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Transport properties and electronic states of anatase $Ti_{1-x}W_xO_2$ epitaxial thin films

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Introduction

$Ti_{1-x}Nb_xO_2$ and $Ti_{1-x}Ta_xO_2$ are transparent conducting oxides with good resistibvity and transmittance [1] [2]. These carrier arises and the resistivity becomes low because Nb and Ta which substitute for Ti exist as Nb^{5+} and Ta^{5+}. There was no report using W which can be hexavalent as a dopant. In this study, in order to clarify the difference of mechanism of conduction between $Ti_{1-x}Nb_xO_2$ and $Ti_{1-x}W_xO_2$, we fabricated anatase $Ti_{1-x}W_xO_2$ epitaxial thin films, measured 4-probe resistance and Hall Effect and performed X-ray photoemission spectroscopy (PES) on these films.

Experiment

$Ti_{1-x}W_xO_2$ (x = 0.01 - 0.09) films were grown on LSAT (100) substrates by pulsed laser deposition and optimize the conditions, i.e. oxygen partial pressure and W content x. Epitaxial growth and W substitution for Ti were confirmed by X-ray diffraction (XRD) measurements. Transport properties are measured in the six terminal geometry. X-ray PES were performed at BL-2C of the Photon Factory, KEK.

Results and Discussion

By XRD measurement, anatase epitaxial growth without secondary phase and W substitution for Ti were confirmed. When $Ti_{0.95}W_{0.05}O_2$ films were deposited under the optimized condition, the resistivities of the films at room temperature were 2 x 10^{-3} Ωcm. These values are 10 times as high as these of $Ti_{0.94}Nb_{0.06}O_2$ films. This is mainly because lower carrier density of the $Ti_{1-x}W_xO_2$ films. Since the result of core level PES indicates that W exists as W^{6+} in the films, the activation ratio which is calculated as about 10 % is very low compared to that of $Ti_{1-x}Nb_xO_2$ film which is almost 100 %. Therefore, there can be states trapping carriers which should have arise from W.

Then in order to observe the states, we performed valence-band PES. Figure 1 shows the valence-band spectra of $Ti_{0.91}W_{0.09}O_2$ films. We can see a state on the top of the valence-band. In the case of $Ti_{1-x}Nb_xO_2$, we cannot find any state like this. To clarify the origin of this state, we performed Ti 2*p*-3*d* resonant PES as shown in Fig. 1 inset. If the state was originated from Ti, the intensity would become strong measured on resonant. But there is no change these spectra. As this state is only observed in and has no relation with Ti, it is regarded as a state assigned from O 2*p* hybridized with W. It is supposed that this state traps many carriers from W. On the other hand, there was no state near the Fermi level (E_F) in $Ti_{1-x}W_xO_2$ films, although there is a state near E_F in the case of $Ti_{1-x}Nb_xO_2$ [3]. This result corresponds to the carrier density measured electrically. These results suggest that the difference of mechanism of conduction between $Ti_{1-x}W_xO_2$ and $Ti_{1-x}Nb_xO_2$ is attributed to the state from W doping.

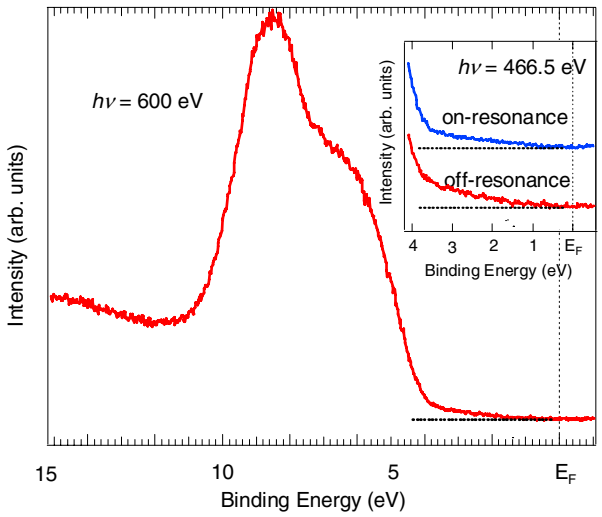

Fig. 1: X-ray photoemission and Ti 2*p*-3*d* resonant photoemission spectra of $Ti_{0.91}W_{0.09}O_2$ films.

References

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