Growth of non-polar (110) and semi-polar (116) AlN and GaN films on the R-plane sapphire

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Growth of non-polar $(11\bar{2}0)$ and semi-polar $(11\bar{2}6)$ AlN and GaN films on the R-plane sapphire

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1 Introduction

III-Nitride LEDs based on multiple quantum wells (MQWs) grown along the conventional [0001] (polar) direction suffer from the quantum confined Stark effect (QCSE), due to the existence of strong electric fields that arise from spontaneous and piezoelectric polarization. One approach to addressing the issue of polarization-induced internal electric fields, is growing wurzite group III-nitride MQW-based devices along the non-polar directions. There are experimental reports indicating the absence of QCSE on the quantum wells grown along the non-polar $[1\bar{1}00]$ [1, 2] and $[11\bar{2}0]$ [3, 4] directions. Another way of reducing the polarization effects is to grow devices on semi-polar planes. Semi-polar planes are those with at least one of the h, k Miller-Bravais indices being non-zero and the l index is also non-zero. The internal electric fields due to polarization effects in nitride MQWs grown on the semi-polar planes are reduced compared to similar QWs grown on the (0001) plane. Theoretical studies by Takeuchi et al. have shown that on specific semi-polar planes, there will be zero net piezoelectric polarization in the growth direction [5]. Currently, there are few reports on the growth of semi-polar $(10\bar{1}3)$ and $(10\bar{1}\bar{1})$ GaN [6, 7]. It has been reported by many groups that, when GaN is grown on R-plane sapphire, it grows with its $(11\bar{2}0)$ A-plane parallel to the sapphire surface [8-10]. In this paper, we report that the crystallographic orientation of the epilayers depends strongly on the nucleation conditions. Thus, a systematic study of the nucleation during the deposition of the AlN buffer was undertaken to clarify how such nucleation conditions affect the crystallographic orientation of the epilayers.

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2 Experimental procedures

The AlN and GaN films were grown on R-plane sapphire substrates by RF plasma-assisted molecular beam Epitaxy (PAMBE) in a Varian Gen-II system. Applied Epi RF plasma source was used to activate the molecular nitrogen. Ga and Al were supplied from Applied Epi SUMO^{TM} effusion cells. The R-plane sapphire substrates were degreased and degassed prior to epitaxial growth. The films were grown in two steps. First an AlN buffer (100-250 nm thick) was grown at 870 °C, followed by the growth of 0.75 µm of GaN at 770 °C. In order to understand the role of the AlN buffer, we have grown a number of thick AlN films under different growth conditions and investigated their structure by x-ray diffraction. Similarly, the GaN films were investigated by XRD studies and in-plane orientation of the films was determined by x-ray pole figure analysis. Pole figures were obtained using a Bruker General Area Detector Diffraction system (GADDS). The pole figure measurements were carried out by setting the four-circle diffractometer for a particular Bragg reflection and by mapping all orientations (χ, Φ) of this reflection above the specimen surface. Here χ is the tilt angle with respect to the sample normal and Φ is the angle rotation about the sample normal. In order to understand the rotational symmetry of the samples, the entire hemisphere of the pole figure data (ranging from Φ =0° to Φ =360°) was collected.

3 Experimental results

Figure 1a shows the θ-2θ scans for two AlN films grown under Al-rich and N-rich conditions of growth. From this data, we notice that films grown under Al-rich conditions have their A-plane $(11\bar{2}0)$ parallel to the R-plane $(1\bar{1}02)$ of sapphire. Weaker peaks at 39° and 67°, which correspond to $(10\bar{1}1)$ and $(10\bar{1}3)$ planes of AlN respectively, provide evidence of some mis-oriented domains, most likely at the interface between the sapphire and the AlN film. On the other hand, the AlN films grown under N rich conditions show only a very low intensity peak corresponding to the $(11\bar{2}0)$ diffraction. This raises the question about the crystallographic orientation of films grown under these conditions.

