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Carrier concentration dependence of donor activation energy in n-type GaN epilayers grown on Si (1 1 1) by plasma-assisted MBE

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ABSTRACT

The n-type GaN layers were grown by plasma-assisted MBE and either intentionally doped with Si or unintentionally doped. The optical characteristics of a donor level in Si-doped, GaN were studied in terms of photoluminescence (PL) spectroscopy as a function of electron concentration. Temperature dependent PL measurements allowed us to estimate the activation energy of a Si-related donor from temperature-induced decay of PL intensity. PL peak positions, full width at half maximum of PL and activation energies are found to be proportional to the cube root of carrier density. The involvement of donor levels is supported by the temperature-dependent electron concentration measurements.

1. Introduction

Gallium nitride (GaN) and its related materials have been widely studied for their unique applications in optoelectronic and high temperature/high power electronic devices with relatively low power consumption [1]. A number of studies have been performed successfully to grow GaN on different substrates such as Al_2O_3, SiC, GaAs and Si [2–5]. Silicon is considered to be one of the most promising candidates for the GaN epitaxy because of its many advantages such as high-quality, large size, low cost and a well-known existing device technology [6]. The origin of the residual n-type conductivity of undoped GaN layers grown on different substrates, by various epitaxial techniques, is still relevant issues. To date, among all the reported buffer layers for GaN on Si heteroepitaxy, the AlN buffer layer approach yields the best results reported in the literature [7,8]. However, the mutual solubility of Al and Si is very high at the buffer-layer growth temperature (~820 °C versus eutectic temperature 577 °C). Therefore, interdiffusion of Al and Si at the interface is severe, resulting in high unintentional doping levels in the epilayers and Si substrates [9]. To overcome this serious drawback, it has been demonstrated that a silicon nitride buffer layer can be used for the low unintentionally doped GaN growth [10–13]. The band-gap narrowing (BGN) effect induced by many body Coulomb interactions is expected to play an important role in the optoelectronic properties of the nitrides because of their large exciton binding energy and effective electron mass [14]. The BGN has been studied experimentally through intentional doping, optical pumping and current injection [15–17]. In addition, it has been reported that the potential fluctuation by randomly distributed impurities significantly influences both electrical and optical properties of GaN [18,19]. Near-band edge (NBE) transition energy and Hall mobility of GaN:Si grown by metal organic chemical vapor deposition (MOCVD), decreased with increasing carrier concentration, indicating strong dependence of the photoluminescence (PL) transition energy on potential fluctuation [20]. In this letter, we have studied the nature of the Si-related donor level in GaN epilayers on Si (1 1 1) substrate by studying the luminescence properties as a function of carrier concentration.

2. Experiments

The samples used for this study were grown by RF-MBE system (OMICRON) equipped with a radio frequency (RF) plasma source and the base pressure better than $\sim 1 \times 10^{-10}$ mbar. The semi-insulating Si (1 1 1) substrates (resistivity > 3000 Ω cm) were ultrasonically degreased in isopropyl alcohol (IPA) for 10 min and boiled in trichloroethylene, acetone and methanol at 70 °C for 5 min, respectively, followed by dipping in 5% HF to remove the surface oxide. The substrates were outgassed at 900 °C for 1 h in ultra-high vacuum. The samples were grown by nitridation–annealing–nitridation process, in which first the nitridation of the substrate was carried out at 530 °C for 30 min, followed by annealing at 900 °C for 30 min and again nitridation at 700 °C for

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30 min [21]. After nitridation, a low-temperature GaN buffer layer of 20 nm was grown at 500 °C, where the Gallium beam equivalent pressure was kept 5.6×10^{-7} mbar. Afterwards, 225 nm thick, undoped (sample (a)) and Si-doped (sample (b)–(e)) GaN epilayers were grown on the buffer layer at 700 °C. Nitrogen flow rate and plasma power were kept at 0.5 sccm and 350 W, respectively for nitridation, buffer layer and GaN growth. The structural characterization of the samples was carried out by HRXRD. The PL spectra were recorded in the temperature range of 5–300 K using a closed cycle optical cryostat and He–Cd laser of 325 nm excitation wavelength with a maximum input power of 30 mW. The Hall effect measurements were conducted in the temperature range from 80 to 300 K at 0.5 T of magnetic field. Samples of 5 mm × 5 mm size were cut from the wafers and metal dots were vacuum evaporated in the four corners to obtain electrical contacts in the Van der Pauw geometry.

3. Results and discussion

Fig. 1 shows the HRXRD 2θ–ω scans of the GaN films grown on Si (1 1 1) substrate. From the figures it can be seen that except the substrate peak, only a strong (0 0 0 2) GaN diffracted peak at $2\theta = 34.59^\circ$ and a weak (0 0 0 4) peak at $2\theta = 73^\circ$ are present, indicating the epitaxial GaN thin film to be highly oriented along the [0 0 0 1] direction of the wurtzite GaN. The transports measurements on the epi-GaN films were done using a Hall mobility setup. Hall Effect measurements revealed a strong n-type conductivity, with donor concentrations of 7.25×10^{17} (sample (a), undoped), 2.69×10^{18} (sample (b), Si-doped), 5.65×10^{18} (sample (c), Si-doped), 1.09×10^{19} (sample (d), Si-doped) and 1.60×10^{19} cm^{-3} (sample (e), Si-doped) at room temperature as shown in Table 1. The estimated electron mobilities are in good agreement with reported values [22].

