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Dislocation-related electron capture behaviour of traps in n-type GaN

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Abstract

Electron capture behaviours for major traps in thin epitaxial and thick free-standing GaN samples have been experimentally and theoretically studied by using deep-level transient spectroscopy (DLTS). According to the logarithmic dependence of the DLTS signal on the filling pulse width, most of the traps in thin epitaxial GaN layers with high dislocation density behave as line defects. In sharp contrast, the same traps in thick free-standing GaN layers with low dislocation density behave as point defects. The most likely explanation for these phenomena is that the electron traps in question tend to segregate around dislocations, when present in large numbers.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The capture kinetics and trapping behaviour of dislocation-related electron traps have been well studied by using deep-level transient spectroscopy (DLTS) in many material systems, such as deformed Si [1] and GaAs [2], lattice-mismatched GeSi/Si [3], and InGaAs/GaAs heterostructures [4]. These traps often show both a logarithmic dependence of the DLTS peak height on the filling pulse width, and broadened asymmetrical peaks. A model of the time-dependent capture barrier associated with extended line defects, i.e., with the capture barrier height proportional to the number of electrons already captured, has been proposed to explain the anomalous electron capture behaviour. Threading dislocations with densities in the 10^8–10^{10} cm^{-2} range are typical in thin epitaxial GaN (epi-GaN) layers grown on sapphire substrates by normal growth techniques. Because of such a high density of dislocations, we anticipate that electron traps in thin GaN layers might often exhibit a dislocation-related capture behaviour. In this paper, we present experimental and theoretical results for six electron traps observed in thin epitaxial GaN layers, grown by reactive molecular beam epitaxy (RMBE) and hydride vapour phase epitaxy (HVPE) techniques. These traps are A_1 (0.89 eV), A (0.67 eV), B (0.59–0.62 eV), C (0.41 eV), D (0.25–0.27 eV), and E_1 (0.18 eV). For these particular samples, almost all of the traps show anomalous electron capture characteristics, behaving as

Table 1. A summary of the n-GaN samples used in the study.

Sample	Growth method	Growth temperature (°C)	Thickness (μm)	N_d, 300 K (10^{16} cm^{-3})	Dislocations (cm^{-2})	Reference
5731	RMBE	750	1.6	10	10^8–10^9	[5, 6]
1106	HVPE	1100	5.0	10	10^8–10^9	[7]
135	HVPE	1030	300	1	5×10^6	[8, 9]

line defects. To illustrate the involvement of dislocations in this phenomenon, we will present comparable results for the same five electron traps, A_1 (1.0 eV), A (0.67 eV), B (0.59 eV), C (0.35 eV), and D (0.25 eV), observed in 300 μm thick free-standing GaN (Ga face), with high electron mobility (1100 cm^2 V^{-1} s^{-1}) and low dislocation density (5×10^6 cm^{-2}). This free-standing GaN (hereafter called bulk GaN) was grown by HVPE and removed from its sapphire substrate by a laser separation process. In contrast to the case for traps found in the *thin* epi-GaN layers, the same traps observed in *thick* bulk GaN show very small electron capture barriers, which were determined by measuring DLTS peak heights as a function of either temperature or filling pulse width. It has been proposed that threading dislocation cores in n-type GaN contain V_{Ga} or V_{Ga}–O acceptor-like defects. However, such defects would be expected to behave as hole traps, and we are observing electron traps. In fact, it is likely that our traps are defects and impurities that simply segregate around the dislocations, rather than forming an integral part of the core structure.

