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Transport properties and electronic states of anatase Li_xTiO_2 epitaxial thin films

Akira CHIKAMATSU*[1], Utahito TAKEUCHI[1], Yasushi HIROSE[1,2], Shoichiro NAKAO[2], Hiroshi KUMIGASHIRA[3], Masaharu OSHIMA[3], Tetsuya HASEGAWA[1,2]
[1]Department of Chemistry, The University of Tokyo, Tokyo 113-0033, Japan
[2]Kanagawa Academy of Science and Technology, Kanagawa 213-0012, Japan
[3]Department of Applied Chemistry, The University of Tokyo, Tokyo 113-8656, Japan

Introduction

$Ti_{1-x}Nb_xO_2$ has been recognized as an excellent transparent conducting oxide with low resistivity and high visible-light transmittance [1]. In this material, each Nb^{5+} substituting for Ti^{4+} releases one conduction electron, which contributes to the low resistivity. It is thus expected that cations intercalated into anatase lattice will produce carriers. In this study, we have synthesized epitaxial thin films of anatase TiO_2 doped with Li, Li_xTiO_2, by using pulsed laser deposition (PLD) technique, and investigated their transparent conducting properties and electronic structures.

Experiment

Epitaxial thin films of anatase $Li_{0.074}TiO_2$ were grown on $(La_{0.3}Sr_{0.7})(Al_{0.65}Ta_{0.35})O_3$ (100) substrates by PLD. The anatase structures of these films were confirmed by X-ray diffraction. Transport properties [i.e., dc resistivity (ρ), carrier density (n_e), and Hall mobility (μ_H)] were characterized based on standard six-terminal geometry under external magnetic field up to 8 T perpendicular to the film surfaces. Valence-band electronic states were measured by soft X-ray photoemission spectroscopy (PES) using BL-2C at the Photon Factory, KEK.

Results and Discussion

Figure 1 plots ρ–T curve of $Li_{0.074}TiO_2$ and $Ti_{0.94}Nb_{0.06}O_2$ thin films. Notably, the ρ–T curves of $Li_{0.074}TiO_2$ show metallic behavior. The ρ(300 K) is ~1×10^{-3} Ωcm, which is approximately five times higher than that of $Ti_{0.94}Nb_{0.06}O_2$ films (2×10^{-4} Ωcm). The n_e(300 K) value is as high as 5×10^{20}-1×10^{21} cm^{-3}, being comparable to that of $Ti_{0.94}Nb_{0.06}O_2$. On the other hand, the μ_H(300 K) value of the $Li_{0.074}TiO_2$ films (10-15 $cmV^{-1}S^{-1}$) is 1/2 -1/3 of that $Ti_{0.94}Nb_{0.06}O_2$. These results indicate that high ρ of $Li_{0.074}TiO_2$ can be almost due to low μ_H.

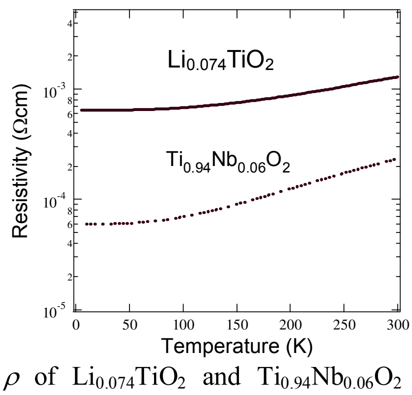

Fig.1: ρ of $Li_{0.074}TiO_2$ and $Ti_{0.94}Nb_{0.06}O_2$ films as functions of temperature.

Figure 2 shows the valence-band spectra of $Li_{0.074}TiO_2$ films near the Fermi level (E_F) obtained by Ti 2*p*-3*d* on- and off-resonant PES with a photon energy of $h\nu$ = 467 eV and 453 eV, respectively. Around the binding energy (E_B) of 0.5-3 eV, in-gap states can be clearly observed. Furthermore, the intensity around E_B = 1-2 eV are enhanced in a Ti 2*p*-3*d* resonance PES, indicating that the in-gap states have Ti 3*d* orbital nature. On the other hand, there was no state near E_F in $Li_{0.074}TiO_2$ films, although there is a state near E_F in the case of $Ti_{1-x}Nb_xO_2$ [2]. These results suggest that the difference of mechanism of conduction between Li_xTiO_2 and $Ti_{1-x}Nb_xO_2$ is attributed to the states from each dopants.

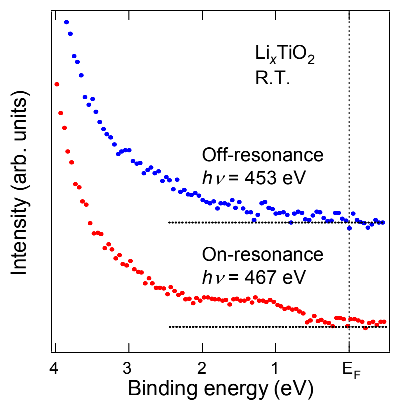

Fig.2: Ti 2*p*-3*d* on- and off-resonant PES of Li_yTiO_2 films obtained with a photon energy of $h\nu$ = 467 eV and 453 eV, respectively.

References

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* chikamatsu@chem.s.u-tokyo.ac.jp