Fabrication and Characterization of $Sn_2M_2O_7$ (M=Nb, Ta) Thin Films

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Oxides containing divalent tin ions have unique valence bands that are constructed from hybridized states of O-2*p* and Sn-5*sp* [1]. This hybridization yields shallow and widely dispersed electronic states near the valence band maximum, indicating their potential for high hole conductivity. Although intensive studies have been conducted on tin monoxide (SnO), a prototypical system of divalent tin oxides and *p*-type semiconductor with relatively high hole mobility, there have been a limited number of reports on the other divalent tin oxides partly because of the difficulty in preparation. $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ with a pyrochlore structure are ternary compounds involving divalent tin ions and have valence band structures similar to SnO as predicted by first-principles calculations [2]. In this study, we fabricated epitaxial thin films of $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ and examined their crystal structures and absorption coefficients.

$Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ thin films were grown on the single crystalline substrates of yttria-stabilized zirconia (YSZ) (100) using pulsed laser deposition (PLD). The substrate temperature was kept at 773 K and 873 K during the deposition of $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$, respectively. The pressure in the chamber was kept at 1.3×10^{-2} Pa by flowing O_2 gas after evacuating down to 5×10^{-4} Pa. The crystal structures and orientations of the thin films were investigated by X-ray diffraction (XRD). The thickness and surface roughness of the films were evaluated by X-ray reflectivity measurements. The absorption coefficients of the films were measured by optical transmission and reflection spectrometry.

Figure 1 shows the XRD 2θ-θ profiles of the thin films on the YSZ (100) substrates. It is found that single phase films were grown with a (100)-oriented pyrochlore structure. The clear fringe structures around the 400 diffraction peaks with narrow full-widths at half maximum of their rocking curves of 0.10 degrees suggest a small distribution of the lattice constants and orientation of the films. The thicknesses estimated from the oscillation intervals of the fringe structure are about 20 nm for both

films. From the systematic XRD analysis, we found that the films are epitaxially grown on the YSZ substrates with a cube-on-cube orientation relationship. A result of X-ray reflectivity analysis on the $Sn_2Nb_2O_7$ thin film is presented in Fig. 2. The film thickness of 21 nm estimated from the X-ray reflectivity measurement is comparable with that from the XRD analysis, indicating high crystal quality throughout the film. The estimated surface roughness of 0.8 nm is close to the lattice constant of $Sn_2Nb_2O_7$ of 1.058 nm, which represents a rather flat surface of the film. Similar values for the thickness and surface roughness are obtained for the $Sn_2Ta_2O_7$ film. The optical spectroscopy shows that the optical band gaps of the $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ films are 2.6 eV and 3.3 eV, respectively, which are slightly larger than the reported absorption thresholds for bulk samples, 2.3 eV and 3.0 eV [3].

Acknowledgments

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References

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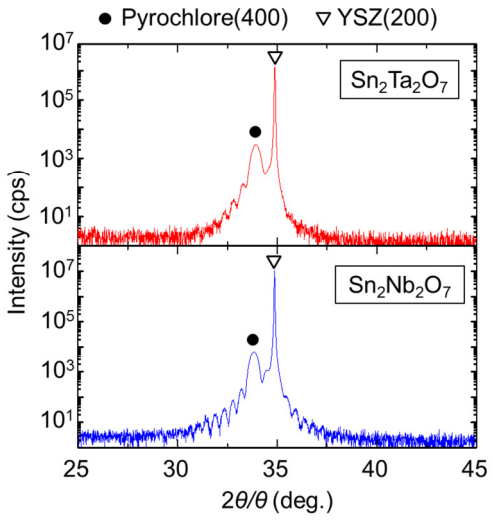

Fig. 1. 2θ-θ XRD profiles of $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$ thin films.

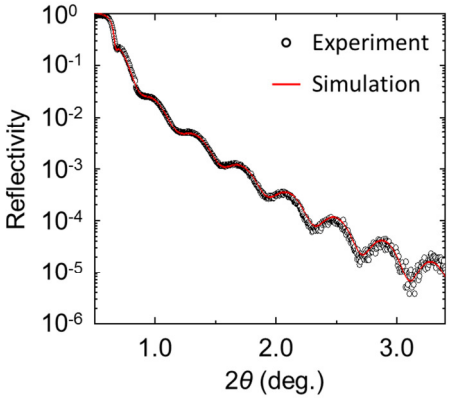

Fig. 2. X-ray reflectivity of a $Sn_2Nb_2O_7$ thin film and a simulated profile with a thickness of 21 nm, roughness of 0.8 nm, and density of 5.5 g/cm^3.