2. Samples and experiment

The major results related to the DLTS centres and dislocation densities for the GaN samples used in the study have already been published [5–9]. The growth technique, growth temperature, 300 K electron concentration, thickness, and dislocation density of the samples are shown in table 1. All GaN layers were grown on sapphire and had Schottky and ohmic contacts fabricated from Ni/Au and Ti/Al/Ti/Au metallizations, respectively. A Bio-Rad DL4600 system with a 100 mV test signal at 1 MHz was used to take capacitance–voltage (C–V) and DLTS data. The 300 K carrier concentration ($n \sim N_d$), obtained from C–V data, was used to calculate trap concentrations from the well-known equation $N_T = 2N_d\,\Delta C/C$, where ΔC is the DLTS signal and C the capacitance at the reverse bias used in the DLTS measurements. In order to study electron capture characteristics, the filling pulse widths (W_f) used in the DLTS measurements were varied from 0.2 to 100 ms. To determine the activation energy (E_T) and capture cross-section (σ_n) of the deep traps, the DLTS spectra were taken at different rate windows (e_ns), from 0.8 to 200 s^{-1}, and were analysed by the standard Arrhenius technique. Furthermore, in order to obtain the temperature dependence of the capture cross-section for some traps, numerical fittings were performed on DLTS peaks taken at different e_ns, assuming exponential capacitance transients (for details see [10]).

3. Results and discussion

In figure 1, we present results for the thick bulk GaN sample (135), which can be seen as a standard for isolated point defects in GaN. The two sets of DLTS spectra shown here have the following parameters: (a) $e_n = 0.8$–80 s^{-1} and $W_f = 1$ ms; and (b) $e_n = 4$ s^{-1} and $W_f = 0.2$–20 ms. In figure 1, five traps can be clearly observed. Their parameters, from Arrhenius analyses, are: A_1($E_T = 1.0$ eV and $\sigma_n = 6.7 \times 10^{-14}$ cm^2), A ($E_T = 0.66$ eV and

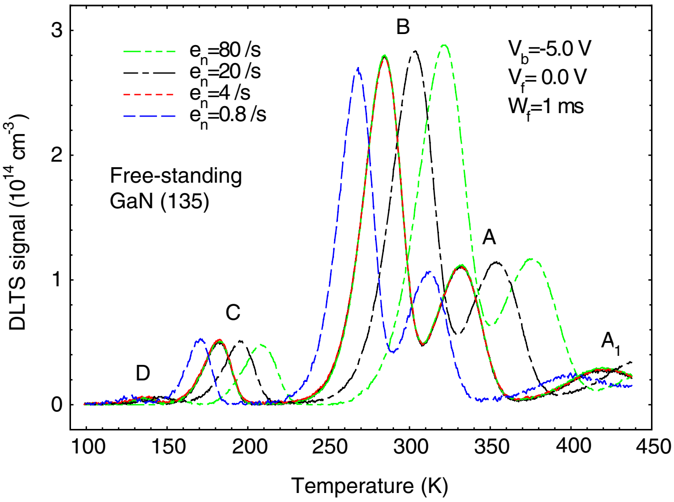

Figure 1. DLTS spectra measured at $e_n = 0.8$–$80\ \mathrm{s}^{-1}$ or $W_f = 0.2$–20 ms for free-standing GaN.

$\sigma_n = 1.3 \times 10^{-15}\ \mathrm{cm}^2$), B ($E_T = 0.59$ eV and $\sigma_n = 4.8 \times 10^{-15}\ \mathrm{cm}^2$), C ($E_T = 0.34$ eV and $\sigma_n = 8.6 \times 10^{-16}\ \mathrm{cm}^2$), and D ($E_T = 0.25$ eV and $\sigma_n = 9.0 \times 10^{-16}\ \mathrm{cm}^2$). Two important observations are:

(i) the peak positions of the five traps shift to higher temperatures as e_n increases, and their peak heights (N_Ts) are almost invariant, as expected for isolated traps; and

(ii) as W_f increases from 0.2 to 20 ms, the N_Ts of five traps show almost no change, which means that even 0.2 ms is a long enough time to nearly fill all of the traps.

