Poster

Understanding complex order in thin film structures with the 3D-DPDF method

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In thin film research, understanding the origin of order parameters and learning how to manipulate them has always been one of the core objectives. The materials often display delicate interactions among spin, orbital, and lattice order parameters. With the development of thin film deposition techniques, one can even introduce various emergent phenomena by artificially engineering heterointerfaces and superlattices of various layers. So far, structural investigation of local order in thin films was mainly achieved through destructive analysis such as Transmission Electron Microscopy (TEM) and/or limited to very small, essentially two-dimensional regions. X-ray investigations were restricted to small reciprocal space sections and could not provide information about local order with atomic resolution.

Here, we report on the non-invasive three-dimensional investigation of polar domains with atomic resolution via large-volume reciprocal space measurements. Specifically, we collected comprehensive three-dimensional diffuse scattering data using synchrotron hard X-rays at ultra-small grazing-incidence geometry (Fig. 1). The data was analyzed with the three-dimensional delta pair distribution function (3D-ΔPDF) method [1]. The investigated structures were superlattices of short-period ferroelectric lead titanate and dielectric strontium titanate having ordered arrays of polar skyrmion bubbles [2]. We will show atomic structure models and the three-dimensional intra- and interlayer correlations of the skyrmions for varying thicknesses of the superlattices as a function of temperature. These observations not only lay experimental groundwork for investigating distributions and correlations of the domains in epitaxially grown thin films with atomic-scale resolution but also contribute to understanding the structure-property relationship in complex oxide heterostructures.

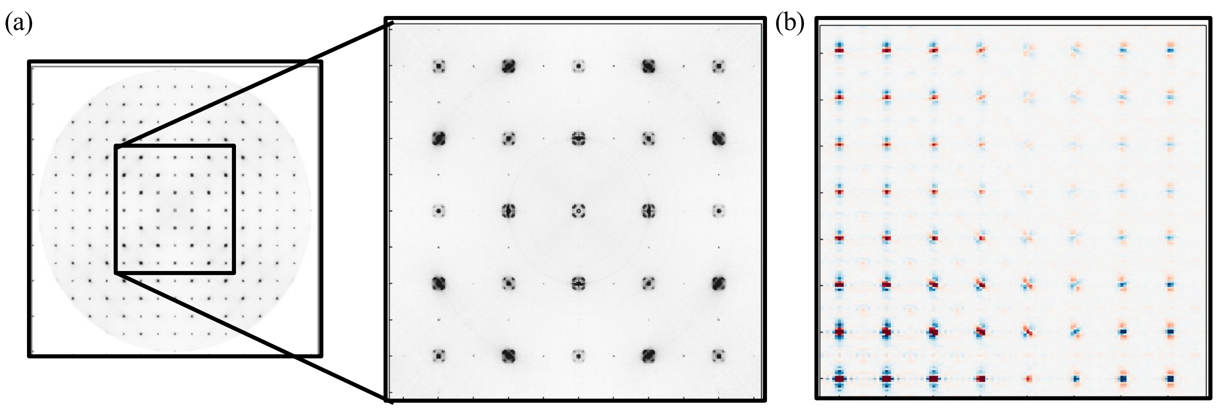

Figure 1. (a) Section from three-dimensional reciprocal space of the thin film. (b) Section from the corresponding 3D-DPDF map.

[1] T. Weber & A. Simonov, (2012) *Z. Kristallogr*. **227**, 238-247

[2] S. Das et al., (2019) *Nature* **568**, 368-372.