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Origin of the metallic states at heterointerface between band insulators $LaAlO_3/SrTiO_3$ studied by *in situ* photoemission spectroscopy

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Introduction

An interesting aspect of the perovskite heterostructures seems to be the appearance of metallic conductivity with extremely high-mobility at the interface between band insulators $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) [1]. Despite intensive theoretical and experimental studies, the mechanism of metallic-state formation is still unclear. One of the scenarios proposed for describing the physics of the metallic states is the "charge transfer" that originates from the charge discontinuity between LAO and STO. On the other hand, some experimental results have suggested that the "oxygen vacancies" in STO layers generated by the deposition of LAO films. In this study, to investigate the origin of the metallic states at LAO/STO heterointerface, we performed *in situ* photoemission spectroscopy (PES).

Experiment

LAO/STO multilayers with an AlO_2-LaO-TiO_2 or AlO_2-SrO-TiO_2 interface were fabricated on atomically flat TiO_2-terminated Nb:STO (001) substrates in a laser molecular-beam epitaxy chamber connected to a synchrotron radiation photoemission system at BL2C. The LAO layer thickness was varied from 0 to 6 ML, while the thicknesses of the "buffer" STO layers were fixed at 20 ML to inhibit the influence of substrates. For the metallic LAO/TiO_2-STO interface, we directly deposited LAO layers on the STO layer, while LAO/SrO-STO was fabricated by depositing a SrO monolayer between the LAO and STO depositions.

Results and Discussion

In order to discuss the possible origin of the metallic states in the LAO/STO heterointerface in terms of the discontinuity in the band structure between the two insulators, we measured the shift of the Ti 2*p* core level as a function of the LAO overlayer thickness for the metallic LAO/TiO_2-STO interface as well as the insulating LAO/SrO-STO interface as shown Fig. 1. Interestingly, the metallic LAO/TiO_2-STO interface clearly shows a peak shift toward higher binding energy as the LAO overlayer thickness increases. In contrast, the insulating interface does not show any detectable shift. The energy shift due to band bending for the metallic interface can be estimated to be -0.25 ± 0.07 eV. Since the conduction band minimum (CBM) in STO is located at 0.2 – 0.3 eV above E_F, the results strongly suggest that the CBM in STO at the metallic interface is nearly attained at E_F. A possible band diagram of the metallic LAO/STO heterointerface, as deduced from the PES experiments, is illustrated in Fig. 1(c). Here, the existence of the notched structure inside the STO layers suggests a mechanism that produces the metallic states while still avoiding the potential divergence in the polar LAO layers. Since the polar LAO layers have alternating ±*e* charge sheets, where *e* is the electron charge, the stacking of the LAO layer on non-polar STO produces a positive electric field. This in turn leads to an electric potential that diverges with an increase in the LAO overlayer thickness. The divergence catastrophe can be avoided by the formation of the long-range electric potential inside the STO whose spatial variation is governed by the carriers in the STO layers. In other words, the accumulation of electrons in the notched structure, where the electrons may be generated by oxygen vacancies in the STO layers, produces the metallic states at the LAO/STO heterointerface.

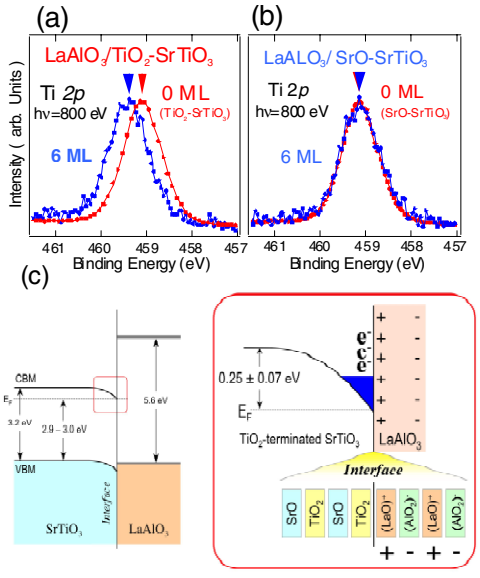

Figure 1: Ti 2*p* core level of (a) metallic LAO/TiO_2-STO and (b) insulating LAO/SrO-STO. (c) Band diagram of the metallic LAO/TiO_2-STO interface determined by the PES experiments.

References

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