A.9: XRD investigations of wurtzite ZnO epitaxially grown over (111) oriented cubic GaP substrate

For effective use of a material in optoelectronic devices, its crystalline and optical qualities are of paramount importance, which are achieved by growing epitaxial thin films of the material on appropriate substrates. Epitaxial ZnO is usually grown on hexagonal symmetry based substrates like $ScAlMgO_4$, Al_2O_3 and SiC. Alternatively, (111) oriented cubic substrates having three fold symmetry are also used for the epitaxial growth of ZnO, in which silicon (Si) is most widely used substrate. However, realization of epitaxial ZnO is hindered due to the presence of interfacial SiO_x amorphous layer formed during the growth. Additionally, large lattice mismatch (~15.4%) and large thermal expansion coefficient mismatch (~48%) between Si(111) and ZnO also pose another difficulty in realizing good quality ZnO layers. In view of this, buffer layers like GaN, AlN, Al_2O_3, ZnS, MgO, Y_2O_3, CeO_2, Lu_2O_3, Sc_2O_3, YSZ, Gd_2O_3, etc. are explored to achieve epitaxial ZnO layer on Si(111) substrate. Gallium phosphide (GaP) material has a lattice mismatch (~15.8%) with ZnO, which is not much different than that of in between Si and ZnO. However, there exists a quite smaller thermal expansion coefficient mismatch (~7%) between GaP and ZnO as compared to Si and ZnO. Additionally, the other inherent advantage of ZnO growth on GaP substrate may be that phosphorous (P) might diffuse from substrate into ZnO layer by post growth annealing process and could lead to p-type conductivity in the ZnO layer. Phosphorous doping has already been shown to produce p-type ZnO layers. Keeping the above mentioned advantages, it is desirable to explore the possibility of epitaxial growth of ZnO over GaP(111) substrate using Pulsed Laser Deposition technique.

In order to determine the crystalline quality and epitaxial relationship, high resolution X-ray diffraction measurements are performed using PANalytical X'Pert Pro MRD diffractometer. Open detector omega scan width is found to decrease with increase in the growth temperature, which indicates that the crystalline quality improves with the growth temperature. 2Theta measurements show well defined XRD peak from (0002) reflection and a very weak peak from (0004) reflection of ZnO in 2theta range of 28^o-80^o other than that of (111) and (222) reflections from GaP substrate. This observation indicates that the grown layers are highly c-axis oriented. Open detector omega scan for (1-101) reflection of ZnO show a very broad peak for the growth temperature of 400 °C, which becomes sharper for the growth temperature of 500 °C. However, there is no signature of (1-101) reflection of ZnO for the growth temperature of 300 C. This observation suggests that the ZnO layer has taken in-plane orientation for the growth temperature greater than 400 °C. In order to confirm the in-plane orientation and to determine the epitaxial relationship, phi scans for (1-101) reflection of ZnO and (220) reflection of GaP are performed and the data is presented in Fig. A.9.1(a), where six peaks for (1-101) reflection of ZnO are clearly seen for the growth temperature of 500 °C.

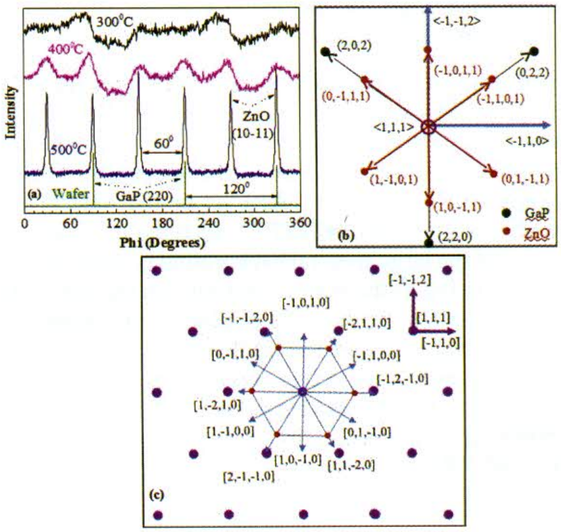

Fig.A.9.1 (a) Phi scans of asymmetric reflections from ZnO layers grown at different temperatures and GaP susbtrate. (b) Superpositions of reciprocal lattice points of ZnO and GaP. (c) In-plane atomic arrangement of wurtzite ZnO and cubic GaP.

This indicates that the ZnO layer has adopted well defined in-plane orientation with hexagonal symmetry. Phi scan of (220) reflection of GaP substrate shows three peaks separated by 120^o. It is also noted that three peaks from the substrate coincide with three peaks from ZnO layer. The three reciprocal lattice points (RLPs) from the GaP substrate are identified to be (022), (202), (220), while six RLPs corresponding to six peaks for (1-101) reflection of ZnO are (-1, 1, 0, 1), (0, 1,-1, 1), (1, 0,-1, 1), (1,-1, 0, 1), (0,-1, 1, 1), and (-1, 0, 1,1). Based on the phi scan measurements, arrangement of RLPs are drawn in Fig.A.9.1(b). Following this, superimposition of direct lattices of ZnO and GaP are shown in Fig.A.9.1(c). It is noted that the [-1, 2, -1, 0] of hexagonal ZnO is parallel to [-1, 1, 0] of cubic GaP. Thus, the out of plane and in-plane epitaxial relationship of ZnO layer with respect to GaP substrate is [0, 0, 0, 1]ZnO || [1, 1, 1]GaP and [-1, 2, -1, 0] ZnO || $[-1, 1, 0]_{GaP}$.

In conclusion, we report the epitaxial growth of wurtzite ZnO on cubic GaP(111) substrate and determine the epitaxial relationship of ZnO layer with respect to GaP substrate. For more details, please refer to S. D. Singh et al., Journal of Alloys and Compounds 617, 921, 2014.

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