The atomic structure of an unusual interface

The physical mechanisms behind the unexpected formation of an ultrathin conducting layer at the interface between the band insulators $SrTiO_3$ (STO) and $LaAlO_3$ (LAO) have been the subject of considerable controversy since its discovery in 2004 [1]. Both STO and LAO belong to a technologically important family of materials called perovskites. In many of these materials, very small movements in the positions of the constituent atoms can have profound effects on their electronic properties, due mainly to the fact that the electrons involved in the bonds are strongly influenced by one another. In the case of the LAO/STO interface, the situation is further complicated by the fact that LAO consists of a stacking of alternating oppositely charged sheets (LaO and AlO_2), while STO contains neutral layers. This causes an electric field to form at the interface, which can be neutralized either by the rearrangement of electrons (i.e., a local change in valence of the ions), or by the rearrangement or removal of atoms. Exactly which mechanisms play the most important role is the essence of the controversy.

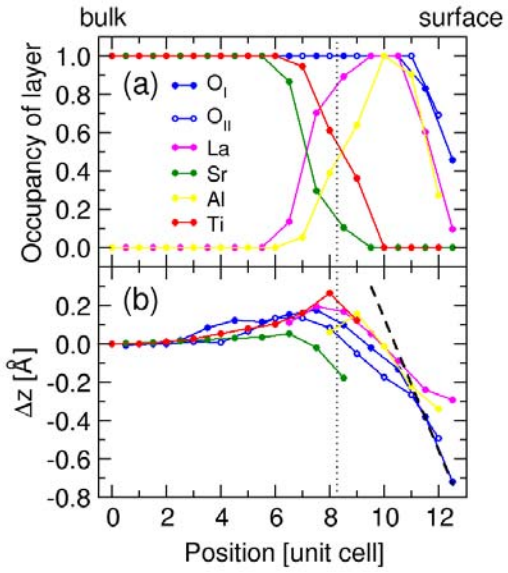

Figure 1: *(a) The occupancies of the component elements at the interface of STO with LAO. (b) The deviations from bulk STO positions of the atoms normal to the interface. Note that the interface region is dilated, caused by the presence of Ti^{3+}, which has a large ionic radius.*

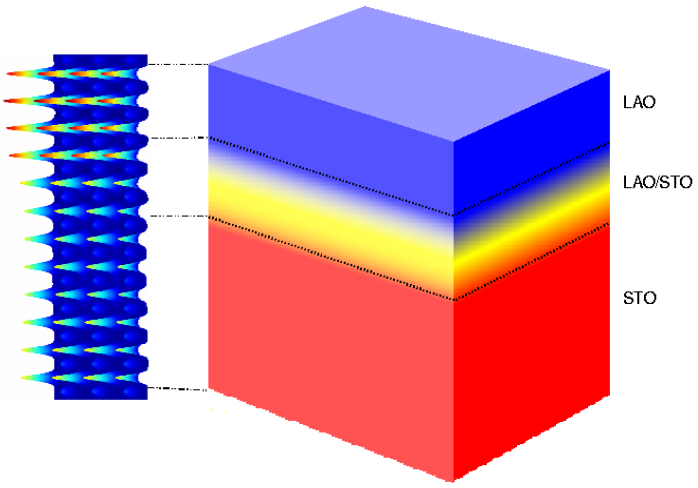

Figure 2: *Left: The electron density map emerging from analysis of the SXRD data using the COBRA phase retrieval method. Right: a schematic of the model, showing the graded interface of around three unit cells' thickness.*

A common conclusion of the investigations to date is that the mechanisms will be better understood if a comprehensive description of the interface with sub-Angstrom resolution is made available. The synchrotron technique of surface x-ray diffraction (SXRD) is ideally suited for this. Briefly, well-defined and atomically flat interfaces and surfaces in crystalline structures result in the generation of a weak but highly predictable signal in between diffraction peaks, from which the interfacial and surface structure can be gleaned.

Using a novel x-ray photon-counting area detector, a large SXRD data set of a 5-monolayer film of LAO grown on STO was recorded, and analyzed with phase-retrieval methods and subsequent structural refinement techniques. It was found that the interface between STO and LAO was not abrupt, but formed a graded layer of approximately 3 unit-cell thickness (see Fig. 1). Importantly, this layer contains a significant fraction of Ti^{3+}, which is incorporated into $La_{1-x}Sr_xTiO_3$ (LSTO), a conducting material in bulk form. Indeed, in this interfacial layer, LSTO is forced to assume a tetragonal structure (it is orthorhombic in the bulk), which should further enhance its conductivity. In this manner, the formation of the conducting layer has been explained based only on simple structural considerations.

The electronic properties of this model were also investigated using a theoretical (density functional theory) calcuations, which confirmed the experimental findings.

References

[1] A. Ohtomo and H.Y. Hwang, Nature **427**, 423 (2004).

Publications

- **Structural Basis for the Conducting Interface between $LaAlO_3$ and $SrTiO_3$**
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