Advanced laboratory-based X-ray scattering

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Historically, high beam flux and large detectors were accessible only at synchrotron light sources. Using the latest generation high-brilliance microfocus rotating anode generator and a large area hybrid photon counting detector in a custom-build diffractometer manufactured by *Bruker AXS,* we now have access to very weakly scattering features, such as non-integer Bragg reflections, that are notoriously hard to capture and were previously inaccessible to laboratory-based XRD tools.

In my talk, I will show some highlights of the research we have performed with this unique tool over the past three years at the MESA+ Institute for Nanotechnology at the University of Twente on epitaxial complex oxide thin films grown by the pulsed laser deposition technique. To showcase the unprecedented scanning and mapping capabilities of the state-of-the-art tool both in real space as well as in reciprocal space, I present four case studies, which all benefit from the availability of an intense, well-collimated, and monochromatic X-ray beam with a small footprint and a 2D detector with high dynamic range (*Eiger2 R 500K* by *Dectris*).

Firstly, I demonstrate how microfocus X-ray reflectivity (XRR) allows us to elucidate the lateral thickness gradient in a complex oxide heterostructure ($LaAlO_3$ / $SrTiO_3$) wedge sample of few unit cells thickness and correlate this data with reflection high-energy electron diffraction (RHEED) data - a widely used tool to study the growth dynamics of thin films, *in situ* and *operando [1]*.

Secondly, I show high-resolution X-ray diffraction (XRD) measurements on lithographically-defined ferroelectric thin films ($BiFeO_3$ / $DyScO_3$ and $PbZr_{0.55}Ti_{0.45}O_3$ (PZT) / $SrTiO_3$), using an X-ray beam size of only 20 micrometer to probe individual microcapacitors and reconstruct 3D reciprocal space maps [2, 3]. The symmetry and domain structure inferred from these measurements serve as crucial input for our new model to explain the amplitude and frequency scaling of the strain, polarization, and loss tangent in epitaxial ferroelectric PZT films.

Thirdly, I briefly illustrate how the same diffractometer can be used to perform grazing-incidence in-plane diffraction on ultrathin epitaxial films ($Hf_{0.5}Zr_{0.5}O_2$ (HZO) on GaN) [4]. The X-ray diffraction analysis contributed to the demonstration of the films polar nature and rhombohedral R3 symmetry.

Last but not least, I highlight recent efforts to implement *operando* measurements on electrostrictive thin films with *in situ* applied electric fields.

References

[1] Smink *et al.*, *Physical Review Materials* **4** (8), 083806 (2020)
[2] Lucke *et al.*, *Advanced Functional Materials* **30** (52), 2005397 (2020)
[3] Haykal *et al.*, *Nature Communications* **11,** 1704 (2020)
[4] Bégon-Lours *et al.*, Physical Review Materials 4 (4), 043401 (2020)