Estimation of the local electric polarization in layered heterostructures using HRTEM and Electron Holography

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Keywords: polarization, layered oxide heterostructures, atom positions, HRTEM, electron holography

Different layered heterostructures containing a constituent with a polarization component perpendicular to the layer like, $SrTiO_3$-$PbTiO_3$ (STO-PTO), $SrRuO_3$-$PbTiO_3$–$SrTiO_3$ (SRO-PTO-STO) or $SrTiO_3$-$LaAlO_3$ (STO-LAO) were prepared recently by epitaxial growth with a high degree of accuracy, showing very interesting behavior for electronic device applications. For example, STO-LAO (fig. 1) exhibits quasi–two-dimensional high mobility electron gas at the interface of the two insulating perovskites [1].

The electric charge distribution in the interfaces results from two competing mechanisms, which aim to reduce the depolarization field at the interface and thereby lower the total energy of the system: (a) the redistribution of ionic charges of the atoms and (b) the electronic charge redistribution, leading to characteristic lattice distortions in the vicinity of the interface [2]. Thus, the local determination of these distortions in combination with a polarization model as provided by the Born effective charge tensor gives quantitative information about the local electric polarization at the interface. Other dielectric properties, such as the magnitude of the interface charge, can be readily derived from the polarization.

The lattice distortions are determined in the following way: Conventional high resolution transmission electron microscope (HRTEM) images and by means of off-axis holography reconstructed waves are fed to a local atom fit procedure. Special emphasis is put on the dedicated parameterization of the fitting model with respect to intensities or reconstructed waves. The thereby obtained atomic coordinates are subsequently analyzed with respect to crystal plane positions, which could be determined with a precision in the order of a few tens of picometer. (fig. 2). The Born effective charge tensor is provided by ab-initio calculations [3].

In all investigated hetero-systems a continuous change of the local polarization across the interface can be observed, whereupon the polarization of the originally non-polar material depends on the dielectric properties, e.g. metallic $SrRuO_3$ ionic screening is both weaker and more localized compared to the screening of the insulating $SrTiO_3$. The lattice strain perpendicular to the layer is comparatively weak in the investigated systems and is not reflecting the polarization behaviour (fig. 2). Unfortunately, the oxygen columns are not yet optimally resolved introducing an uncertainty in the determination of the polarization.

W. Grogger, F. Hofer, P. Pölt (Eds.): MC2009, Vol. 3: Materials Science,
DOI: 10.3217/978-3-85125-062-6-513 , © Verlag der TU Graz 2009

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4. The authors acknowledge financial support from the European Union under the Framework 6 program under a contract for an Integrated Infrastructure Initiative. Reference 026019 ESTEEM.

