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Deep centers in \( n \)-GaN grown by reactive molecular beam epitaxy

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Deep centers in \( n \)-GaN layers grown by reactive molecular beam epitaxy have been studied by deep-level transient spectroscopy as a function of growth conditions. Si-doped GaN samples grown on a Si-doped \( n^+ \)-GaN contact layer at 800 \(^\circ\)C show a dominant trap \( C_1 \) with activation energy \( E_T=0.44 \) eV and capture cross-section \( \sigma_T=1.3\times10^{-15} \) cm\(^2\), while samples grown at 750 \(^\circ\)C on an undoped semi-insulating GaN buffer show prominent traps \( D_1 \) and \( E_1 \), with \( E_T=0.20 \) eV and \( \sigma_T=8.4\times10^{-17} \) cm\(^2\), and \( E_T=0.21 \) eV and \( \sigma_T=1.6\times10^{-14} \) cm\(^2\), respectively. Trap \( E_1 \) is believed to be related to a \( N \)-vacancy defect, since the Arrhenius signature for \( E_1 \) is very similar to the previously reported trap \( E \), which is produced by 1-MeV electron irradiation in GaN materials grown by both metalorganic chemical-vapor deposition and hydride vapor-phase epitaxy.

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Rapid progress in the development of blue light-emitting diodes, ultraviolet detectors, and high-temperature transistors in the III–V nitride system (GaN, AlGaN, and InGaN) has led to great activity in the growth and characterization of these materials.\(^1,2\) Due to the high dislocation densities in the usual GaN layers, which are grown on sapphire, and the self-compensation tendencies of wide-gap semiconductors, point defects are expected to be prevalent. A number of deep centers in \( n \)-GaN, measured by deep-level transient spectroscopy (DLTS), with activation energies in the range of 0.15–0.8 eV and trap densities in the range of \( 10^{13}–10^{15} \) cm\(^{-3}\), have been reported by several groups.\(^3–5\) Most of the studies have so far dealt with \( n \)-GaN materials grown by either metalorganic chemical-vapor deposition (MOCVD) or hydride vapor-phase epitaxy (HVPE). The origin of the observed deep centers remains an open question. Based on the effects of 270-keV \( N^{2+} \) implantation and annealing, Haase \textit{et al.} have suggested that two centers, \( D_2 \) and \( D_3 \), with activation energies of 0.60 and 0.67 eV, are the \( N \) antisite and \( N \) interstitial, respectively.\(^4\) Recently, some of the present authors have reported an electron-irradiation-induced trap, located at \( E_C=0.18 \) eV, in both MOCVD and HVPE GaN. This trap is most likely associated with the \( N \) vacancy.\(^6,7\) Interestingly, the energy of this trap is close to that found in an unirradiated, undoped, semi-insulating (SI) reactive molecular beam epitaxial (RMBE) layer by the thermally stimulated current (TSC) technique.\(^8\) However, there are very few DLTS studies on any type of MBE-grown GaN, perhaps due to the difficulty of fabricating good Schottky barrier diodes (SBDs), with small leakage currents. In this letter, we present a detailed DLTS study of deep centers in RMBE-grown GaN, which has led to the observation of two centers at \( E_T=0.20 \) and 0.44 eV. To the best of our knowledge, these centers have not been observed before in \( n \)-type GaN grown by either MOCVD or HVPE.

Two sets of Si-doped \( n \)-GaN films, with AlN buffer layers (about 650 \( \AA \) thick), were grown on sapphire by RMBE, employing ammonia flow rates between 20 and 73 sccm. Set I, grown at 750 \(^\circ\)C, contained an undoped Si GaN layer of about 1.6-\( \mu \)m thickness, while set II, grown at 800 \(^\circ\)C, had a 2-\( \mu \)m-thick Si-doped \( n^+ \)-GaN contact layer in this position in order to reduce series resistance in the SBDs. The \( n \)-GaN samples in set I were about 1.6-\( \mu \)m thick, while the samples in set II were about 0.5-\( \mu \)m thick. The electron Hall mobilities for both types of samples changed with the ammonia flow rate, and the highest mobility, 220 cm\(^2\)/V s, was found to occur at an ammonia flow rate of 50 sccm. SBDs on these samples were fabricated using Ti/Al/Ti/Au as the Ohmic contact and Ni/Au as the Schottky contact. For the samples in set II, 0.6-\( \mu \)m-high mesas were etched by a Cl-based reactive ion process, and 250-\( \mu \)m-diam Schottky dots were formed on the surface of the mesa while Ohmic contacts were fabricated on the \( n^+ \)-GaN contact layer. All the measurements were performed on wire-bonded samples.

