XPS study on composition and band structure of aluminum alloyed β-gallium oxide bulk crystals and thin films

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Beta-phase gallium oxide is a transparent, wide-gap semiconductor with a band gap of 4.85eV [1] and promising prospects for applications in high-power devices and UV photodetectors. Considering its higher calculated breakdown field [2], β-gallium oxide is predicted to outperform well established materials such as silicon carbide and gallium nitride for high-power switching. To further increase the high-power capabilities, as suggested by the Baliga figure of merit, $BFOM = \epsilon\mu E_b^3$ [3], it is required to increase the electron mobility μ and electric breakdown field E_b. The electron mobility is highly dependent on the material's crystallinity and lack of defects, thus highly dependent on the growth technique. Moreover, the electric breakdown field can be increased by alloying the oxide with aluminum. The present work discusses structural and electronic properties of β-$(Al_xGa_{1-x})_2O_3$ thin films grown by metal organic vapor-phase epitaxy and bulk crystals grown by the Czochralski method. The targeted Al content ranges up to 30%. The Al concentration has been determined by X-ray photoelectron spectroscopy (XPS) from weighted core-level analysis, an approach pre-validated using reference gallium oxide and aluminum oxide single crystals. Also, the thin films have been investigated for homogeneity by XPS depth profiling obtained by sequential Argon ion sputtering, revealing lower aluminum content at the sample surface, indicating possible surface segregation of gallium. Furthermore, the band gap has been determined by the electron loss onset in the XPS core-level spectra, as illustrated in Fig.1. Using the concentration dependence of the band gap based on optical absorbance measurements [4], our experimental band gap suggests an Al concentration of 4% (cf, Fig. 2), at variance with the XPS analysis, which resulted in a value of about 7.5%. Similar data have been recorded and analyzed for several thin films and bulk crystals of varying aluminum concentration and have also been compared to the Al content calculated from the lattice parameter measured by X-ray diffraction (XRD) for thin films and inductively coupled plasma optical emission spectrometry (ICP-OES) for bulk samples.

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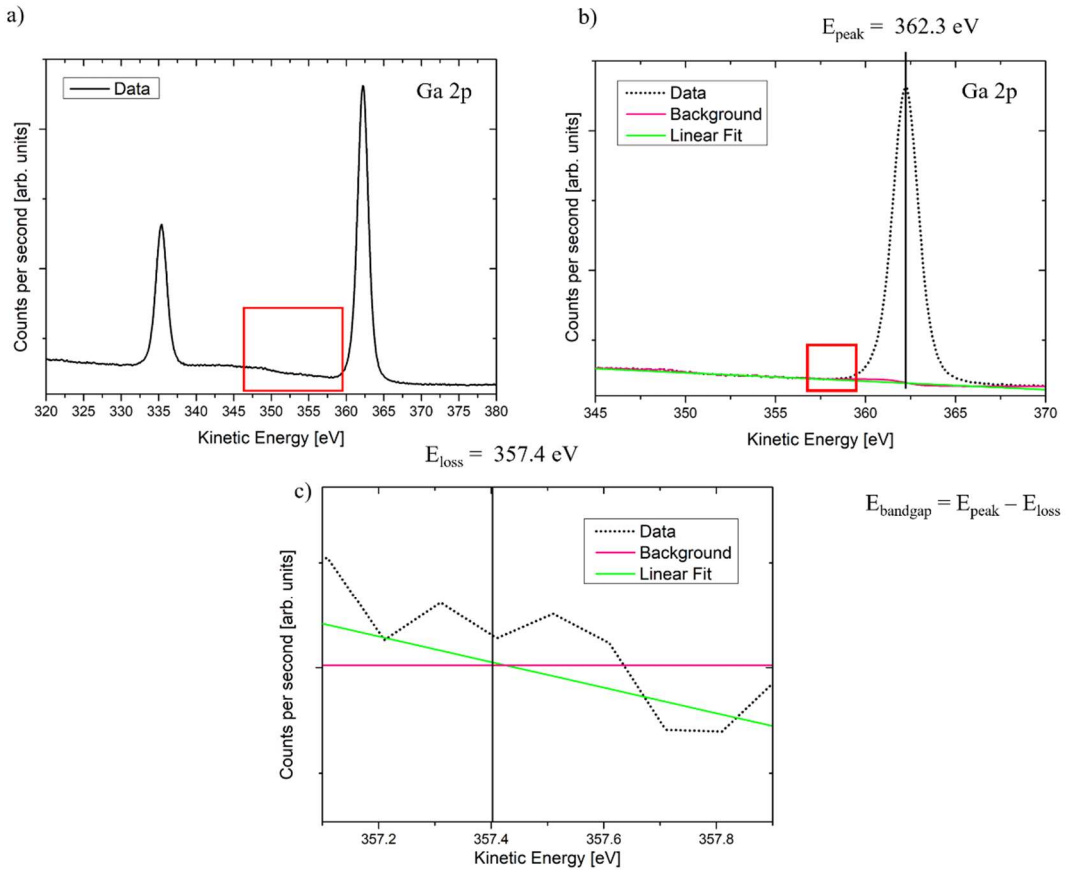

Fig. 1 a) Gallium 2p peak measured using monochromatized aluminum $\boldsymbol{K_\alpha}$ radiation, with the onset of band-to-band losses of the Ga 2p-3/2 peak (highlighted in red). b) Ga 2p-3/2 core level with background and linear fit to the loss onset; the peak energy corresponds to 362.3eV. c) The band gap is represented by the minimum possible energy loss, i.e., by the interception of the linear fit and the background of the peak (at 357.4eV), resulting in $E_{bandgap} = E_{peak} - E_{loss}$.

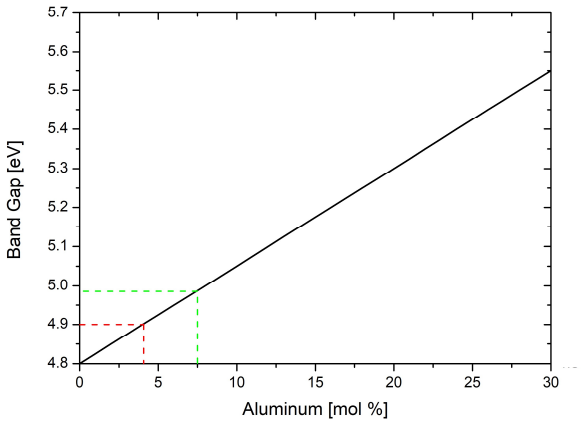

Fig. 2 Band gap variation with Al concentration (black solid line, from [4]). The red data point resembles the Al concentration according to the measured band gap of 4.9 eV, whereas the bandgap value of 4.98 eV as suggested by the 7.5% Al concentration of weighted core level XPS analysis is illustrated by green color.