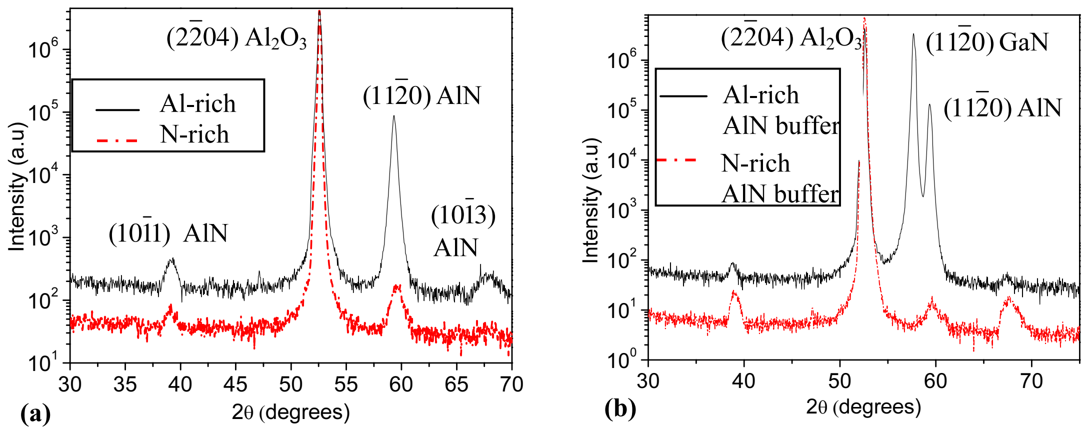
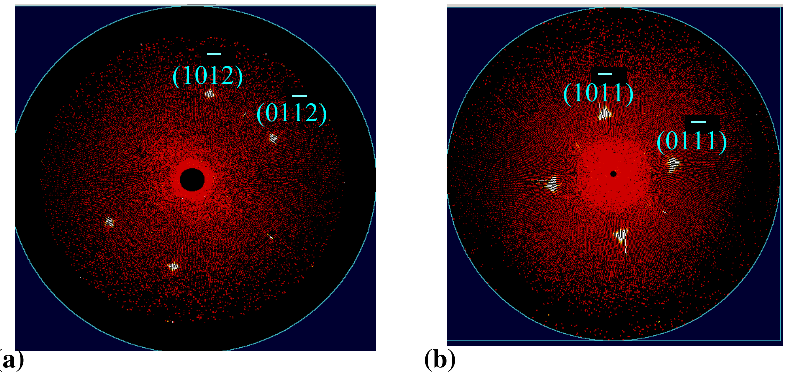


Fig. 1(a) θ-2 θ scans for two AlN films grown under Al-rich conditions and N-rich conditions. (b) θ-2 θ scans for two GaN films grown using AlN buffers as described in the insert of the figure.

Figure 1b shows the θ-2θ x-ray diffraction scans of two identical GaN films grown on the previously discussed AlN buffers. Again we observe that the GaN film, grown on the Al-rich AlN buffer, grows with its A-plane $(11\bar{2}0)$ parallel to the R-plane of sapphire, while the GaN film grown on N-rich AlN buffer does not show any diffraction peaks related to GaN. The only diffraction peaks seen in this figure are those of the sapphire substrate and low intensity peaks corresponding to the AlN buffer as discussed in Fig. 1a. Again this raises the question about the crystalline quality of the film or a change in the texture. In order to address this issue, we have carried out pole figure analysis on the two samples described in Fig. 1b. Figure 2 shows the $(10\bar{1}2)$ and $(10\bar{1}1)$ pole figures for the GaN film grown on the Al-rich AlN buffer. Due to the hexagonal symmetry of GaN, there are 6 equivalent planes $\{10\bar{1}2\}$. Also due to the rectangular symmetry of the A-plane unit cell, one expects to see poles corresponding to 180˚ rotation. In Fig. 2 (a) one clearly sees the poles corresponding to $(10\bar{1}2)$ and $(01\bar{1}2)$ as well as those corresponding to the two fold rotational symmetry. In addition one expects to see one extra diffraction spot at $\chi = 90°$ corresponding to the $(1\bar{1}02)$ pole. This diffraction has not been observed in our films because of the limitations of the diffraction geometry due to the defocusing effects close to $\chi = 90°$. Figure 2(b) shows the poles corresponding to $(10\bar{1}1)$ and $(01\bar{1}1)$ which again shows the 180˚ symmetry.



(a) **(b)**

Fig. 2 Pole figures for the GaN film grown on Al-rich AlN buffer (a) $(10\bar{1}2)$ poles, (b) $(10\bar{1}1)$ poles.

Using the angular relationships between $(10\bar{1}2)$ and $(10\bar{1}1)$ poles, we calculated the following in-plane orientation between the substrate and film: [0001] GaN || $[\bar{1}101]$ sapphire, $[1\bar{1}00]$ GaN || $[11\bar{2}0]$ sapphire [see Fig. 3]. This relationship agrees with the previous reports for GaN films grown on R-plane sapphire [8-10]. R-plane sapphire is a rectangular plane with unit cell dimensions 15.34 Å x 4.75 Å and A-plane GaN is also a rectangular plane with unit cell dimensions 5.18 Å x 5.5 Å. Thus to form a good epitaxy, three unit cells of A-GaN may fit in one unit cell of R-plane sapphire. The lattice mismatch is calculated to be 1.3% and ~15% in $[\bar{1}101]$ and $[11\bar{2}0]$ directions of sapphire respectively [8]. This type of extended epitaxy is schematically shown in Fig. 3.