Besides Arrhenius analyses, all of the traps were also fitted numerically, assuming exponential capacitance transients; an example (for $e_n = 4\ \mathrm{s}^{-1}$) is shown in figure 2. For all traps, but especially for A_1, the trap parameters (E_Ts and σ_ns) determined from the numerical fittings were very similar to those obtained from Arrhenius analyses. By using σ_n-values deduced from numerical fittings at eight different e_ns, capture cross-section temperature dependences of four traps can be obtained, and these are shown in figure 3 (open symbols). From the figure, we find that all traps, except for trap C (which has been proved to be due to surface damage [11]), show very small electron capture barriers ($E_\sigma = 0.01$ to 0.02 eV). The results indicate that all traps found in this free-standing GaN sample behave as point defects, distributed at random in the sample.

Now, we present results for two thin epi-GaN samples. DLTS spectra for RMBE-GaN sample 5731, measured as a function of e_n and W_f, are shown in figures 4(a) and (b). From the figures, we find that the peak heights of traps B, D, and E_1 clearly increase as e_n or W_f increase; this behaviour is in sharp contrast to that found for the free-standing GaN sample. Data fittings were performed on low-temperature portions (including traps D and E_1) of the DLTS spectra. It turns out that the D/E_1 region can be well fitted by decomposing it into three components, as exemplified in figure 5. The trap parameters are: $E_T = 0.25$ eV and average $\sigma_n = 1.4 \times 10^{-15}\ \mathrm{cm}^2$ for D_1; $E_T = 0.16$ eV and average $\sigma_n = 2.8 \times 10^{-18}\ \mathrm{cm}^2$ for D_2; and $E_T = 0.18$ eV and average $\sigma_n = 2.1 \times 10^{-16}\ \mathrm{cm}^2$ for E_1. From the fitted values of N_T and σ_n, we can plot N_T versus logarithmic W_f (figure 6), and σ_n versus $1/T$ (figure 3, solid symbols), for traps D_1, D_2, and E_1. From figure 6, where experimental data for trap B were also added,

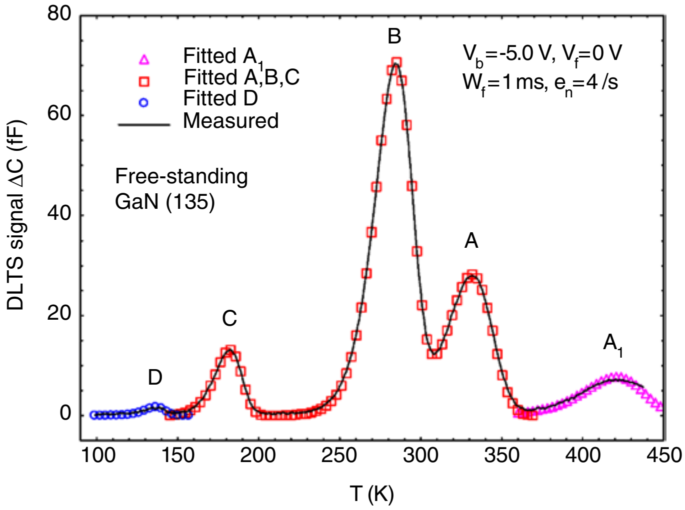

Figure 2. Measured and fitted DLTS spectra for free-standing GaN.

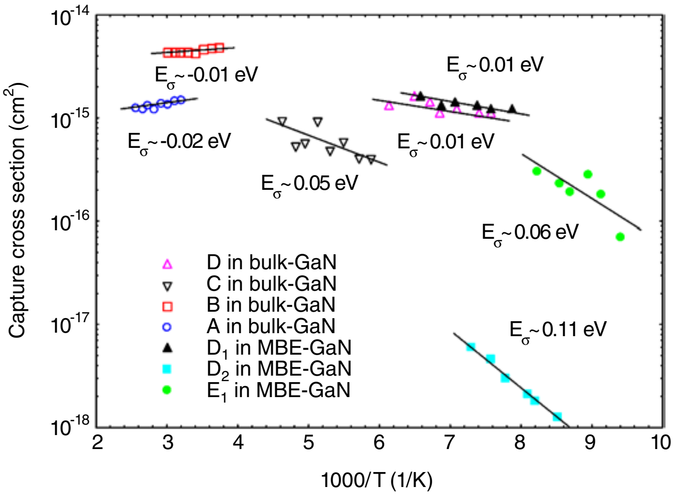

Figure 3. The temperature-dependent capture cross-section for traps in two GaN samples.

