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Electronic structure of anatase $Ti_{1-x}Nb_xO_2$ studied by synchrotron-radiation photoemission spectroscopy

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Introduction

Transparent conducting oxides have been established as essential materials for opto-electronic devices, such as flat-panel displays, light-emitting devices and solar cells. We have recently reported that anatase $Ti_{0.94}Nb_{0.06}O_2$ (TNO) thin films epitaxially grown on $SrTiO_3(100)$ substrate by using pulsed laser deposition (PLD) show low resistibity of 2.1×10^{-4} Ωcm at room temperature and a high internal transmittance of ~95% in the visible region.[1] In order to clarify the origin of these electrical properties, it is important to investigate how the electronic structures change as a function of electron doping (Nb concentration x). In this study, we have fabricated TNO thin films with a variety of Nb concentration and have performed synchrotron-radiation photoemission spectroscopy (PES) measurements of these materials.

Experiments

$Ti_{1-x}Nb_xO_2$ (x = 0, 0.06, 0.1, 0.2, 0.3) thin films were grown on $LaAlO_3$ (100) substrates by PLD techniques at substrate temperature of 650°C and oxygen pressure of $7 \times 10^{-6} - 1 \times 10^{-5}$ Torr. X-ray diffraction measurements confirmed epitaxial growth of (001) oriented anatase TiO_2 phase, without any impurity phases. PES measurements were carried out at beam-line 2C of the synchrotron radiation source at Photon Factory in Tsukuba.

Results and discussion

Figure 1 shows the Ti 2p 3/2 core-level spectra of TNO. This figure exhibits a major Ti^{4+} peak together with a minor Ti^{3+} peak at lower binding energy. The peak intensity of the Ti^{3+} systematically increases with increasing x, which reflects increasing career electron by Nb doping. Ti 2p 3/2 core level monotonically shifts toward higher binding energies as x is increased. This result indicates the chemical-potential shift of TNO with electron doping [2]. Moreover, we have clearly observed that the density of states near the Fermi level originated from Ti 3d conduction bands increase with increasing x measured by Ti 2p-3d resonant PES. These results suggest that the behaviour of the electronic structure in TNO can be described as the rigid-band model in principle.

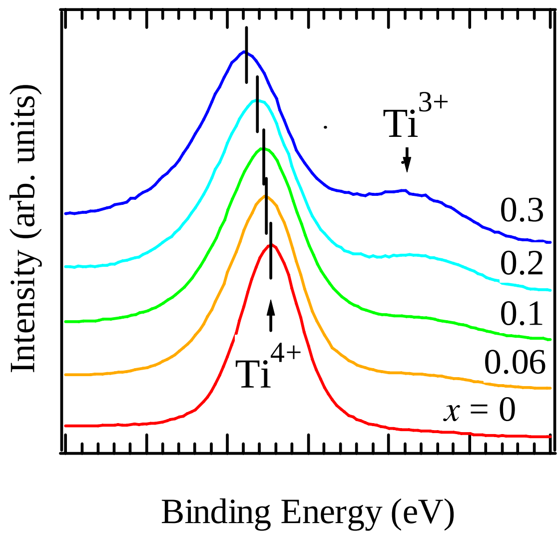

Fig.1: Ti 2p 3/2 core-level spectra of $Ti_{1-x}Nb_xO_2$

References

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