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Optical properties of $(Al_xGa_{1-x})_2O_3$ on sapphire

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ABSTRACT

The $(Al_xGa_{1-x})_2O_3$ and Ga_2O_3 films are epitaxially grown on sapphire by pulsed laser deposition (PLD). From X-ray photoelectron spectroscopy (XPS) and X-ray diffraction measurements, the $(Al_xGa_{1-x})_2O_3$ films with Al compositions of 0.39, 0.49 and up to 0.53 are all single crystal and there is an out-of-plane tensile strain in $(Al_xGa_{1-x})_2O_3$ films within the range from 0.164% to 0.345%. The optical properties are investigated by Spectral Ellipsometry (SE) together with the optical transmission method. The spectral dependence of the refractive index (n) by SE is in accordance with the reported experiment results. The thicknesses of the Ga_2O_3 and $(Al_xGa_{1-x})_2O_3$ films obtained by SE fitting are 201, 116.8, 40 and 84.61 nm, respectively, which is consistent with the field emission scanning electron microscopy (FESEM) measurement results. In addition, with the Al composition increasing, the bandgaps of the $(Al_xGa_{1-x})_2O_3$ films determined from the SE are both increase from 4.95 to 5.49, 5.7 and 5.75 eV, almost identical to the values determined by the transmittance spectra, which is larger than some extent compared to reference [13] for the compressive strain in the $(Al_xGa_{1-x})_2O_3$ films.

1. Introduction

Monoclinic β-Ga_2O_3 has attracted increasing interests as a strong candidate for next generation devices such as solar-blind photodetector [1], Schottky barrier diode (SBD) and field-effect transistor (FET) [2] owing to its advantageous material properties, e.g., a wide bandgap of ~4.8 eV, a breakdown field of 8 MV/cm, a Baliga's figure of merit that is more than 4 times larger than that of SiC and GaN [3] and an easy, low cost and mass-producible availability of single crystal substrates to support the β-Ga_2O_3 homoepitaxial growth. The band-gap engineering of β-Ga_2O_3 can be achieved by alloying with Al or In to expand the range of applications. Especially with the incorporation of Al into β-Ga_2O_3, the bandgap of $(Al_xGa_{1-x})_2O_3$ can be continuously tuned from ~4.8 to ~8.7 eV [4–6] by adjusting the Al concentration, which is of great value to realize the wavelength-tunable opto-devices, metal-oxide-semiconductor field-effect transistors (MOSFETs), high electron mobility transistors (HEMTs) and so on. Until now, most studies on $(Al_xGa_{1-x})_2O_3$ system have been concentrated on the film epitaxy [6–11], the crystal structure, surface morphology and optical transmission characteristics. However, there have been a few theoretical studies and experimental measurements of the essential optical parameters of β-$(Al_xGa_{1-x})_2O_3$ with high Al composition, such as refractive index n and extinction coefficient k to the best of our knowledge. Spectroscopic ellipsometry

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(SE) has been used as a nondestructive technique to determine the film thickness and investigate the optical characteristics of semiconductors using a suitable model.

In this letter, we present the results of SE and optical transmission measurements on $(Al_xGa_{1-x})_2O_3$ films on sapphire substrate for the wavelength larger than 200 nm. In addition, the film thicknesses and Al compositions are also evaluated using scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS).

2. Experimental

The $(Al_xGa_{1-x})_2O_3$ films were deposited on sapphire (0001) substrates by pulsed laser deposition (PLD). The substrate temperature was fixed at 610 °C and the base pressure of the PLD growth chamber was 1.5×10^{-8} torr. The cylindrical stoichiometric $(Al_xGa_{1-x})_2O_3$ targets with different Al content x_t, ($x_t = 0$, 0.4, 0.5 and 0.55), were irradiated by focused KrF excimer laser beam and the corresponding $(Al_xGa_{1-x})_2O_3$ samples were referred to as sample A, sample B, sample C and sample D, respectively. The distance between the target and substrate was 5 cm. The repetition rate and pulse energy density were fixed at 3 Hz and 2 J/cm^2, respectively. During growth, the working pressure in the chamber was maintained at 0.01 mbar. The thicknesses of the epitaxial layers were about 80–210 nm, determined by the total number of laser pulses. The structural properties of the films were examined by high resolution X-ray diffraction (HRXRD). The stoichiometries of $(Al_xGa_{1-x})_2O_3$ films were investigated by XPS measurement using Mg $K\alpha$ X-ray source. Before XPS measurement, the surface of the samples was etched using *in situ* Ar^+ plasma and the peaks were calibrated by adventitious C 1*s* of 284.6 eV. The Spectral Ellipsometry (SE) and optical transmission method were used to determine the optical parameters, refractive index n, extinction coefficient k and absorption coefficient α.

