INVESTIGATION OF Si RELATED DEEP ACCEPTOR LEVEL IN AS GROWN GaN BY DLTS

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In this study, we have investigated the origin of an acceptor level in as grownGaN thin films grown by MBE on Si substrate. DLTS measurements revealed the presence of anacceptor defect level in the band gap of GaN with activation energy E_a = 0.23±0.01eV, capture cross section 3.18 × 10^{-18} cm^2 and trap concentration 6.0 × 10^{14} cm^{-3}. This defect level may be correlated to the silicon incorporation into GaN due to high substrate temperature during GaN film growth and the same might be responsible for the so called p-type conductivity of GaN layer. The transport of out-diffused Si atoms into GaN is through the voids presents in the grown film. The density of carriers at GaN/Si interface is high as compared to surface of GaN demonstrated by depth profiling of carriers. The presence of Si in GaN is further justified using photoluminescence and Raman spectroscopy measurements.

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1. Introduction

The III-nitrides especially GaN have attracted great interest in the recent years for potential applications in ultra-violet (UV), blue, green, white light emitting diodes and short wavelength optoelectronic devices [1-4].However, the performance of these electronic devices strongly dependsupon the nature of intrinsic and extrinsic defects present in the as grown GaN [5]. Therefore the investigation of various deep level defects in GaN has fundamental importance. Various researchers have reported donor deep level defects in GaN grown on sapphire substrate. For example; F. D. Auretet. al. characterized GaN layers grown by ELO-OMVPE and found energy levels at 0.15, 0.22 and 0.30 eV below the conduction band [6]. M. Asghar et. al. performed DLTS on p-n diodes of GaN grown on basal plane sapphire by MOVPE and observed deep level defects at 0.59, 0.76 and 0.96 eV [7]. D.C. Look et.al.reported five electron levels having activation energy 0.16, 0.25, 0.35, 0.60, 0.67 and 1.0 eV in GaN grown on sapphire substrate by HVPE [8]. But there are very few reports about the deep acceptor levelsin as grown GaNon Si substrate. Therefore there is still work need to be done to understand the nature of deep acceptor level present in the band gap of GaN.

In this paper, we have investigated the origin of a deep acceptor level in as-grownGaN on Si substrate by MBE. Deep level transient spectroscopy measurements revealed an acceptor level in the band gap of GaN having activation energy E_a = 0.23±0.01 eV above the valence band, capture cross section 3.18 × 10^{-18} cm^2 and trap concentration 6.0 × 10^{14} cm^{-3}. With the first principle theory, this acceptor level is related with Si_N(silicon on nitrogen site) defect. The mechanism of Si incorporation in as grown GaN was discussed in detail. Furthermore, the presence of Si atom in GaN was justified with the help of photoluminescence and Raman spectroscopy measurements. Experimental details, results, discussion and conclusion have been presented in the subsequent sections.

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2. Experimental details

MBE chamber was prepared for the growth of GaN on undoped Si(1 1 1) substrate of 3 inch diameter wafer. During the 4 hours growth procedure, the chamber pressure, substrate temperature and gallium cell temperature were set as 1.4×10^{-9} Torr, 1050°C and 930°C, respectively. The nitrogen plasma was generated by RF power supply maintained at 250W. The thickness of grown sample was found by film thickness monitor as 1 micro-meter. Contrary to the general understanding that GaN is instrinsically an n-type material, the Hall measurementssurprisingly revealedthe p-type conductivity of grown GaN film having hole concentration of the order of 1×10^{15} cm^{-3}. For electrical characteracterization, Schottky contacts of diameter (1mm, 2mm and 3 mm) of Au-Cr (2000Å, 200Å) were deposited on GaN using electron beam evaporation technique.The deposition parameters such as chamber pressure and deposition rate were kept as $1.7x10^{-5}$ torr and 20Å, respectively. Ohmic contact of metal Aluminum of thickness 2000Å was deposited on the Si (back) surface followed by heat treatment for 10 minutes at 450°C. The characterization of the grown film has been performed using following equipments: DLTS (DLS 83D Hungry), PL and Raman spectroscopy (mini PL/Raman) having laser wavelength 248nm and XRD (Bruker D8). Photoluminescence, Raman, Hall measurements and XRD measurements were performed at room temperature.

3. Results and Discussion

3.1 X-Ray Diffraction

The quality of GaN layers grown on Si(111) substrate was investigated by x-ray diffraction using Bruker D8. Figure 1 displays one of the representative x-ray spectra of GaN samples. Here, diffraction peaks are observed at 2θ ~ 28 ± 0.41, 34 ± 0.57, 36± 0.01, 58 ± 0.83, 72 ± 0.93, 94 ± 0.93 and 126 ± 0.21, respectively. Peaks observed at 2θ ~ 28 ± 0.41, 57, 58 ± 0.83 and 94 ± 0.93 are due to the silicon substrate and 34 ± 0.57, 72 ± 0.93 and 126 ± 0.21 are related to the crystalline phase of GaN. Miller indices calculated for these diffraction peaks were found to be (111), (222) and (333) for silicon and (0002), (0004) and (0006) for GaN, respectively [9-17].

