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

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Deep centers in Si-doped *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 °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 °C on an undoped semi-insulating GaN buffer show prominent traps D_1 and E_1 , with E_T =0.20 eV and σ_T =8.4×10⁻¹⁷ cm², and E_T =0.21 eV and σ_T =1.6×10⁻¹⁴ cm², 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. © 1998 American Institute of Physics. [S0003-6951(98)02818-6]

Rapid progress in the development of blue light-emitting diodes, ultraviolet detectors, and high-temperature transistors in the III–V nitride system $(GaN, AIGaN, and InGaN)$ 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 *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_c -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 Å thick), were grown on sapphire by RMBE, employing ammonia flow rates between 20 and 73 sccm. Set I, grown at 750 °C, contained an undoped Si GaN layer of about 1.6- μ m thickness, while set II, grown at 800 °C, had a 2- μ 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- μ m thick, while the samples in set II were about 0.5 - μ m thick. The electron Hall mobilities for both types of samples changed with the ammonia flow rate, and the highest mobility, $220 \text{ cm}^2/\text{V}$ 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 - μ 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 $(350-100 \text{ K})$ 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 $(80-350 \text{ K})$, the DLTS system can display the trap density versus temperature di-

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FIG. 1. *I*-*V* characteristics, measured at temperatures from 100 to 350 K, for sample 5962 in set II.

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 σ_T , the DLTS spectra were taken at different rate windows, from 20 to 1000 s^{-1} .

The temperature-dependent $(100-350 \text{ K})$ 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. 9 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

This a FIG. 2. DLTS spectra measured on sample 5731 in set L_e using different rate subject to the samples of set I, with trap densities in the mid-10⁻ cm windows. 128.172.48.58.On:

FIG. 3. DLTS spectrum measured on sample 5962 in set II, with a rate window of 50 s^{-1} .

 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 σ_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 8.4×10^{-17} cm², 0.21 eV and 1.6 $\times 10^{-14}$ cm², and 0.44 eV and 1.3×10^{-15} cm², 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 \times 10¹⁵ cm⁻², 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 $(0.665 \text{ eV})^3$ and *D*3 $(0.67 \text{ eV})^4$. Trap *B*, peaked at \sim 335 K with E_T = 0.62 eV and σ_T = 7.4 $\times 10^{-15}$ cm², 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 found⁷ to be a dominant trap in both MOCVD and HVPE GaN layers, with trap densities from 1 to 2×10^{14} cm⁻³. Trap *D*, peaked at ~160 K with $E_T = 0.24 \text{ eV}$ and $\sigma_T = 2.0 \times 10^{-15} \text{ cm}^2$, which is close to E_1 (0.264 eV)³ and DLN₁ (0.25 eV),⁵ was also found⁷ in both MOCVD and HVPE GaN, but with trap densities in the low-10¹⁴ cm⁻³. Trap *C*, peaked at \sim 220 K with E_T =0.45 eV and σ_T =1.5×10⁻¹³ cm², 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 the 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- to mid-10¹⁵ 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_I) are produced at equal rates, about 1 cm^{-1} , by the irradiation.¹⁰ 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 Nvacancy-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 $750 \degree C$ and under a high ammonia flow rate (73 sccm), a TCS center with an activation energy of 0.17 eV was found.⁸ 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 $D2⁴$, 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,⁴ 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 $\sigma_T = 1.3 \times 10^{-15}$ cm², 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 $\sigma_T = 8.4 \times 10^{-17} \text{ cm}^2$, and $E_T = 0.21 \text{ eV}$ and $\sigma_T = 1.6$

FIG. 4. Arrhenius plots of T_m^2/e_n for deep centers observed in *n*-GaN materials grown by both reactive MBE (solid lines) and MOCVD (dashed lines).

 $\times 10^{-14}$ cm², 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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