Kyushu Synchrotron Light Research Center

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Experiment Report for Prefectural Beamline

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Electronic states of Mg, Sn-doped Ga_2O_3 thin films on ultra-smooth sapphire substrates using a NiO seed layer

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1. Summary (Note: Please include conclusions)

1) For analyzing band gap of Ga_2O_3 thin films with different dopant, we have measured Ga_2O_3, Mg doped Ga_2O_3 and Sn doped Ga_2O_3 thin films. We complete the Sn doped Ga_2O_3 (Sn-Ga_2O_3) measurement as complement this time. We measured its valence band using synchrotron XPS and Ga *L* edge and O *K* edge using NEXAFS.
2) We also measure interface layer of $LaAlO_3$thin films on $SrTiO_3$ substate. We found the valence band changes with thickness. The O *K* edge also change. But there is no change in Al *L* edge and La *M* edge. These is not reasonable if consider $LaAlO_3$ as an isolated system. We should consider the interface interaction.

2. Purpose of experiment and background

In these years, the thermodynamically stable β phase of gallium oxide (Ga_2O_3) film has attracted the increasing interest as one of TCOs (transparent conducting oxide) thin films. [1] In fact, Ga_2O_3 is a transparent insulator with band gap of 4.85 eV. But with the donor doping, such as Si^{4+}, Sn^{4+}, or oxygen vacancy, it can be tuned to high electrical conductivity (38 S/cm) and colorful transparency. [2-4] These behaviors make it promising in the potential applications of solar-blind photodetectors, [5] solar cells, [6] and also field effect transistors. [7] Recently, based on the previous NiO (111) epitaxial seed layer on sapphire substrate, we obtained device-qualified crystalized Ga_2O_3 using KrF excimer laser annealing. Because of the laser effect during the thin film processes, there may be a new interface layer composite of Ga, Ni, and Al. To compare this interface layer, we would like to measure the typical $LaAlO_3/SrTiO_3$ interface structure.

3. Experimental（Note: Description of sample，method of experiment and analysis, etc.）

The NEXAFS and XPS data of Pd@HKUST-1 and HKUST-1 were recorded at BL12, SAGA Light Source. During NEXAFS experiment, both a total electron yield and a fluorescence yield were collected. The total electron yield mode can probe the materials with the order of several nanometers beneficial for the study of nanomaterials. While the probing depth for fluorescence measurements of the order of 100 nm for the fluorescence X-rays, used for the bulk references. The overall resolution is 0.1 eV. For the valence band measurement, we used Synchrotron X-ray source. For the core level measurement, we used Al Kα source. The detector of photoelectron is 16-input muti-channel detector (MCD). The peaks were calibrated by C 1s from the absorbed air on the sample surface. The spectrum resolution is 0.1 eV

4. Results and Discussions

1) Band gap and absorption edge of Sn-Ga_2O_3 thin film

Before we chose three samples, pure Ga_2O_3, Sn doped Ga_2O_3 (Sn-Ga_2O_3) and Mg doped Ga_2O_3 (Mg-Ga_2O_3). But for the Sn-Ga_2O_3 film, it is difficult to obtain clear signal. After analysis, we guess there may be an amorphous layer at its surface resulted from the laser annealing from sample top. The instantaneous high temperature results in the thin films have an extra process from crystallized phase to amorphous again. Then we controlled the laser energy carefully and keep its homogeneousness on the surface of the sample. Then the clear profiles are show as in Fig. 1~3. The features of these spectra are similar to the results before, but much smoother. Especially, we observed the clear Ga d-electron state at 10 eV in Fig. 1, double peak at 1120 eV in Fig. 2 and double peak around 535 in Fig. 3.

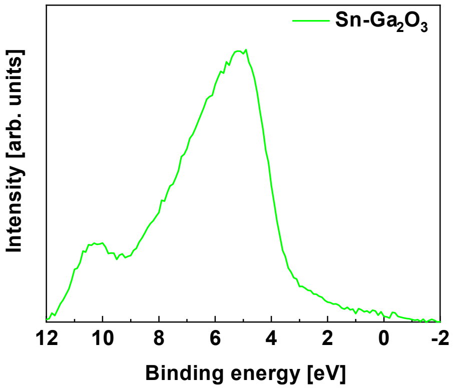

Fig. 1 XPS valence band of Sn-Ga_2O_3thin film.