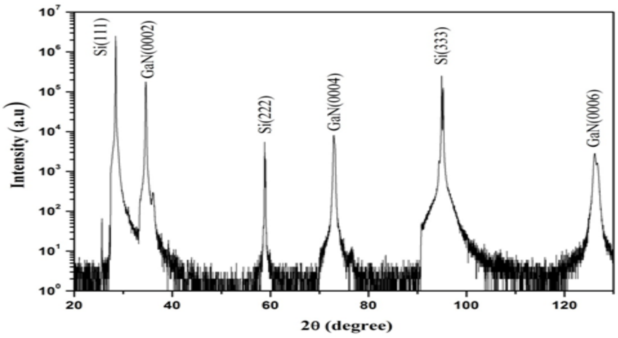

Fig. 1 X-Ray Diffraction pattern of as-grown GaN thin films on Si substrate by MBE

3.2 Deep Level Transient Spectroscopy

Deep level transient spectroscopy (DLTS) was performed to investigate the presence and identification of deep level defects in the bandgap of GaN. It is very powerful technique that provides quantitative information about the deep energy level position, trap concentration and capture cross-section [18]. Figure 2 displays the representative DLTS spectrum of un-doped GaN/Si thin film measured in the temperature under the following conditions: reverse bias U_R= -1, filling pulse V_p= 0V and filling time t_p= 20 sec.

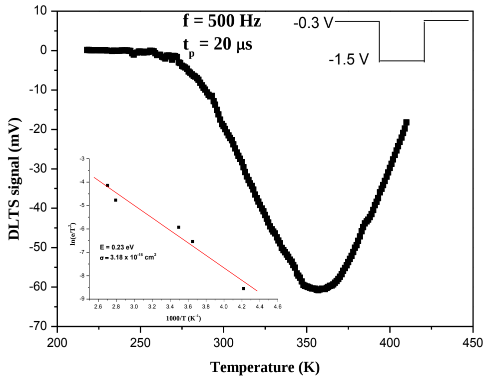

Fig.2 Typical DLTS spectra of GaN grown on Si substrate by MBE at 1500 Hz. Inset shows representative emission rate signature (Arrhenious plot) of deep acceptor level in MBE grown GaN on Si substrate.

In the measured spectrum, only a single acceptor level at 357 K was observed. From the DLTS measurements, Arrhenius plot (inset) was prepared to calculate the electrical parameters of the observed deep level defect i.e. activation energy and capture cross-section that are 0.23 eV ± 0.01 eV and 3.18 × 10^{-18} cm^2 respectively using the following equation

$$\ln\left(\frac{e_n}{T^2}\right) = \gamma_n \sigma_n + e^{-\frac{\Delta E}{kT}} \tag{1}$$

where e_n emission rate (s^{-1}), T temperature (K), σ capture cross-section (cm^2), γ is constant ($cm^{-2}s^{-1}$) and equal to$2k^2m^*\left(\frac{2\pi}{h^2}\right)^{\frac{3}{2}}(3)^{\frac{1}{2}}$, ΔE activation energy (eV) and$k$ Boltzmann constant (eV/K) [19, 20]. Trap concentration of the observed acceptor level was estimated as 6.0 × 10^{14} cm-3 with the help of formula given as $N_T = 2N_D\ (\Delta C/C)$ [18]. In the literature, Si can be considered as acceptor as well as donor replacing N and Ga respectively. For example Gotz et al reported Si as donor in GaN with activation energy 0.17 eV [21]. However the acceptor energy level may be related to the silicon atoms sitting at the nitrogen site in the lattice structure of GaN[22-24]. The presence of the silicon related defect in GaN layer is most probably related to the substrate temperature during growth i.e. 1050 oC. We argued that at such high substrate temperature in MBE chamber, the Si atom diffused out of the substrate and penetrates into the GaN film. Jakielaet at demonstrated that at high substrate temperature during growth, the Si out diffusion becomes prominent [25]. The out-diffused Si atoms transport into the GaN thin film through the voids which are present in the grow film. This argument is further strengthened by the free carrier concentration depth profile exhibiting maxima near the GaN/Si junction. Doping concentration (N_D) is calculated by using the slope of V–$(A/C)^2$ plot obtained (see figure 3) by theoretical fitting of its linear region as,

$$N_D = \frac{-2}{q\varepsilon_0\varepsilon_r \dfrac{d\left(A/C\right)^2}{dv}}$$

Where q (1.6×10^{-19} C) is the charge on an electron, ε_o (8.85×10^{-14}) is the permittivity of the free space, ε_r is the relative permittivity of the medium, A is the area of the Schottky contact and C is the background capacitance in pF. The width of space-charge region can be calculated using formula$W(\mu m) = \dfrac{A\varepsilon_0\varepsilon_r}{C}$. The graphical representation of width versus doping concentration $N_D\left(cm^{-3}\right)$ is known as depth profiling. The presence of low density of carriers at top and high density of carriers at GaN/Si interface also justified our argument that Si atoms diffused into the

GaN which are originated from Si substrate. We have performed Ramanand photoluminescence measurements to support our argument.

