Orientation-dependent band offsets at MOCVD grown β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces

A F M Anhar Uddin Bhuiyan[1], Zixuan Feng[1], Lingyu Meng, Jared M. Johnson[2], Hsien-Lien Huang[2], Jinwoo Hwang[2], and Hongping Zhao[1,2]

[1]Department of Electrical and Computer Engineering, The Ohio State University, Columbus, OH, USA

[2]Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA

Because of its large bandgap (~4.8 eV) and high breakdown field strength (8 MV/cm), β-Ga_2O_3 is considered as one of the most promising ultrawide bandgap semiconductor material systems for next generation energy efficient power and radio frequency electronics. Alloying β-Ga_2O_3 with Al_2O_3 can expand the energy bandgap and provide opportunities for the formation of high mobility two-dimensional electron gas (2DEG) with high sheet charge density in β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces with large band offsets. Our recent studies [1-3] show that β-$(Al_xGa_{1-x})_2O_3$ epitaxy on top of β-Ga_2O_3 substrates is highly dependent on the substrate orientation such as (010), (100) and $(\bar{2}01)$. Recent theoretical calculations based on density functional theory (DFT) revealed a distinct dependence of the band offsets between β-$(Al_xGa_{1-x})_2O_3$ and β-Ga_2O_3 on crystal orientation [4]. However, experimental measurements of the band offsets at β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 interfaces with different orientations are still limited.

In this work, for the first time we experimentally determined the band offsets of MOCVD grown β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces grown along (100) and (010) orientations, with different Al compositions. Phase pure β-$(Al_xGa_{1-x})_2O_3$ epitaxial films were grown on (100) and (010) β-Ga_2O_3 substrates via MOCVD. The valence and conduction band offsets at β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces along (100) [x= 0.10, 0.33 and 0.52] and (010) [x= 0.16, 0.26 and 0.35] orientations were determined by using x-ray photoelectron spectroscopy (XPS). By examining the onset of the inelastic energy loss in core-level atomic spectra, the bandgaps of β-Ga_2O_3 and β-$(Al_xGa_{1-x})_2O_3$ alloys with different Al compositions were measured from 4.83±0.12 eV (x=0) to 5.85±0.08 eV (x = 0.52). The valence band offsets were determined to be -0.06±0.06 eV (x=0.10), -0.11±0.06 eV (x=0.33) and -0.19±0.06 eV (x=0.52). The conduction band offsets up to 1.21±0.16 eV (x=0.52), were determined from the extracted bandgaps of (100) β-$(Al_xGa_{1-x})_2O_3$ alloys. Similarly, for (010) oriented β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces, the valance and the conduction band offsets of -0.13±0.06 eV and 0.57±0.06 eV were extracted for 35% Al composition. The determined band offsets revealed the formation of type-II (staggered gap) heterojunctions for all Al compositions investigated along (100) and (010) orientations. The bowing parameters extracted from the quadratic fitting of the conduction band offsets along (100) and (010) orientations were 1.25 eV and 0.75 eV, respectively. The (100) orientation exhibited larger conduction band offsets as compared to that of the (010) orientation. Both valence and the conduction band offsets were found to increase as the Al composition increases. The experimentally measured band offsets agreed well with the theoretically predicted values [5].

In summary, we investigated the band offsets at MOCVD grown β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces grown along (100) and (010) orientations with the variation of Al compositions up to 52%. Results from this study will provide guidance for future device designs and fabrications.

Acknowledgment: The authors acknowledge the funding support from the Air Force Office of Scientific Research No. FA9550-18-1-0479 (AFOSR, Dr. Ali Sayir) and NSF (1810041, 2019753).

References:

1. Bhuiyan et al., APL Mater. 8, 031104 (2020).
2. Bhuiyan et al., Cryst. Growth Des. 20, 6722 (2020).
3. Bhuiyan et al., Appl. Phys. Lett. 117, 142107 (2020).
4. Mu et al., Appl. Phys. Lett. 117, 252104 (2020).

Orientation-dependent band offsets at MOCVD grown β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces

A F M Anhar Uddin Bhuiyan, Zixuan Feng, Lingyu Meng, Jared M. Johnson, Hsien-Lien Huang, Jinwoo Hwang, and Hongping Zhao

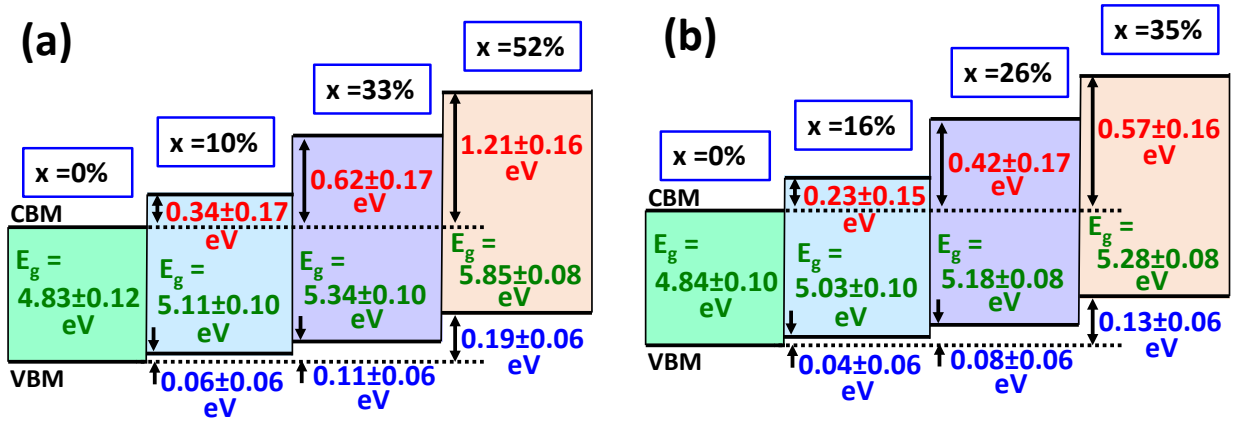

Figure 1 Band offsets at β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces for (a) (100) oriented β-$(Al_xGa_{1-x})_2O_3$ alloys with Al compositions of 10%, 33%, and 52% and (b) (010) oriented β-$(Al_xGa_{1-x})_2O_3$ alloys with Al compositions of 16%, 26%, and 35%. The bandgaps and the conduction and valence band offset values are represented in green, red, and blue, respectively.

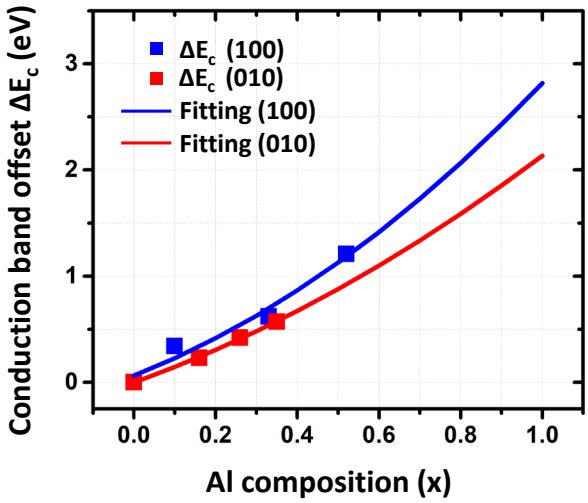

Figure 2 Conduction band offsets, ΔE_c for β-$(Al_xGa_{1-x})_2O_3$/β-Ga_2O_3 heterointerfaces oriented along (100) and (010), as a function of Al composition.