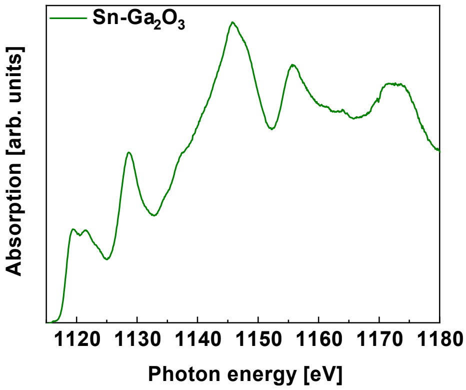

Fig. 2 NEXAFS Ca *L* edge of Sn-Ga_2O_3thin film.

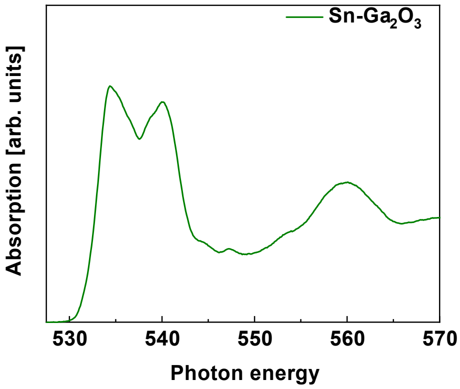

Fig. 3 NEXAFS O *K* edge of Sn-Ga_2O_3 thin film.

2) Interface layer of $LaAlO_3$ thin films

We measured the $LaAlO_3$ thin films with thickness from 1.2 nm to 25 nm. In this kind of epitaxial thin films deposited by PLD, the interface layer should be several nanometers. From valence band shown in Fig. 4, the edge of main peak shifts to higher binding energy with the thickness increasing roughly, except the film with 1.2 nm thick. This maybe result from the charging effect during measurement. We have to consider about the calibration in this kind of interface phenomenon later. We also noticed a small peak near the Fermi edge. This is an abnormal feature in the valence band. The origin of this small peak is still unclear. From NEXAFS, we observed the corresponding result that the observation edge shift to higher photo energy in O *K* edge. Especially, the observation edge change little from 5 nm, which means the interface layer under 5 nm with different electronic states. But the Al *L* edge and La *M* edge do not show any shift. Then we have to consider the reason of this phenomenon existed isolately in oxygen element.

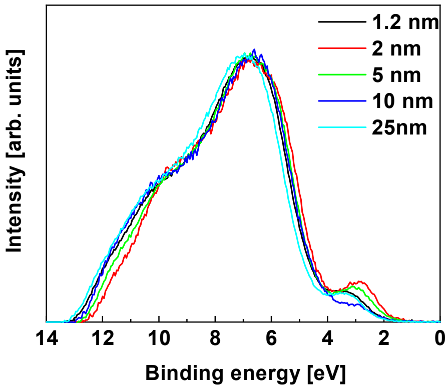

Fig. 4 XPS valence band of $LaAlO_3$thin film.

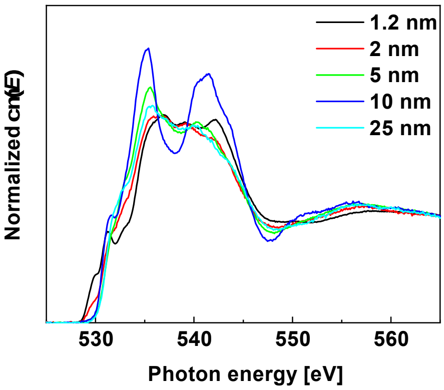

Fig. 5 NEXAFS O *K* edge of $LaAlO_3$thin film.

5. Future issues

For Ga_2O_3 thin films, we are writing pater reporting these results together with X-ray diffraction and extended X-ray absorption fine structure. About $LaAlO_3$ thin films, we have to consider the calibration of XPS and consider about the reason why we observed such specular results.

6. References

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７. Publications, patents（Note: Typical deliverables related to this proposal. ）

Not yet.

８. Keywords（Note: 2-3 words about samples and experimental methods. ）

Gallium oxide, Thin film, Electronic structure

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