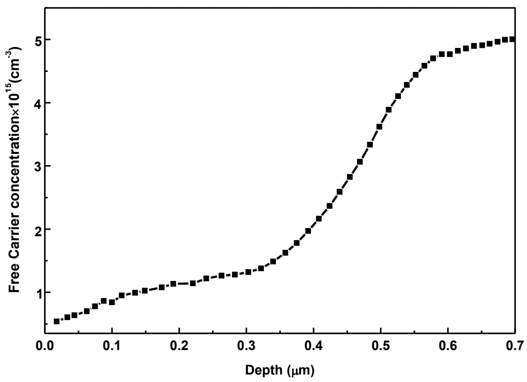

Fig. 3 Graph between depth verses carrier concentration of GaN on Si substrate

3.3Raman Spectroscopy

Fig. 4 shows the Raman measurement of GaN thin film grown on Si substrate by MBE. A number of vibrational modes corresponding to the GaN and silicon are observed. A strong peak at 300 cm^{-1} is due to acoustic phonon mode of Si in GaN film along with Si substrate peak at 520 cm^{-1} [26]. Furthermore, we have observed E_2 (high) and A1 (LO) modes of GaN at 577 cm^{-1} and 740 cm^{-1}, respectively [27, 28]. Compared to the characteristic E_2 (high) of GaN, we see red shift in E_2 (high) mode in our as grown GaN sample, we tentatively link this shift in the Raman peak to the presence of compressive stress which is originated due to the presence of Si atom in GaN crystal [9, 29]. The peaks present at 980 and 1287 cm^{-1} are due to acoustics-optical combination and optical combination modes of GaN, respectively [30].

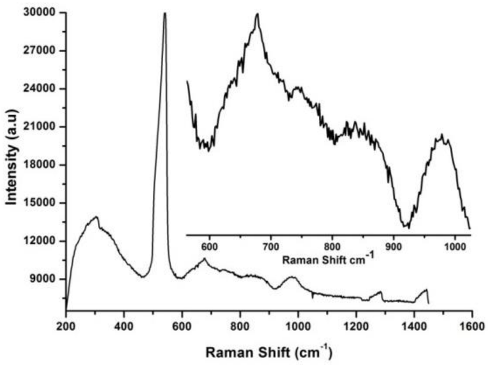

Fig. 4 Raman shift of GaN illustrating the presence of E_2 and A1(LO) modes.
The inset is the highlighted part of original graph in the range of 600 to 1000 cm^{-1}

3.4 Photoluminescence

Photoluminescence (PL) spectroscopy is a relatively simple, non-destructive but useful technique to probe information about the intrinsic bandgap, defect states, quality and crystallinity of the material. PL spectrum of GaN is shown in fig. 5. A number of emission peaks are observed in the PL spectrum at 2.2, 2.62, 2.86, 3.2 and 3.3 eV. A broad band at 2.2 eV is due to the yellow emission.The full width at half maximum (FWHM) of this broadband is consistent with the commonly observed YL i.e. 600 meV [31]. A doublet emission line observed at 3.2 and 3.3 eV is assumed to be originated from the silicon atoms sitting at the position of nitrogen in the lattice of GaN i.e. Si_N[32]. However, the lines originated from 2.62 eV and 2.86 eV are related to the Y_i lines.

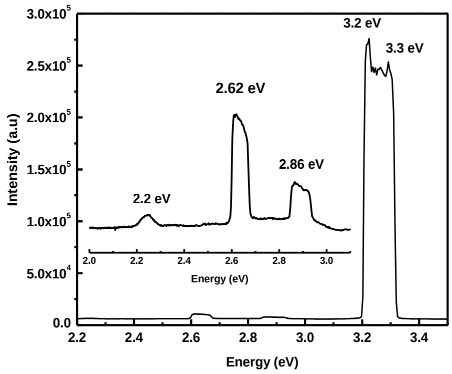

Fig. 5 Room temperature photoluminescence spectrum of as-grown GaN layer. The peak at 3.2 eV related to Si atom at nitrogen site

4. Conclusions

In this study, we have investigated the origin of an acceptor level in un-doped GaN thin films grown by MBE on Si substrate. DLTS measurements revealed the presence of a defect level in the band gap of GaN with activation energy E_a = 0.23 eV and capture cross section σ = 3.18 × 10^{-18} cm^2. The free carrier (hole) concentration measured by C-V methodof the as grown intrinsic GaN interestingly happens to be nearly of same amount, this indicates to argue that the observed acceptor defect level at 0.23 eV above the valence band maxima might be the key factor of p-type conductivity in our as grown GaN film.This defect level may be correlated to the silicon incorporation into GaN due to high substrate temperature during GaN film growth. The out-diffused silicon atom travel to the GaN layer either through the thinner part of the layer and/or voidstherein. The presence of Si in GaN was further confirmed using photoluminescence and Raman spectroscopy measurements.

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