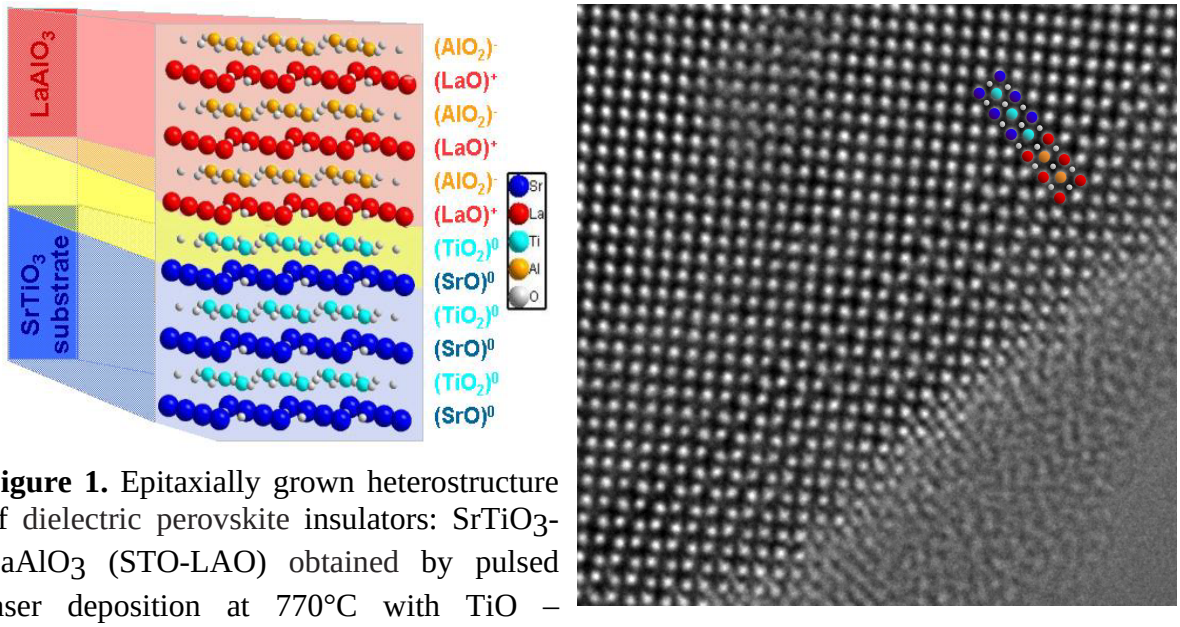

Figure 1. Epitaxially grown heterostructure of dielectric perovskite insulators: $SrTiO_3$-$LaAlO_3$ (STO-LAO) obtained by pulsed laser deposition at 770°C with TiO – terminated (001) $SrTiO_3$.

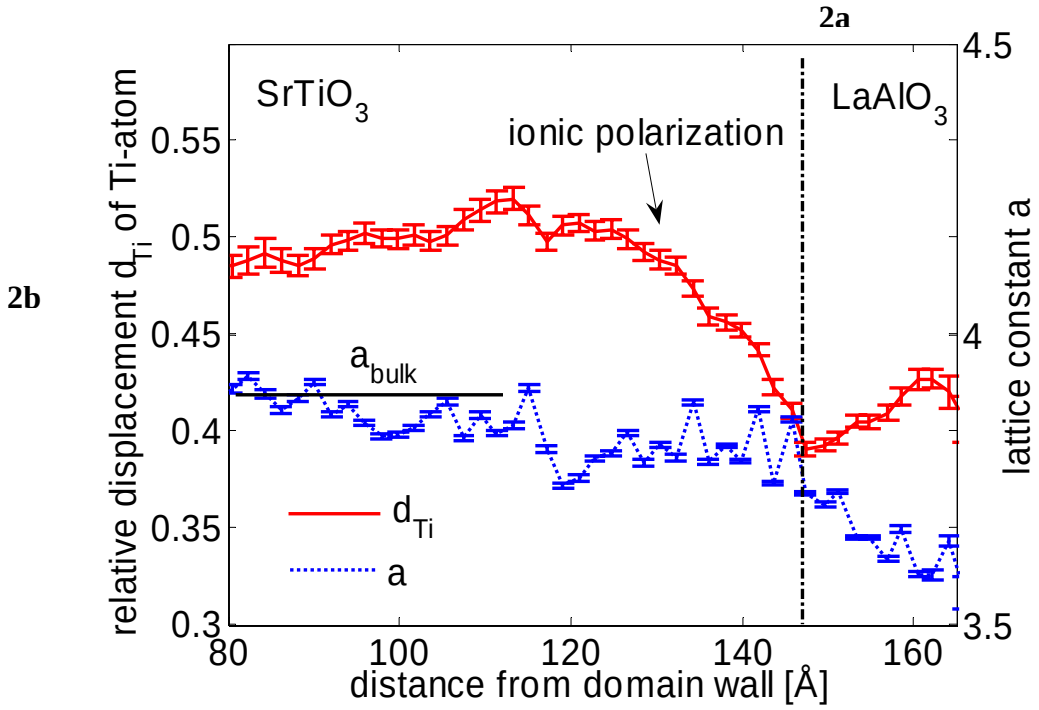

Figure 2. a) HRTEM image of a specimen with four unit cell thick LAO on STO. b) The Ti- displacement perpendicular to the interface accounts for existing polarization across the last ~2 nm.

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