we observe that there exist fairly good linear relationships between N_T and logarithmic W_f for the four traps. On the basis of the models proposed for dislocation-related traps in various semiconductors [1–4], these logarithmic dependences indicate that traps D_1, D_2, E_1, and B exhibit a line defect type of behaviour. From figure 3, we find that $E_\sigma = 0.01$ eV for D_1, 0.11 eV for D_2, and 0.06 eV for E_1. Interestingly, we note that D in the bulk GaN (behaving as a point defect) and D_1 in the RMBE-GaN (behaving as a line defect) have similar electron capture barriers (0.01 eV) but very different peak-height temperature dependences (actually, D and D_1 are due to identical traps).

Finally, we turn to the thin HVPE-GaN sample (1106), and to the dependence of the DLTS signal strength on W_f, as shown in figure 7. First of all, we find that the trap *species* in this thin GaN sample are exactly the same as those found in the thick free-standing GaN—not

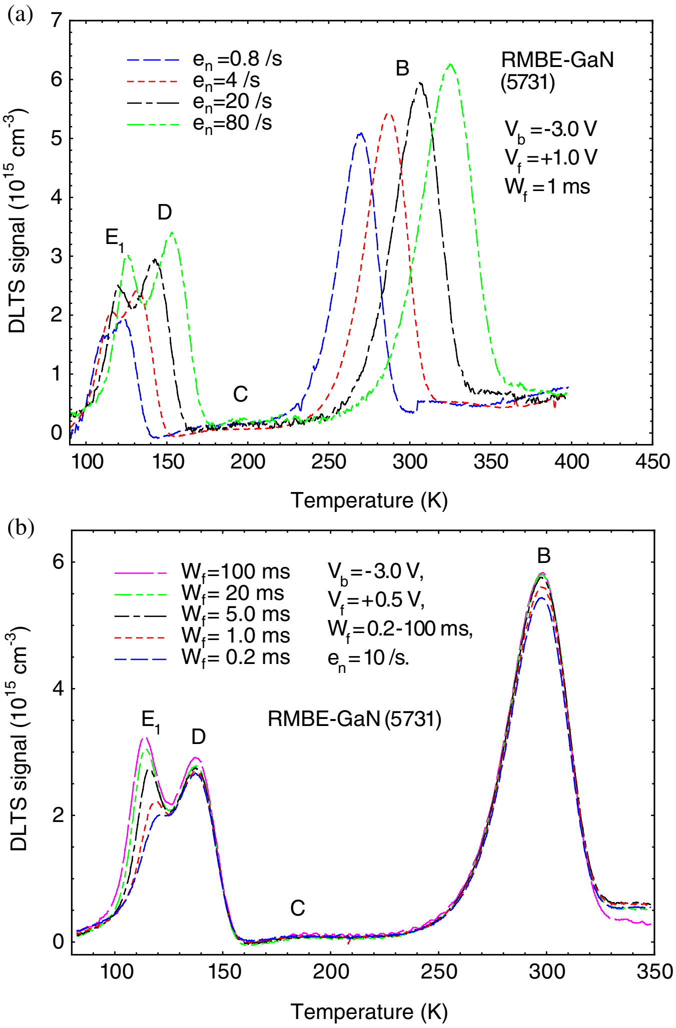

Figure 4. (a) DLTS spectra measured at $e_n = 0.8$–$80\ \mathrm{s}^{-1}$ for RMBE-GaN. (b) DLTS spectra measured using $W_f = 0.2$–100 ms for RMBE-GaN.