The current–voltage (\( I–V \)) characteristics were first checked at room temperature and only those SBDs with small leakage currents were chosen for the capacitance–voltage (\( C–V \)) and DLTS measurements. A Bio-Rad DL4600 system with a 100-mV test signal at 1 MHz was used to take \( C–V \) and DLTS data. The \( C–V \) data, which are used to determine the carrier profile, were also taken at different temperatures (350–100 K) to establish if the carrier concentration was changing with temperature. As long as the carrier concentration is much larger than the concentrations of deep centers at all temperatures (80–350 K), the DLTS system can display the trap density versus temperature di-
rectly. During the DLTS measurements, the bias (1-ms width) was pulsed from \(-1.0\) to \(0\) V in order to fill the traps. To determine the apparent parameters of the deep centers, i.e., the activation energy \(E_T\) and capture cross section \(\sigma_T\), the DLTS spectra were taken at different rate windows, from \(20\) to \(1000\) s\(^{-1}\).

The temperature-dependent (100–350 K) forward and reverse \(I-V\) characteristics for sample 5962, in set II, are presented in Fig. 1. From the forward \(I-V\) curves, the ideality factor \(n\) was found to be 1.5 at 300 K, which is in agreement with the value of 1.4 reported by Kribes et al. for MBE-grown GaN.\(^5\) Our reverse \(I-V\) characteristics show very low leakage currents, 105 nA at 350 K and 14 nA at 100 K, respectively, under a bias of \(-5\) V.

Figure 2 presents typical DLTS spectra measured on sample 5731 in set I, with rate windows from 50 to 1000 s\(^{-1}\). Two electron traps, labeled as \(D_1\) and \(E_1\), are clearly observed at the low temperatures. On the other hand, a typical DLTS spectrum measured on sample 5962 in set II (note the different temperature range) is pictured in Fig. 3. In contrast to the samples in set I, samples in set II always show a dominant electron trap \(C_1\) peaked at around 250 K, and also some other traps, like \(A\), \(B\), and \(E\). The Arrhenius plots of \(T_m^2/e_n\) versus \(1000/T_m\) for the major traps observed in RMBE-grown GaN SBDs, as shown in Fig. 4, reveal that the apparent activation energy \(E_T\) and capture cross-section \(\sigma_T\) for \(D_1\) and \(E_1\) in sample 5731 (set I) and \(C_1\) in sample 5962 (set II) are 0.20 eV and \(8.4\times10^{-17}\) cm\(^2\), 0.21 eV and \(1.6\times10^{-14}\) cm\(^2\), and 0.44 eV and \(1.3\times10^{-15}\) cm\(^2\), respectively. In the Arrhenius plots, for comparative purposes, we also present the signatures for traps \(B\), \(C\), \(D\), and \(E\), which were obtained on MOCVD GaN SBDs irradiated by 1 MeV electrons.\(^6\) Three of the traps, i.e., \(B\), \(C\), and \(D\), are preexisting in the material and not affected by the irradiation, while trap \(E\) is induced by the electron irradiation, with a production rate of at least 0.2 cm\(^{-1}\), and is believed to be due to the N vacancy. By comparing the signatures of \(E_1\) and \(E\), we find that they have similar activation energies, but some difference in the capture cross section. The signatures of \(D_1\) and \(D\) are also similar.