3. Result and discussion

Fig. 1 presents the XPS measurement results of the $(Al_xGa_{1-x})_2O_3$ samples. With Al composition increasing, The Al 2*p* peak shifts to higher binding energy gradually and the intensity also increases, which is quite the reverse for Ga $2p_{3/2}$ peaks. We consider the shift can be ascribed to the fact that the charge transfer contribution changes with the increase of Al concentration for a more ionic character for Ga than Al element [5]. Based on the area of the peaks and the corresponding sensitivity factors, the relative ratios of Al to Ga in $(Al_xGa_{1-x})_2O_3$ films are calculated to be 39:61, 49:51 and 53:47 for sample B, C, and D, respectively and the oxygen atom percent in all $(Al_xGa_{1-x})_2O_3$ films is between 51% and 54%, indicating the formation of a large number of oxygen vacancies during film growth. In our previous study we have carried out the Energy-dispersive X-ray spectroscopy (EDS) measurement to confirm our XPS result [12].

To investigate the crystal structure of the grown $(Al_xGa_{1-x})_2O_3$ thin films, θ-2θ HRXRD patterns were recorded in the 2θ range of 15°–65°, as shown in Fig. 2. There are three diffraction peaks located at the vicinity of 18.95°, 38.4° and 59.19°, corresponding to the $(\bar{2}01)$, $(\bar{4}02)$ and $(\bar{6}03)$ faces, respectively. Apart from these peaks, no other peaks representing other

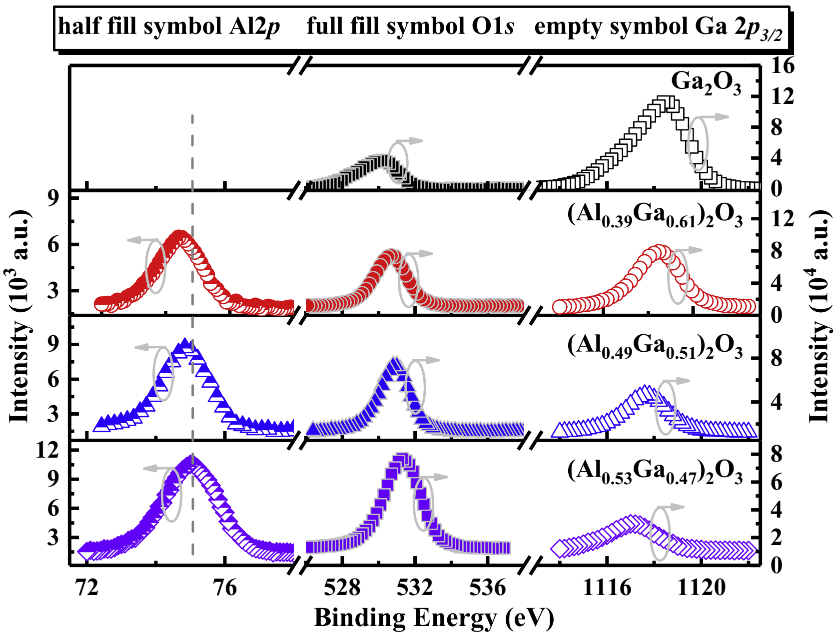

Fig. 1. Ga $2p_{3/2}$ and O 1*s* XPS spectra of Ga_2O_3 and the XPS results of the Ga $2p_{3/2}$, O 1*s* and Al 2*p* peaks of sample B, C, and D.