High-resolution electron holography of ferroelectric nanolayers

M. Linck¹, H. Lichte¹, A. Lubk¹, F. Röder¹, K. Honda²

1. Triebenberg Laboratory, Institute of Structure Physics, Technische Universität Dresden, Zum Triebenberg 50, 01328 Dresden

2. Fujitsu Laboratories Ltd., Device and Materials Lab, 10-1 Morinosato-Wakamiya, Atsugi 243-0197, Japan

Martin.Linck@Triebenberg.de Keywords: Electron Holography, Ferroelectrics, Thin Films, Electric Fields

Ferroelectric thin films are a hot topic in materials science. The competition for the cheapest and biggest non-volatile mass storage is pushing forward the process of miniaturization. At the same time, the tools of analysis have to be improved to investigate the properties of the related structures. Already, the evaluation of the atomic displacements from Cs-corrected HRTEM micrographs has shown that the ferroelectric polarization can be determined not only in direction but also in quantity on the nanometer scale [1].

However, HRTEM does not recover all information present in the object exit wave, especially large area information stemming from charging and electric fields is not accessible from conventional methods. Off-axis electron holography allows reconstructing the complete complex object wave, i.e. amplitude and phase of the object-modulated electron wave with all details from largest area information up to the resolution limit of the microscope. Therefore, it is capable to recover atomic details and large area fields at the same time [2].

The ferroelectric polarization is closely connected to surface charges that build up the dielectric displacement and compensate the electric field. Otherwise the remaining electric field would depolarize the ferroelectric structure. Therefore, the remaining electric field cannot be interpreted in terms of polarization directly. However, if accessible, the screening charges at the surface of the ferroelectric layer could directly indicate the polarization direction without knowledge about the specific atomic displacements in the unit cells.

By means of high-resolution off-axis electron holography the atomic structure and large area potential variations, e.g. screening charges, can be studied at the same time. Although the signal arising from surface charges is close to the holographic signal detection limit, there are promising results that directly indicate these surface charges. As an example, Figure 1 shows a phase image of a PbTiO₃ layer of 12 unitcells thickness on a SrTiO₃ substrate. The direction of polarization can be derived from the atomic displacements of the ferroelectric unitcell. Additionally, a reduction of the phase shift is found at the interface position that could correspond to a negative screening charge as it is expected from the polarization direction. Subsequently, in Figure 2 a ferroelectric layer of PbTiO₃ in between an electrode of SrRuO₃ und an insulating layer of SrTiO₃ has been evaluated in terms of local lattice distortion and center atom displacement. These data will allow determining the local polarization and connecting it to the findings with respect to surface charges. These possibilities offer a comprehensive analysis of ferroelectrics on the atomic scale, which is essential for a precise understanding of ferroelectric phenomena in thin films and beyond. [3]

- 1. C.L. Jia, S.B. Mi, K. Urban, I. Vrejoiu, M. Alexe and D. Hesse, Nature Materials Vol. **7** Issue 1 (2008), 57-61.
- 2. H. Lichte, P. Formanek, A. Lenk, M. Linck, C. Matzeck, M. Lehmann and P. Simon, Annual Review of Materials Research, Vol. **37** (2007), 539-588, ISBN 978-0-8243-1737-9.
- 3. The authors appreciate the enlightening discussions within the Triebenberg group. Financial support through ESTEEM and the DFG is gratefully acknowledged.



Figure 1. The phase image of a ferroelectric layer of $PbTiO_3$ (middle) on a substrate of $SrTiO_3$ (top) allows determining the direction of polarization from the displacement of the atoms within the unit cells. Additionally, the smaller phase shift at the interface position suggests a negative screening charge at the interface.



Figure 2. From the complex object exit wave of a ferroelectric $PbTiO_3$ layer (middle) in between an electrode of $SrRuO_3$ (bottom) and a layer of $SrTiO_3$ (top), the center atom displacements and the unitcell distortions have been analyzed (right). Within the $PbTiO_3$ layer a significant tetragonal distortion is found. The evaluation of the center atom position within the unit cell indicates strong atomic displacements in the PbTiO3. This behavior is also reaching out to the neighboring $SrTiO_3$ and $SrRuO_3$ layers.