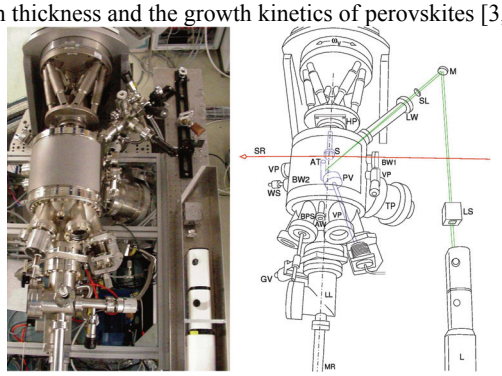

Fig. 1. The pulsed laser deposition chamber.

Results

The (001) surface structure of TiO_2-terminated $SrTiO_3$ (STO) was determined from a data set of more than 1800 structure factors (recorded in less than 10 hours). The surface consists of coexisting (2×2), (2×1), and (1×1) domains. A punitive (Keating energy) term associated with bond-length deviations from equilibrium values was introduced to the fitting procedure to stabilize the structure during optimization, which could however be removed for the final model. Debye-Waller factors were also included. The χ^2-minimization of the 350 fit parameters (oversampling factor ≈ 5) necessary to model the complexity of the surface, used a grid-search algorithm. An example of measured intensities and fits are given in Fig. 2.

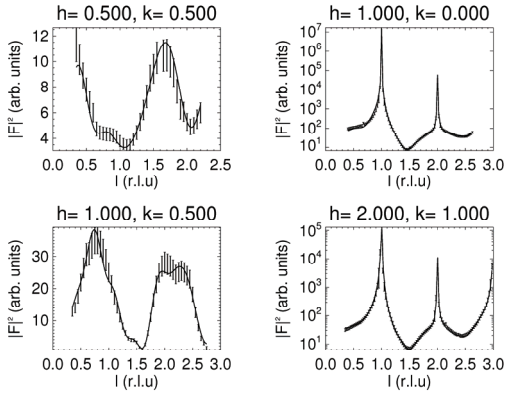

Fig. 2. Measured and calculated intensities of STO.

$La_{1-x}Sr_xMnO_3$ has been heteroepitaxially grown on STO(001). We studied both the growth kinetics [4] and structure as a function of film thickness.

Discussion

The complexity of CMOs means that their surface structure determination requires large data sets. The unprecedented acquisition rate at our station enables us to record a full data set within typical beamtimes, even with a high degree of oversampling. The area detector sets standards in speed and in reliability: Figure 3 shows five equivalent crystal truncation rods (CTRs) of the surface of $LaAlO_3$(001) (LAO). We also believe direct/phase retrieval methods to be of crucial importance for future SXRD studies of these complex systems.

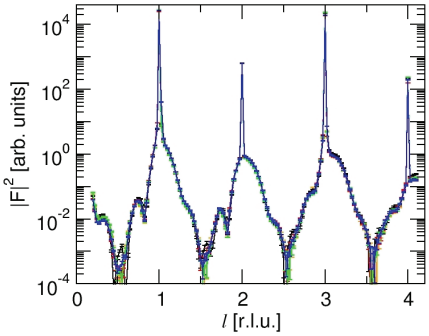

Fig. 3. Five equivalent CTRs of LAO(001).

Acknowledgements

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References

[1] P.R. Willmott et al., Appl. Surf. Sci. 247, 188 (2005).
[2] C.M. Schlepütz et al., Acta Cryst. A 61, 418 (2005).
[3] R. Herger et al., in preparation.
[4] P.R. Willmott et al., Phys. Rev. Lett 96, 176102 (2006).