unexpected, since both were grown by HVPE. However, the traps in the thin sample show clear increases in their peak heights, as W_f increases, especially for A_1, A, and B. A new species A_2 appears in the spectrum with $W_f = 100$ ms, which might be due to a charge-state-related defect reaction. DLTS spectra were also measured using different e_ns. The results (not shown here) reveal that as e_n increases, the major traps show an increase in their peak heights. The two experimental observations, i.e., that the DLTS peak heights for many traps in the thin samples increase as either e_n or W_f increase, seem to be always correlated with each other. A change in DLTS peak height for a trap as a function of temperature is usually explained by a temperature dependence in its capture cross-section. However, this is not true, at least for trap D_1 in the RMBE-GaN sample, as mentioned above. The correlation between the two observations could be related to the automatic setting of the pulse repetition period (PRP) for different e_ns. Most DLTS systems select specific combinations for the values of e_n and PRP,

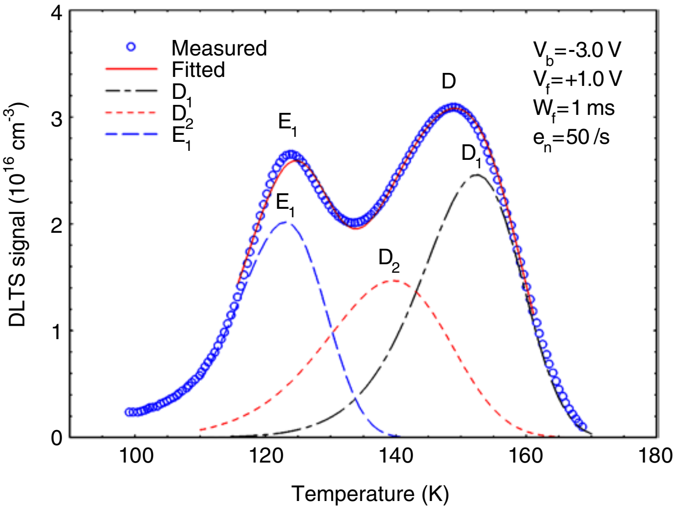

Figure 5. Measured and fitted DLTS spectra in the low-temperature portion for RMBE-GaN.

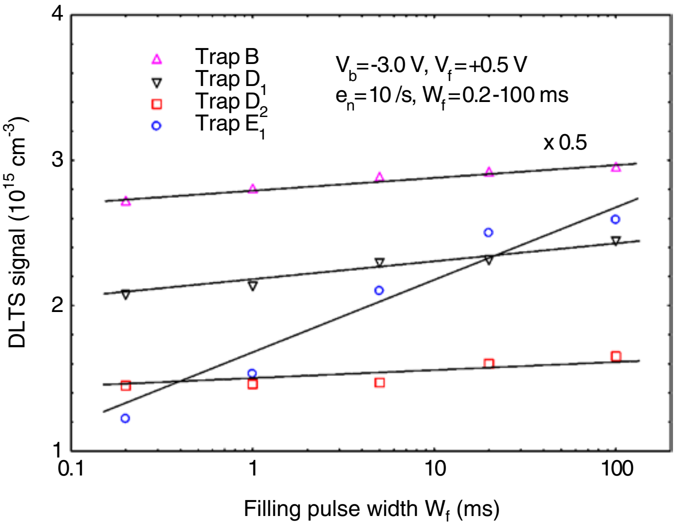

Figure 6. The logarithmic dependence of the DLTS peak height on W_f for traps in RMBE-GaN.

to obtain an optimal signal-to-noise ratio; i.e., the smaller the e_n, the longer the PRP. If W_f is unchanged, the equivalent pulse width, which is proportional to the ratio W_f/PRP, would be longer for larger e_n, and vice versa. Thus, if a trap behaves as a line defect, we would expect a higher peak height for a larger e_n, since the trap is subjected to more filling pulses over same time period. This is true for many traps in thin epi-GaN samples studied in our laboratory.

