

Plane-direction dependence of the surface electronic structure of SrTiO₃

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Introduction

Recently, the in-plane anisotropy of (110)-oriented perovskite oxide single-crystal substrates have been applied to control the film properties of materials, such as High-T_c superconductors or those showing colossal magnetoresistance. Moreover, owing to the fixed charge of each atomic layer irrespective of cation valence states, (110) orientations have been anticipated to solve the problem of charge discontinuity at heterointerfaces. However, detailed studies on their surface electronic structures, which could greatly affect epitaxial growth and interface structure, have not been carried out so far. In this study, we have performed photoemission spectroscopy (PES) measurements to probe the chemical bonding states in the surface region of (110)-oriented SrTiO₃ (STO).

Experiments

Atomically flat surfaces of (110)- and (001)-oriented, 0.05 wt% Nb-doped STO (Nb:STO) substrates, were obtained in a laser molecular beam epitaxy (MBE) chamber connected to a synchrotron radiation PES system at BL2C [1]. Substrate temperature and oxygen pressure were kept at 1050 °C and 1×10⁻⁷ Torr in the first stage annealing, and at around 400 °C and 760 Torr during the post-annealing. Surface morphology was characterized by *in-situ* reflection high-energy electron diffraction (RHEED) and *ex-situ* atomic force microscopy (AFM), confirming atomically flat terrace structures with (110) unit-cell steps. The PES spectra were taken *in-situ* with a total energy resolution of 100 meV at *hν* = 500 eV for Sr 3*d* core levels. Photoelectron emission angles of 0° (=normal to the surface), 45°, and 60° were used, enhancing surface sensitivity.

Results and Discussions

Figure 1 shows the Sr 3*d* core level spectra of Nb:STO substrates. It is evident for (001) surfaces that as the emission angle increases (surface sensitive increases), a component with chemical shift of ~1 eV (S₁₀₀) increases in intensity, indicating its surface nature. Judging from the energy shift amount and full width at half maximum (FWHM), this component is assigned to the amorphous Sr-oxide segregated during thermal treatment [2]. To

one's surprise, such segregation peaks are not observed in (110) substrates. This result suggests that (110) surfaces can be stabilized without segregation of Sr-oxides, in contrast with (001) surfaces.

It has been reported that high-polar (110) surfaces are stabilized by the presence of oxygen vacancies [3]. It has also been shown by recent classical shell model calculations, that a surface reconstructed (1×2)(110) O-termination is the most stable (110) structure [4]. Thus, by taking into account the reduced conditions of annealing in this study, the formation of stable, reconstructed O-terminated surfaces during first stage annealing may be responsible for the suppression of Sr-oxide segregation.

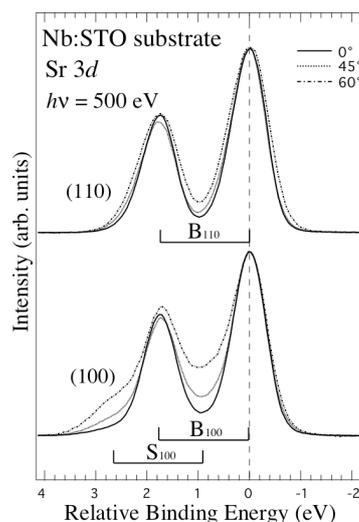


Figure 1: Sr 3*d* core level spectra of (110) and (100) Nb:STO substrates (B: bulk component, S: surface component).

References

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