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MS-3-P-3239 A direct bond analysis of SrTiO3/SrIrO3 (3 bilayers)/(111) SrTiO3 oxide heterostructures based on aberration-corrected HRTEM images

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Oxide heterostructures have been intensively studied in recent years due to their novel physical properties, e.g. metal-insulator transition, ferromagnetism and superconductivity. These phenomena are related to the interplay between the lattice, charge, orbital and spin degree of freedom at the interface. Hence, a direct measurement of strain, cation displacement and oxygen octahedral rotation-tilt is essential for understanding the structure-property relation of these materials. In this work, we demonstrate a direct measurement of the bond length and bond angle of each oxygen octahedron across the interface based on aberration-corrected HRTEM.

Figure 1 shows the TEM image of a SrTiO3/SrIrO3 (3 bilayers) film grown on (111) SrTiO3 oriented along [110] zone axis. Negative spherical aberration imaging condition is used in the experiment and thus the image reflects the projected atomic structure of the heterostructure. To understand the structure of the heterostructure, we carried out a direct measurement of the atom positions by fitting the intensity of individual atomic column to a two-dimensional Gaussian peak. Based on the fitting results, the projected bond length and bond angle of each oxygen octahedron (defined in the inset of Fig. 1) is analyzed and the results are shown in Figure 2. We first note that the Sr-Sr bond lengths of the SrIrO3 film (6th to 8th oxygen octahedron) are larger than that of the substrate. It is interesting to point out that the Sr-Sr bond length of the 7th oxygen octahedra is much shorter than its neighboring octahedron. This may be due to the variation of Sr-Sr bond length projected along [1 0] direction for orthorhombic SrIrO3, which are 2.88 Å and 2.69 Å, respectively. The projected Sr-Sr bond length along [001] direction is consistent with the bulk value ~3.94 Å. We also note that the projected bond length and bond angle between B-site cation and oxygen changes abruptly at the SrIrO3/SrTiO3 interface and extends only several atomic layers. Furthermore, from Fig. 2b and 2c, it is clearly that the bond length and bond angle between B-site atoms and oxygen is maximum/minimum. These results are not compatible with the bulk SrIrO3 structure and indicate that the ultrathin 3 bilayers thick SrIrO3 film is possibly in a new displacive polar state.

In summary, we have shown that the bond length and bond angle of oxygen octahedron across the SrTiO3/SrIrO3 interface can be directly measured from an aberration-corrected HRTEM image. We found that the ultrathin SrIrO3 film has a new displacive polar state different from its bulk structure. Although the exact crystal structure of the film remains unclear, our work provides an insight into the atomic structure of these materials with peculiar properties at the interface.

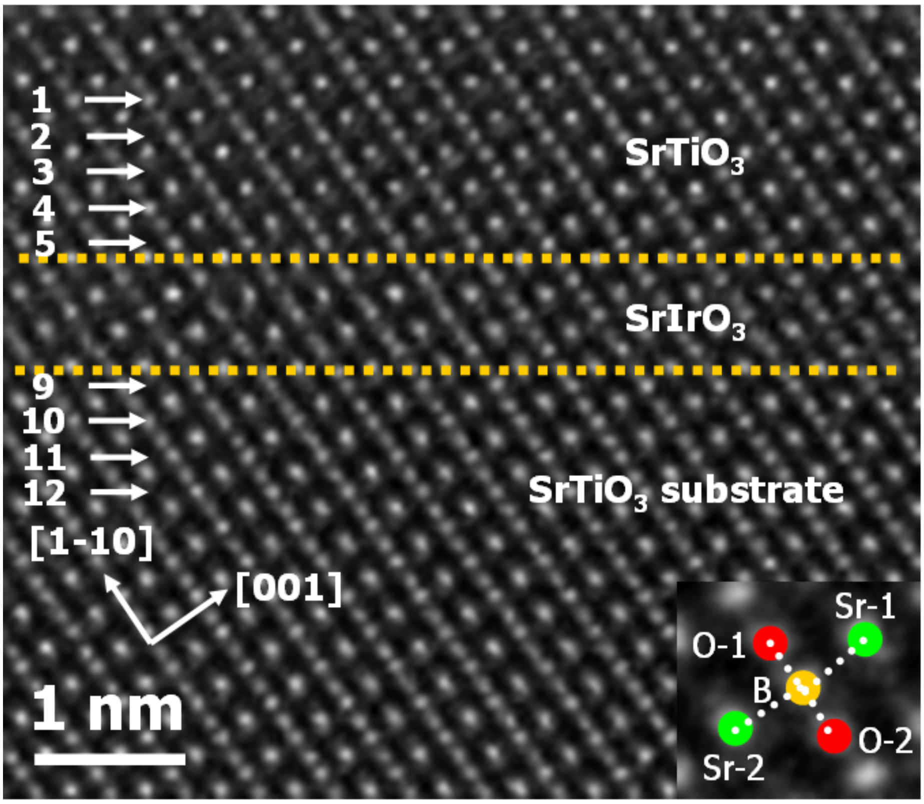

Fig. 1: HRTEM image of [110] $SrTiO_3$/$SrIrO_3$/(111) $SrTiO_3$. The projected bond length and bond angle of the oxygen octahedron is defined in the inset and the number in the image indicates the n-th oxygen octahedron used for the analysis.

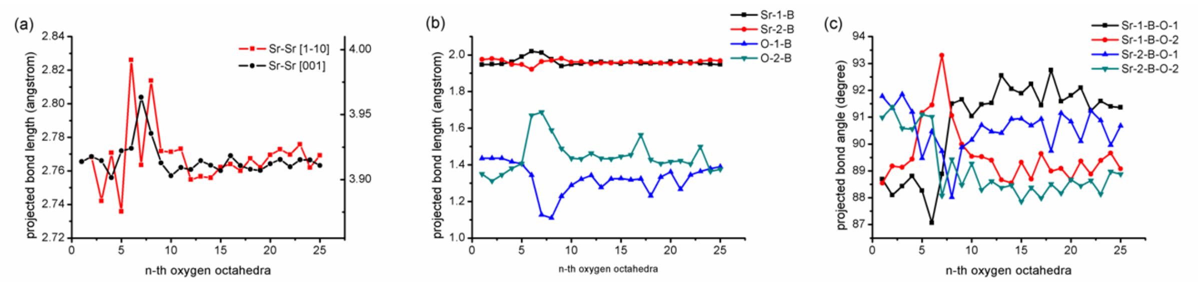

Fig. 2: The projected bond length of (a) Sr-Sr atoms and (b) Sr-B and O-B atoms and the projected bond angle of (c) Sr-B-O atoms. It is clear that the bond lengths of Sr-Sr and O-B and bond angle between cations and oxygen of the film deviate from the substrate substantially.