Determination of Energy Band-Offsets of Ga_2O_3 for Device Modeling

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Background/Relevance

- Gallium Oxide is a large bandgap material that is of interest for use in high power applications
- Silicon is being replaced with materials more suited for use as semi-conductors such as Gallium Nitride. Certain figures of merit show Ga_2O_3 to be ~4000 times more suitable than Si.

Innovation

- Collaboration with industry partner Agnitron allows for quantity and quality of samples necessary for extensive data collection.
- Measurements on multiple instruments (XPS, AFM, Shimadzu) increases confidence in results

Approach

- X-ray photoelectron spectroscopy (XPS) directly measures core level energies of elements
- Valance band maximum (VBM) energy levels found by linear extrapolation of valance band edge.
- Valance band offset (VBO) is calculated from core level energies and VBM energies:

$$\Delta E_V = (E_{Al2pCL}^{AlGaO}(i) - E_{Ga3dCL}^{GaO}(i)) + (E_{Ga3dCL}^{GaO} - E_V^{GaO}) - (E_{Al2pCl}^{AlGaO} - E_V^{AlGaO})$$
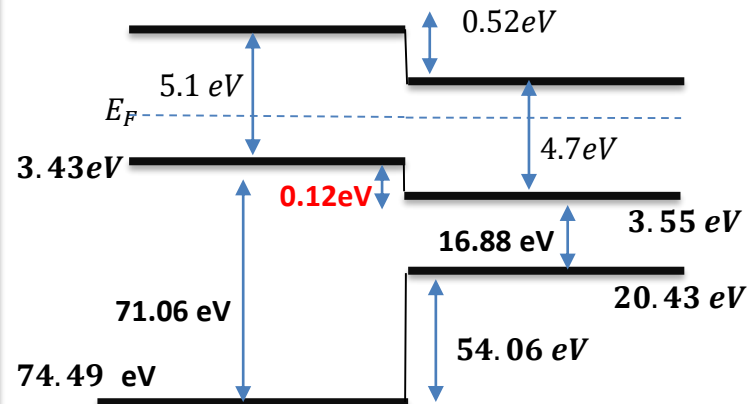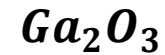

1.5nm AlGaO Ga 3d
Ga 3d
20.51 eV
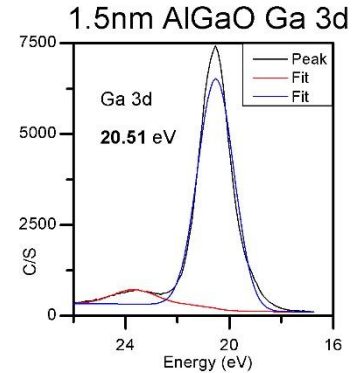
Ga 3d energy peak of AlGaO measured by XPS

Key Results

Measured energy peak positions (avg. at bottom):

Ga 3d	Al 2p	Ga 3d(i)	Al 2p(i)	GaO VBM	AlGaO VBM
20.38 eV	74.75 eV	20.34 eV	74.38 eV	3.45 eV	3.75 eV
20.36 eV	74.76 eV	20.51 eV	74.60 eV	3.53 eV	3.65 eV
20.37 eV	**74.76 eV**	**20.43 eV**	**74.49 eV**	**3.49 eV**	**3.70 eV**

VBO = -0.12 eV

Conclusions

$(Al_{.21} Ga_{.79})_2O_3$ Ga_2O_3

$0.52 eV$
$5.1\ eV$
E_F
$3.43 eV$
$4.7 eV$
$0.12 eV$
$3.55\ eV$
$16.88\ eV$
$20.43\ eV$
71.06 eV
$54.06\ eV$
74.49 eV

With the available data the VBO was determined to be 0.12 eV.

Confidence in this value still needs to be accurately determined.