A.15: Determination of core level binding energies free from differential charging: A case for β-Ga_2O_3/NiO heterojunction

β-Ga_2O_3 is an important large bandgap semiconductor with n-type conductivity that can be varied by suitable doping with Sn, Si, and Ge etc. However, p-type conductivity in large bandgap semiconductors is far from reality. Hence, potential use of these large bandgap semiconductors in opto-electronic devices depends on suitable p-type semiconductor with larger bandgap like NiO, Ir_2O_3, Cr_2O_3 etc. to make p-n heterojunction (HJ). Among them NiO has a reliable p-type conductivity that can be varied with Li doping. Thus, NiO and β-Ga_2O_3 material system is a good choice for making reliable p-n HJ opto-electronic devices. Band offset (BO) at HJ is an important physical quantity responsible for device properties. The determination of BO HJ requires accurate knowledge of the core level (CL) binding energies of constituting materials across interface. However, differential charging in large bandgap semiconductors originating due to defect induced traps levels with different time constants hinders determination of accurate value of CL binding energies. X-ray photoelectron spectroscopy (XPS) data of NiO/β-Ga_2O_3 HJ shows presence of differential charging. We thus present a procedure to remove the differential charging effect to determine accurate value of CL energies.

For this, two sets of HJ samples with β-Ga_2O_3 (Set A) and NiO (Set B) top layers on NiO/GaN/Al_2O_3 and β-Ga_2O_3/NiO/Al_2O_3 templates respectively, were grown using RF sputtering. β-Ga_2O_3 (NiO) top layer thickness were 1.55 (1.22) nm, 3.46 (2.64) nm, and 5.76 (4.62) nm for SA1(SB1), SA2(SB2), and SA3 (SB3) samples, respectively. XPS data has been collected after 120 minutes of x-ray exposure on samples, which has been found adequate to saturate the charging effects.

XPS data from Ga 3d and Ni 3p core levels for set A samples is shown in Figure A.15.1(a) as a representative. CL energy difference between Ga 3d and Ni 3p have been marked. Increase (decrease) in CL intensity of Ga 3d (Ni 3p) is due to increase in thickness of β-Ga_2O_3 top layer for Set A samples. It is to be noted that CL energy difference is varying with change in top layer thickness, which should otherwise be independent of top layer thickness, if differential charging effect is absent. Similarly, CL energy difference data for Set B samples also indicate presence of differential charging, as noted from Figure A.15.1(b). Hence, it becomes necessary to remove the effect of differential charging to determine CL energy difference accurately. This issue originates due to presence of trap levels in the top layer. Hence, if one measures difference in CL energy with zero top layer thickness, then, there will be

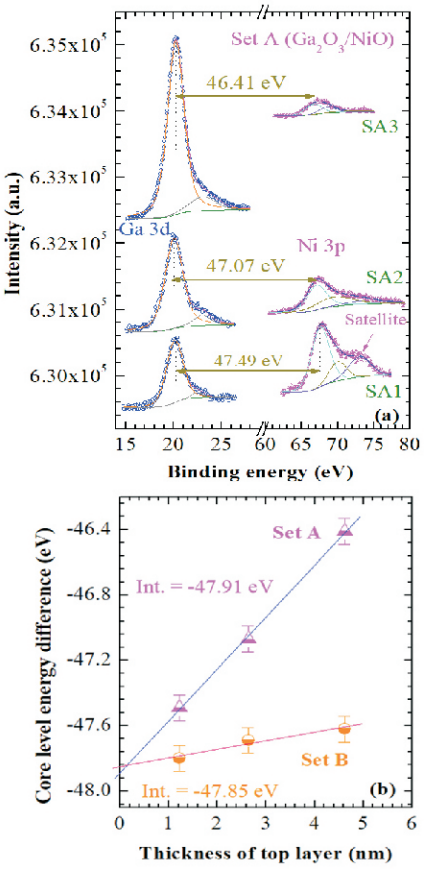

Fig. A.15.1: (a) XPS spectra Set A samples. Ga 3d and Ni 3p CL peaks and BE difference between them have been marked. The symbols and solid lines represent experimental and fitted XPS data, respectively. (b) CL energy difference with top layer thickness for Set-A and Set-B samples. The symbols and solid lines represent experimental and fitted data, respectively. The intercept values for Set A and Set B are also indicated.

no trap levels to affect it. It is experimentally not possible to have zero thickness of top layer and determine CL energy difference from XPS. However, if one plots the difference in CL energy as a function of top layer thickness and extrapolates it for zero value of top layer thickness, then, the CL binding energy difference will be free from differential charging effects. Similar plot for Set A and Set B samples have been shown in Figure A.15.1(b), where value of intercept gives the CL energy difference for zero top layer thickness. It is to be noted that both sets of samples give same value for CL energy difference within error, which shows the correctness of method adopted. For more details, please see *S. Ghosh et. al., Appl. Phys. Lett. 115, 251603 (2019).*

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