## L.7: Crystalline structure and band alignment property of InAs/Ge(111)

Recently, Ge substrate is being investigated for the replacement of Si for next generation high carrier mobility devices. On the other hand, InAs is a promising material for infrared photodetectors and high-speed electronics. Therefore, integration of InAs with Ge substrate can lead to high speed and low power devices by combining the best performance of InAs and advantageous properties of Ge. In this direction, InAs/Ge(111) sample was grown by Metal Organic Vapor Phase Epitaxy (at SPDL) using Trimethylindium and Arsine sources at a growth temperature of 400°C. The structural and band alignment properties were investigated using X-ray diffraction (at Semiconductor Physics & Devices Laboratory and INDUS-2) and photoelectron spectroscopy (Angle integrated photoelectron spectroscopy beam line at INDUS-1), respectively.

Omega/2 theta scan of high resolution XRD shows (111) to (444) reflections of InAs layer and Ge substrate, which allowed to infer that the layer is highly oriented and structurally coherent with the substrate. Further, value of strain relaxation between substrate and layer was estimated to be 95% through reciprocal space map measurements (RSM) for (513) asymmetric reflections, Fig. L.7.1(a). Six intense peaks observed in the phi scan for InAs/Ge indicates that the layer is either of wurtzite phase or there is a coexistence of domains with different stacking configurations. In order to distinguish these structural phases, RSM measurement was performed between InAs(331)ZB and Ge(331)ZB peaks. No InAs(105) WZ related peak was observed confirming two domain ZB structure of the grown InAs layer, Fig.L.7.1(b).

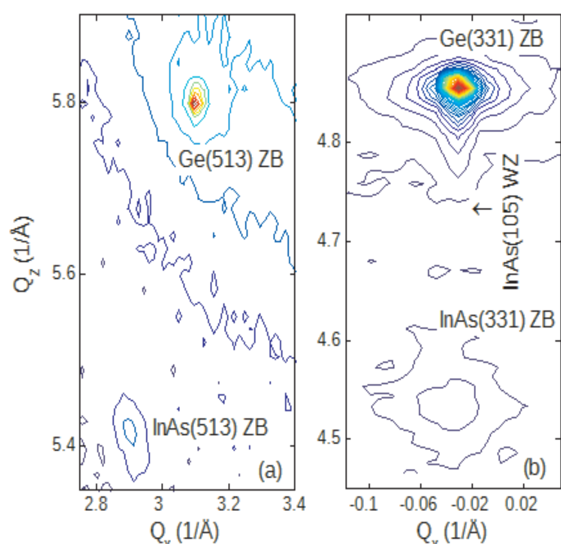


*Fig. L.7.1: Reciprocal space map of the InAs(111) layer for (a) (513) and (b) (331) reflections.*

For device design and modeling, the accurate knowledge of the band offsets and band alignment at the heterojunction interface is required. We calculated the valence band offset ($\Delta E_v$) across different interfaces of the InO/InAs/Ge structure using the difference in valence band onsets measured from PES experiment, which was carried out with a photon energy of 100 eV. The sample was sputtered for 5, 9, 11 min to access different interfaces (InO/InAs, InAs/Ge etc.). For unsputtered InAs substrate, a valence band onset as large as 3.72 eV is observed, which is attributed to the possible native oxides related to $As_2O_3$. A valence band offset of 1.45 eV is calculated for $InO_x$/InAs. The valence band spectrum shown in the inset of Fig. L.7.2 shows three valence band onsets at 0.32±0.20, 0.62±0.20 and 2.75±0.20 eV, which have been identified as related to top InAs layer, Ge substrate and $GeO_x$, respectively.

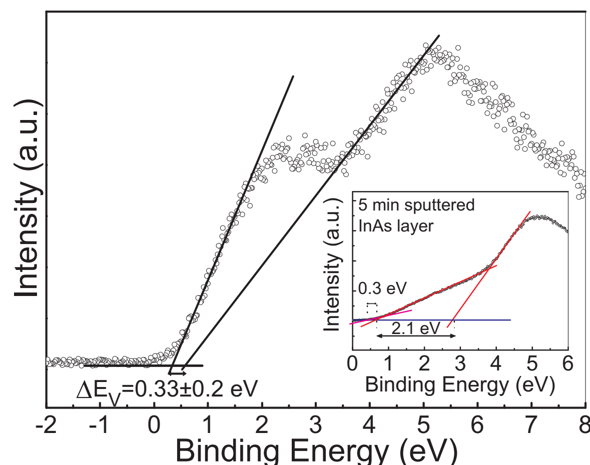


*Fig. L.7.2: Valence band spectrum after 9 min sputtering showing the onsets from InAs layer and Ge substrate. Inset shows three onsets for InAs layer, Ge substrate and $GeO_x$.*

It is therefore understood that the value of $\Delta E_v$ for InAs/Ge heterojunction is 0.30±0.20 eV. Comparing the $\Delta E_v$ value obtained in the present study with that reported in the literature, we find that the growth sequence (InAs/Ge or Ge/InAs) and crystal plane [(001) or (111)] causing different atomic arrangement at the interface do not change the value of $\Delta E_v$ in case of InAs/Ge heterojunction. It is also found that band alignment for both InAs/Ge and InAs/InO hetrojunctions are type I. Very low value of band offsets suggest that InAs/Ge system can be used for low power device application. For more details, please refer to *Suparna Pal et al., J. Alloy Compd. 646 (2015) 393*.

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