We earlier reported the line defect nature of traps A_1 (0.89 eV) and C_1 (0.44 eV) in RMBE-GaN samples grown at 800 °C [12], and of traps A_x (0.77 eV) and D (0.28 eV) in plasma-assisted MBE-GaN grown at 725 °C on a MOCVD-GaN template [13]. In work from other groups, some traps, such as ER5 (0.95 eV, similar to A_1) introduced in MOCVD-GaN during He-ion irradiation [14], E_1 (0.19–0.23 eV, similar to D) in MOCVD-GaN [15], and

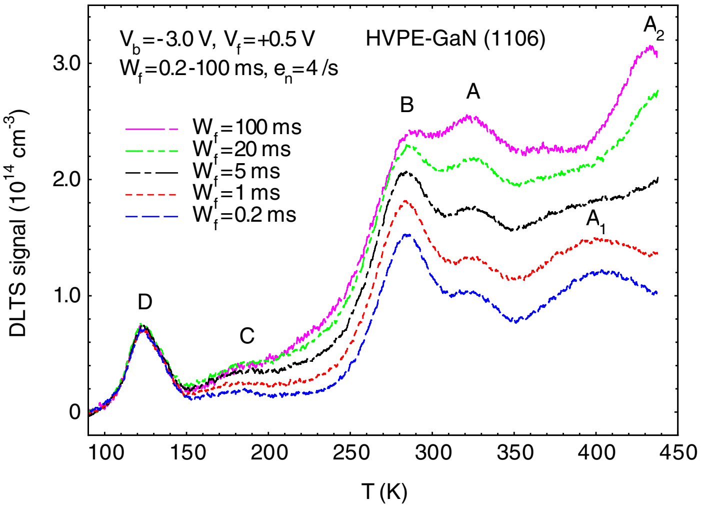

Figure 7. DLTS spectra measured using $W_f = 0.2$–100 ms for HVPE-GaN.

E (0.91 eV) in MBE-GaN grown on a MOCVD-GaN template [16], were explained to be line defects, based on a logarithmic dependence of their DLTS signals on the filling pulse width. Thus, we can conclude that traps behaving like line defects in thin epi-GaN layers with high dislocation densities are omnipresent, no matter how the layers were grown and which substrates were used (sapphire or a GaN/Al_2O_3 template). However, in the thick free-standing GaN, with low dislocation density, the same traps turn out to behave as point defects.

According to DLTS and optical DLTS studies on HVPE-GaN samples with different thicknesses from 68 to 2.6 μm, both electron and hole traps were found to increase with decreasing thickness, which was thought to be associated with an increase in the number of threading dislocations near the surface [7, 17]. Threading dislocations in n-type GaN have been predicted to have V_{Ga} or V_{Ga}–O acceptor-like defects in their core structures [18, 19]. Indeed, the presence of high concentrations of V_{Ga} or V_{Ga}–O in the same HVPE-GaN samples has been verified by positron annihilation spectroscopy [20]. Usually, such defects would be expected to behave as hole traps, such as one at $E_v + 0.90$ eV [17]. However, what we observe in both thick bulk GaN and thin epi-GaN samples are electron traps with normal capture cross-sections in the 10^{-15}–10^{-14} cm^2 range for most of the traps, except for E_1 and D_2. It is likely that our traps are defects or defect–impurity complexes which are simply segregated around the dislocations, rather than belonging to integral parts of the core structure. The identities of some of the major traps, such as E_1, were discussed earlier, mainly on the basis of electron irradiation studies [7, 10, 12].

4. Conclusions

Electron capture behaviours for major traps found in both *thick* free-standing GaN, with low dislocation density (5×10^6 cm^{-2}), and *thin* epi-GaN samples, with high dislocation density (10^8–10^9 cm^{-2}), have been studied by means of experimental DLTS measurements and theoretical data fittings. According to the logarithmic dependence of the DLTS signal on the filling pulse width, many traps in the thin epi-GaN samples were found to behave as line defects. In sharp contrast, these same traps in thick free-standing GaN show normal electron capture characteristics and small capture barriers ($E_b = 0.01$–0.02 eV), behaving as point defects. These electron traps, which are believed to be due to point defects or their complexes with impurities in n-type GaN, are likely to segregate around the threading dislocations, rather than to form integral parts of the core structure.

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