# 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. Therefore β-gallium oxide has become a hot research topic due to its potential use to improve future power grids and reduce the global $CO_2$ footprint.

To further increase the high-power capabilities of a material with dielectric constant $\varepsilon$, as suggested by the Baliga figure of merit (BFOM)

$$BFOM = \varepsilon \mu E_b^3 \text{ [3]},$$

it is required to fine-tune the electron mobility $\mu$ and electric breakdown field $E_b$ of β-gallium oxide. The electron mobility is highly dependent on the material's crystallinity and lack of defects, thus highly dependent on the growth technique. Additionally, it is possible to dope gallium oxide to further increase electron mobility, although high doping concentrations may result in additional crystal defects, thus lowering the mobility [4]. Moreover, the electric breakdown field can be significantly increased to further improve the β-gallium oxide properties: Similarly to the mobility, the breakdown field is also related to the crystal quality; however, it is additionally possible to improve it by alloying the oxide with aluminum, resulting in further challenges for the crystal growth.

The present work discusses the ideal content and distribution of Al in epitaxial gallium oxide thin films and bulk crystal samples, combining multiple characterization techniques with a particular emphasis on depth-profiling X-ray photoelectron spectroscopy (XPS) measurements. These measurements revealed a potential surface segregation of gallium for the thin films grown by metal-organic vapor phase epitaxy (MOVPE). In particular, the influence of possible experimental artifacts originating from the destructive ion bombardment, as well as the surface sensitive nature of XPS on the estimation of sample composition is discussed. Additionally, the band gap has also been determined by energy loss measurements in XPS combined with UPS, revealing a dependency on the aluminium content.

**References**

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