The investigations of the luminescence properties of GaN layers were studied at room temperature by recording the photoluminescence spectra and are shown in Fig. 2. From the figure it can be seen that the PL spectra of all samples are dominated by NBE band, which generally contains the band-to-band transition as well as the transition from neutral donor level to the valence band (DBE). Since donor levels form a band in the forbidden gap, the redshift of the NBE peak with increasing carrier concentration (i.e., higher doping levels) is consistent with the DBE emission and may indicate the broadening of the Si-related donor band as well BGN effect [15]. Fig. 3 represents the PL peak positions of the sample as a function of the cube root of carrier density, and in fact manifests the BGN effect due to Si doping. BGN effect can be evaluated by an

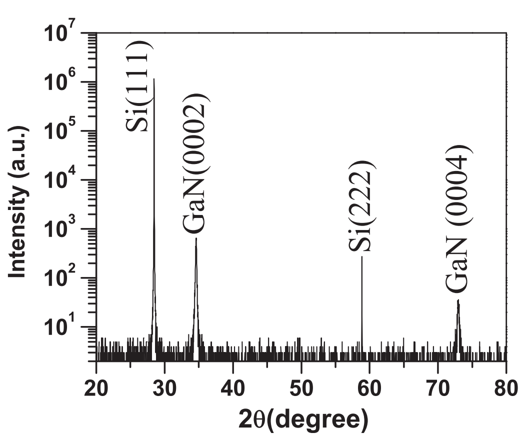

Fig. 1. HRXRD 2θ–ω scans of GaN on Si (1 1 1) substrate.

Table 1
Room-temperature electronic properties of n-type GaN on Si (1 1 1).

Sample name	Electron concentration (cm^{-3})	Carrier mobility (cm^2/V s)
(a)	7.25×10^{17}	371.9
(b)	2.69×10^{18}	247.3
(c)	5.65×10^{18}	185.6
(d)	1.09×10^{19}	78.8
(e)	1.60×10^{19}	48.4

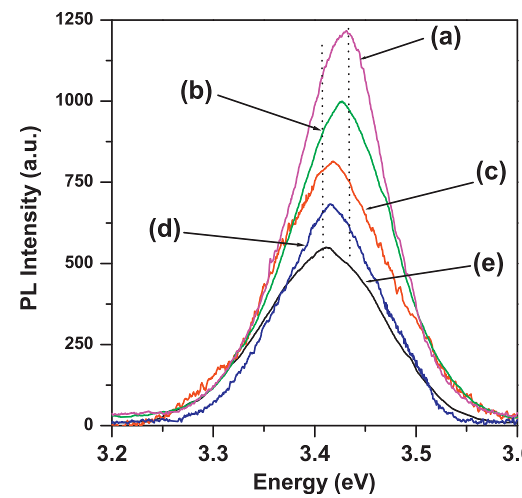

Fig. 2. NBE photoluminescence spectra of samples (a)–(e) taken at room temperature. The peaks are at 3.4309, 3.4253, 3.4205, 3.4155 and 3.4123 eV, respectively.

empirical relation, as reported by Lee et al. [23],

$$\Delta E_G = E_G(0) - E_G(n) = Kn^{1/3} \quad (1)$$

where $E_G(0)$ is the band-gap energy of pure sample, $E_G(n)$ the band-gap energy depending on doping density, and n the electron density. The $n^{1/3}$ dependence of ΔE_G resembles the prevailing exchange contribution of electron–electron interaction [24]. As shown in Fig. 3, our experimental data are fitted well by the relation shown in Eq. (1). The BGN coefficients (K) evaluated by fitting were estimated to be $\sim -1.15 \times 10^{-8}$ eV cm.

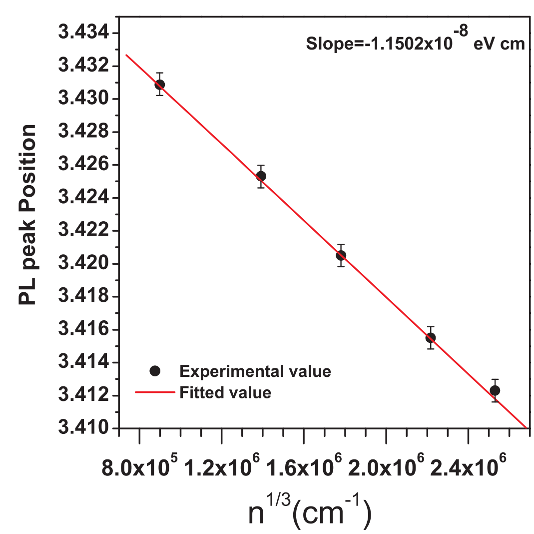

Fig. 3. Peak position of NBE transition as a function of $n^{1/3}$, showing clear band-gap narrowing effect. The solid lines are from the least square fit. The error in PL peak position is $\sim\pm 1$ meV.