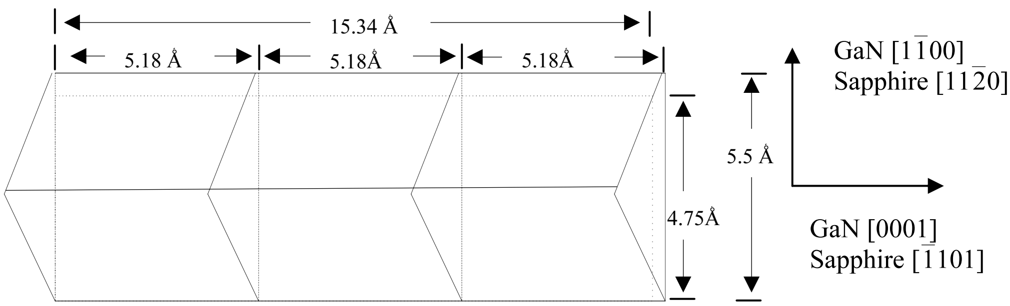


Fig. 3 Schematic illustration of epitaxial growth of A-plane $(1\bar{1}02)$ GaN on R-plane $(1\bar{1}02)$ sapphire.

Figure 4 shows the pole figures for the GaN sample grown on N-rich AlN buffer. The $(10\bar{1}2)$ pole figure is shown in Fig. 4(a). Contrary to the data of Fig. 2(a), we now see six $(10\bar{1}2)$ poles instead of three. In addition to these, we also see poles corresponding to the 180° rotation. The presence of two poles in the (0002) pole figure (Fig. 4(b)) indicates the presence of twin structures. For this sample, the pole figure analysis indicates that the $(11\bar{2}6)$ plane of GaN is parallel to $(1\bar{1}02)$ plane of sapphire. Due to the presence of the 180º rotational symmetry of the substrate, there is a possibility for the occurrence of twin structures in GaN films grown both along $[11\bar{2}0]$ and $[11\bar{2}6]$ directions. However, for the GaN film grown along the $[11\bar{2}0]$ direction, the c-axis is in the plane of growth and it is difficult to identify the presence of twinning using X-ray analysis. The sharpness of the diffraction peaks in both the GaN films indicates good epitaxial relationship with the substrate.

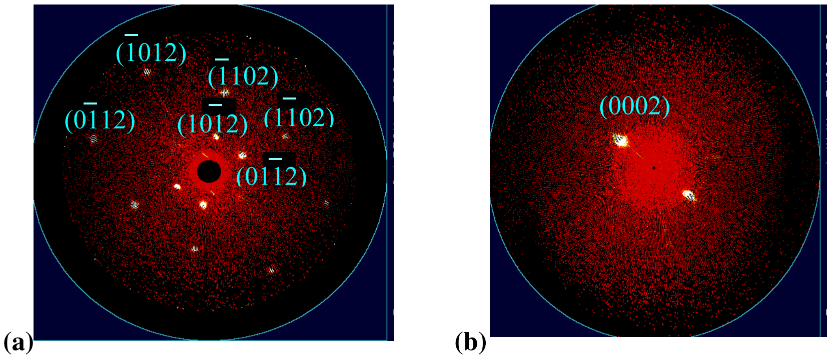


Fig. 4 Pole figures for the GaN film grown on N-rich AlN buffer (a) $(10\bar{1}2)$ poles, (b) (0002) poles.

Currently there is no available theory explaining the epitaxial growth of AlN and GaN on the R-plane sapphire. However there is such theoretical literature on the growth of these materials on the C-plane sapphire. Felice and Northrup reported that the relative stability of AlN films on the C-plane sapphire depends on the chemical potentials of Al and N. Specifically they found that Al-rich conditions lead to AlN having (0001) polarity, while N-rich conditions lead to AlN having $(000\bar{1})$ polarity [11]. We postulate that our observation on the crystallographic orientation of AlN and GaN on the R-plane sapphire is also affected by the chemical potentials of Al and N during growth.

4 Conclusions

In conclusion, we have shown that two different epitaxial relationships can occur when growing GaN on R-plane of sapphire depending on growth kinetics of the AlN buffer. The well known GaN orientation with its A-plane parallel to the R-plane of sapphire is only favoured when an Al-rich AlN buffer is used. In this case the in-plane epitaxial relationship between the sapphire and GaN is found to be [0001] GaN || $[\bar{1}101]$ sapphire, $[1\bar{1}00]$ GaN || $[11\bar{2}0]$ sapphire. On the other hand, when a N-rich AlN buffer is used, GaN epilayer grows with its $(11\bar{2}6)$ plane parallel to the R-plane of sapphire.

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