A.7: Determination of band gap bowing parameter for β- $(Al_xGa_{1-x})_2O_3$ alloys

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. In addition to this, band gap engineering can also be performed on β-Ga_2O_3 host material by making an alloy of β-$(Al_xGa_{1-x})_2O_3$ through Al substitution. The biggest advantage of preparing an alloy of β-$(Al_xGa_{1-x})_2O_3$ is that the band gap can be tuned over a wide range, from 4.8 eV to 6.9 eV. However, the band gap for an alloy can not be simply predicted by linear interpolation from the band gap values of the end points. The band gap of an alloy generally deviates from the linear variation by a factor termed as band gap bowing. Thus, knowledge of band gap bowing parameter is extremely necessary for the better understanding of physical properties of an alloy system.

For determination of band gap bowing parameter, several samples of β-$(Al_xGa_{1-x})_2O_3$ were prepared from solid state reaction route. The starting precursors were 99.99% pure β-Ga_2O_3 and α-Al_2O_3 powders, which were mixed in a desired ratio and ground to prepare β-$(Al_xGa_{1-x})_2O_3$ alloys. The mixture was then pelletized and provided a heat treatment at 1400 °C in air for about 14 hours to enhance the solid-state reaction. Finally, the furnace was naturally cooled to room temperature. For uniform mixing, the pellets were re-ground and re-pelletized. Then, a second heat treatment at the same temperature for about 14 hours in air was performed. 10 K optical reflectivity (OR) experiments were carried out on the same pellets by mounting them on a He based closed cycle refrigerator. A light from deuterium lamp was dispersed by using a monochromator (IHR 320). Incident light, chopped by an optical chopper at a frequency of ~190 Hz, was allowed to fall on the pellet and reflected light was detected by a photomultiplier tube using lock-in technique.

The phase purity and crystalline quality of prepared β-$(Al_xGa_{1-x})_2O_3$ alloys were checked using x-ray diffraction (XRD) experiments (graphs not shown here). It is found that the prepared β-$(Al_xGa_{1-x})_2O_3$ alloys are of single phase with monoclinic β-phase for Al composition of $x \leq 0.35$. The lattice parameters (a, b, c) and volume of the unit cell were found to decrease indicating the incorporation of Al atom at Ga site. This is because the atomic size of Al atom is smaller than that of Ga atom and substitution of Al atom leads to decrease in the unit cell volume. Figure A.7.1(a) depicts 10 K OR spectra from β-$(Al_xGa_{1-x})_2O_3$. A dip at around 4.8 eV in OR spectrum of β-Ga_2O_3 sample is noted and the energy position of this dip is found to be shifted towards larger energy as Al composition (x) is increased. Hence, this dip is related to the band edge feature of β-$(Al_xGa_{1-x})_2O_3$ alloys, whose energy position increases with increase in Al composition. The band gap values as obtained from the OR data have been plotted in Figure A.7.1(b) for different Al composition. The band gap of an alloy is given by Equation (1) as given below:

$$E_g(x) = x * E_g(Al_2O_3) + (1-x) * E_g(Ga_2O_3) - b * x * (1-x) \quad (1)$$

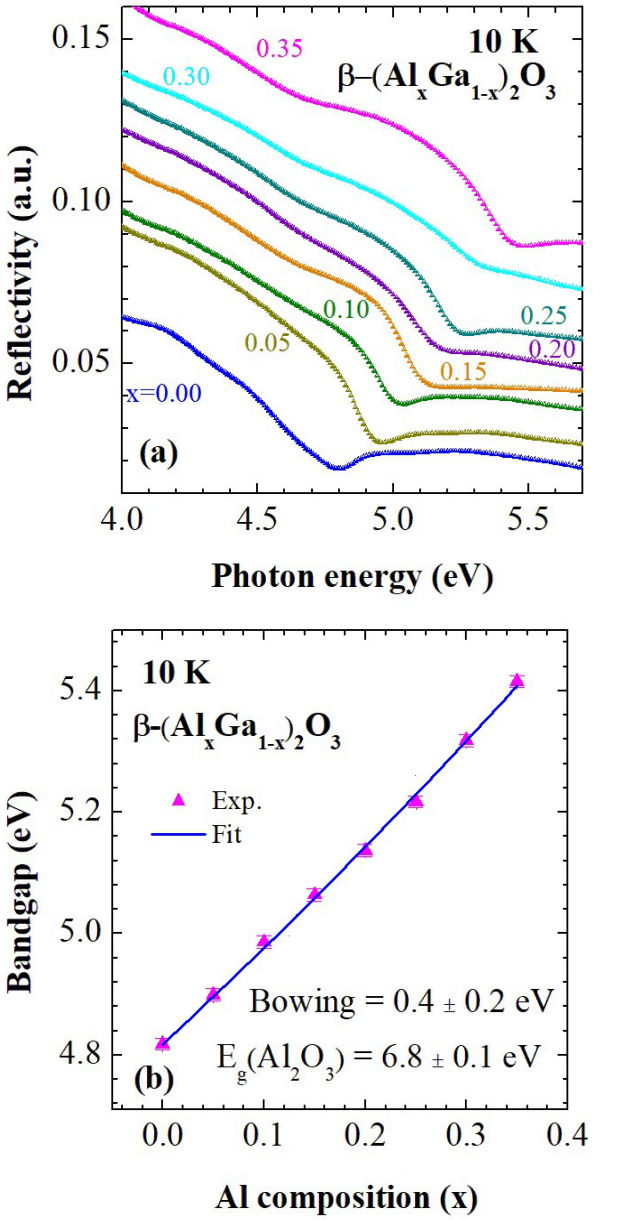

Fig. A.7.1: (a) 10 K optical reflectivity (OR) spectra from β-$(Al_xGa_{1-x})_2O_3$ alloys. The OR spectrum from each sample has been shifted along vertical direction for clarity of presentation, and (b) the band gap of β-$(Al_xGa_{1-x})_2O_3$ alloys as determined from OR data as a function of Al composition. Symbols indicate the experimental data and solid line is the fit to Equation (1). The values of bowing parameter and band gap of θ-Al_2O_3 have also been indicated.

where, first and second terms denote the band gap of Al_2O_3 and Ga_2O_3 materials, respectively, *b* is the bowing parameter and *x* is the Al composition. Solid line in Figure A.7.1(b) is the best fit to Equation (1), with *b*=0.4 ± 0.2 eV and $E_g(Al_2O_3)$=6.8 ± 0.1 eV.

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