Trap \(A\), which appears as a shoulder at \(\sim 385\) K in Fig. 3, is close to \(E_3\) (0.665 eV) and \(D_3\) (0.67 eV).\(^4\) Trap \(B\), peaked at \(\sim 335\) K with \(E_T=0.62\) eV and \(\sigma_T=7.4\times10^{-15}\) cm\(^2\), which is close to \(E_2\) (0.58 eV), \(D_2\) (0.60 eV), and DLN\(_3\) (0.59 eV) reported by Hacke et al.,\(^3\) Haase et al.,\(^4\) and Götz et al.,\(^5\) respectively, was also found to be a dominant trap in both MOCVD and HVPE GaN layers, with trap densities from 1 to \(2\times10^{14}\) cm\(^{-3}\). Trap \(D_1\) peaked at \(\sim 160\) K with \(E_T=0.24\) eV and \(\sigma_T=2.0\times10^{-15}\) cm\(^2\), which is close to \(E_1\) (0.264 eV) and DLN\(_1\) (0.25 eV), was also found in both MOCVD and HVPE GaN, but with trap densities in the low-\(10^{14}\) cm\(^{-3}\). Trap \(C\), peaked at \(\sim 220\) K with \(E_T=0.45\) eV and \(\sigma_T=1.5\times10^{-13}\) cm\(^2\), which was first reported by Fang et al.,\(^7\) is not a dominant trap in either material. However, by comparing the DLTS spectra obtained from GaN SBDs grown by RMBE and other techniques, we found some unique features for the traps in \(n\)-GaN grown by RMBE. First, trap \(C_1\), peaked at \(\sim 250\) K, was found to be a dominant trap in the samples of set II, with trap densities in the low-\(10^{15}\) cm\(^{-3}\); this trap has not been reported so far in MOCVD or HVPE material. Second, traps \(D_1\) and \(E_1\), peaked at \(\sim 145\) and \(\sim 115\) K, respectively, for a rate window of 50 s\(^{-1}\), were found to be dominant traps in the samples of set I, with trap densities in the mid-\(10^{15}\) cm\(^{-3}\) range. Trap \(D_1\) is similar to trap \(D\) reported for both
MOCVD and HVPE GaN materials, while trap $E_1$ is similar to trap $E$ reported only for the electron-irradiated MOCVD and HVPE GaN. Third, in comparison with the best MOCVD and HVPE GaN that we have studied, the GaN films grown by RMBE show higher overall trap densities; i.e., low-$10^{14}$ cm$^{-3}$ for the MOCVD and HVPE layers versus low- to mid-$10^{15}$ cm$^{-3}$ for the MBE layers. Note that there was a difference in film thicknesses between MOCVD (or HVPE) and reactive MBE films, which might be causing the difference in trap density.

Based on a temperature-dependent Hall-effect study of a HVPE GaN layer subjected to 1-MeV electron irradiation, Look et al. concluded that a defect donor ($V_N$) and a defect acceptor ($N_f$) are produced at equal rates, about 1 cm$^{-1}$, by the irradiation. Although there is a significant difference in the activation energy for the electron-irradiation-induced Hall donor center (0.07 eV) and the DLTS center (0.18 eV), we still believe that the DLTS center, trap $E$, might be related to the N vacancy, since an activation energy for the capture cross section could be involved in the apparent DLTS activation energy of 0.18 eV. Moreover, both centers have similar production rates and annealing behavior. The similarity of traps $E_1$ and $E$ implies that there exist N-vacancy-related defects in RMBE GaN material due to possible nonstoichiometry. The prominent trap $E_1$ found in the samples of set I might be associated with the use of an undoped Si GaN layer as a buffer or the use of a lower growth temperature as compared to that used for the samples in set II, i.e., 750 versus 800 °C. In a similar undoped Si RMBE GaN, grown also at 750 °C and under a high ammonia flow rate (73 sccm), a TCS center with an activation energy of 0.17 eV was found. If the 0.17 eV center is really related to a N-vacancy defect, rather than a possible Ga-vacancy defect, as discussed in Ref. 8, the crystal stoichiometry or the N richness of RMBe GaN films seems to be determined mainly by the growth temperature, rather than the ammonia flow rate. (Note that the ammonia cracking rate is strongly temperature dependent.) On the other hand, the dominance of trap $B$, which is close to trap $D^2$, in both MOCVD and HVPE GaN materials, implies that these materials are more N rich, since the center $D^2$ has been tentatively identified to be related to the N-antisite defect, based on a study of N$_2$ implantation and annealing, as mentioned above.

In summary, deep centers in RMBE GaN layers have been studied by DLTS in conjunction with growth conditions. Si-doped $n$-GaN samples grown on Si-doped $n^+$-GaN contact layers at 800 °C show a dominant trap $C_1$ with $E_T = 0.44$ eV and $\sigma_T = 1.3 \times 10^{-15}$ cm$^2$, while samples grown on undoped semi-insulating GaN buffer layers at 750 °C show prominent traps $D_1$ and $E_1$, with $E_T = 0.20$ eV and $\sigma_T = 8.4 \times 10^{-17}$ cm$^2$, and $E_T = 0.21$ eV and $\sigma_T = 1.6 \times 10^{-14}$ cm$^2$, respectively. Trap $E_1$ is believed to be related to a N-vacancy defect, since the Arrhenius signature for $E_1$ is very similar to that for trap $E$, which is induced by 1-MeV electron irradiation in MOCVD and HVPE GaN materials.

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