Termination dependence of the Schottky barrier height for \( \text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3/\text{Nb}:\text{SrTiO}_3 \) heterojunctions

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Introduction

The height of the Schottky barrier \( \Phi_B \) that forms at a metal/insulator junction is an essential and fundamental parameter that dominates the device performance. A perovskite oxide heterojunction (ABO\(_3\)/A′B′O\(_3\)) has two types of interfacial structures that are AO/BO\(_2\)/A′O/B′O\(_2\) and BO\(_2\)/AO//B′O\(_2\)/A′O layer sequences, and consequently different interfacial electronic structures emerge depending on the interfacial termination [1]. Thus, the precise determination of the band diagrams for interfacial termination-layer controlled oxide heterojunctions is indispensable for designing spintronic devices, such as tunneling magnetoresistance devices using a half-metallic ferromagnetic material like \( \text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3 \) (LSMO).

In this study, we report on the band diagrams of interfacial termination-layer controlled oxide heterojunctions determined by \textit{in situ} photoemission (PES) studies.

Experimental

LSMO/TiO\(_2\)-Nb:STO and LSMO/SrO/Nb:STO (n-type and p-type LSMO/Nb:STO, respectively) heterojunctions were fabricated in a laser molecular beam epitaxy chamber connected to a synchrotron-radiation photoemission system at BL-2C. The Nb:STO substrate was annealed at 1050 °C and an oxygen pressure of \( 1 \times 10^{-7} \) Torr to ensure an atomically flat TiO\(_2\) layer terminated surface. For p-type structure, we initially deposited SrO on the TiO\(_2\)-terminated Nb:STO substrate to change its termination from the TiO\(_2\) to SrO layer. During LSMO depositions, the substrate temperatures and the ambient oxygen pressures were 1000 °C and \( 1 \times 10^{-4} \) Torr, respectively. The film thicknesses were controlled on an atomic scale by monitoring the intensity oscillations of the reflection high-energy electron diffraction specular spot during growth. The PES spectra were taken \textit{in situ} a total energy resolution of 150 meV in the energy range of 600 to 800 eV. The work functions (\( \Phi_m \)) and electron affinities (\( \chi_i \)) were determined from the secondary electron emission spectra recorded with the He I (21.2 eV) resonance line.

Results and discussion

The measurement of core-level spectra enables us to determine \( \Phi_B \) formed at the heterojunctions directly. For both junctions, a peak shift towards a lower binding energy was clearly observed as the overlayer film thickness increased. Judging from the saturation level of the peak shift, \( \Phi_B \) could be estimated to be \( 1.2 \pm 0.1 \) and \( 0.6 \pm 0.1 \) eV for the n-type and p-type heterojunctions, respectively. The band diagrams for the (a) n-type and (b) p-type LSMO/Nb:STO heterojunctions derived from the present PES experiments, are illustrated in Fig. 1. \( \Phi_m \) of n-type LSMO/Nb:STO is much higher than the prediction from the Schottky-Mott rule \( (\Phi_B = \Phi_m - \chi_i) \) by 0.5 eV, indicating the formation of an “interface dipole” [2]. In contrast, for p-type LSMO/Nb:STO, \( \Phi_B \) is lower by 0.4 eV. These results suggest that the direction of the interface dipole is inverted by changing the termination layer owing to the inversion of the polarity discontinuity at the polar/nonpolar interface.

References


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