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On the main irradiation-induced defect in GaN

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We show that the usual Arrhenius analysis of the main electron-irradiation-induced defect trap in *n*-type GaN, observed by deep-level transient spectroscopy (DLTS), is not sufficiently accurate. Instead, an exact fitting of the DLTS spectrum for this trap reveals two components, each of which has a thermal energy near 60 meV, not the apparent 140–200 meV, as given in other DLTS studies. This result resolves the discrepancy between Hall-effect and DLTS determinations of the thermal energy of this defect center. © 2000 American Institute of Physics. [S0003-6951(00)02615-2]

The recent great interest in III-nitride semiconductors is due to their unique optical and electronic properties. Commercial light-emitting diodes¹ as well as laser diodes,² heterostructure field-effect transistors,³ and ultraviolet detectors⁴ are presently being developed. For space-based applications, in particular, GaN-based devices will have to operate in a radiation environment; it is then of fundamental importance to achieve a detailed knowledge of radiation-induced defects, which have often been shown to affect the electrical and optical properties of semiconductor materials. Moreover, it is well known that in wide-gap semiconductors, such as GaN, defects are often important as donors and acceptors.⁵ Recently, a strong effort by several groups has been devoted to the study of irradiation-induced defects in GaN and related compounds.^{6–10} Most of the results are still not fully understood, but some useful conclusions have already emerged. As an example, for 30 years the N vacancy V_N has been considered to be the dominant donor in GaN,¹¹ but it has just recently been shown that this assumption is not true,⁷ at least for the best, present-day material.

The dominant Hall-effect defect produced by 1 MeV electrons is a donor with energy $E_C - E_T = 0.06$ eV, and has been assigned to the N vacancy.⁷ (Here, E_C and E_T denote the energies of the conduction-band minimum and trap, respectively.) However, the dominant deep-level transient spectroscopy (DLTS) defect, for several different types of irradiation, is an electron trap, with an Arrhenius-determined energy of about 0.14–0.20 eV below the conduction band.^{8,10,12} In this letter, we show that the usual Arrhenius analysis is not sufficient and that the true thermal energy (i.e., $E_C - E_T$) is indeed about 60 meV. Our findings are supported by a detailed analysis of the DLTS peaks.

A Schottky barrier diode with planar structure was fabricated by evaporation and lithographic processes on an unintentionally doped *n*-type GaN layer grown by metalorganic vapor-phase deposition on sapphire.^{8,12} The layer was 4.5 μm thick, and had a 300 K carrier concentration $n = 2.3 \times 10^{16} \text{ cm}^{-3}$, and a mobility $\mu = 765 \text{ cm}^2/\text{Vs}$, as determined from Hall-effect measurements. Electron irradiation was carried out in a Van de Graaff accelerator at a voltage of 1

MeV. A previous experiment with this sample⁸ had involved two irradiation steps, each at a fluence of $0.5 \times 10^{15} \text{ cm}^{-2}$. The sample was subsequently annealed at 250 °C, showing a 50% decrease in the irradiation-induced trap. For the present study, three further steps of irradiation were carried out, each at $2 \times 10^{15} \text{ e cm}^{-2}$. Assuming that the effective fluence after the initial anneal was roughly $0.5 \times 10^{15} \text{ cm}^{-2}$, the total fluences after the three irradiation steps in this study were: $\phi_3 = 2.5 \times 10^{15} \text{ cm}^{-2}$, $\phi_4 = 4.5 \times 10^{15} \text{ cm}^{-2}$, and $\phi_5 = 6.5 \times 10^{15} \text{ cm}^{-2}$. The DLTS experiment was carried out in the temperature range 80–400 K, at a quiescent reverse bias $V_r = -3$ V, and a forward-filling bias $V_f = +1$ V. Three levels were detected in the as-grown material: trap B ($E_C - 0.62$ eV, $\sigma = 7.4 \times 10^{-15} \text{ cm}^2$), trap C ($E_C - 0.45$ eV, $\sigma = 1.5 \times 10^{-13} \text{ cm}^2$), and trap D ($E_C - 0.24$ eV, $\sigma = 2.0 \times 10^{-15} \text{ cm}^2$). The irradiation did not affect the preexisting levels, but introduced a new trap (designated E) located at about $E_C - 0.18$ eV (Arrhenius analysis), with $\sigma = 2.0 \times 10^{-15} \text{ cm}^2$, as already reported in previous works.^{8,12}

The trap E density clearly increases with irradiation fluence, and its DLTS peak shows a very broadened shape (see Figs. 1 and 2), also observed by Auret and co-workers¹⁰ in He-ion-irradiated GaN. (In Figs. 1 and 2, N'_T denotes the usual DLTS signal, which, in a simple case, is equal to the actual trap concentration N_T at the peak of the DLTS curve. In this case, $N'_T \neq N_T$ even at the peak, as discussed later.) Broadening is usually an indication of the spreading of defect states over a larger energy range.¹³ At higher fluences,

FIG. 1. DLTS spectra at different pulse widths ($e_n = 200 \text{ s}^{-1}$, fluence $\phi_3 = 2.5 \times 10^{15} \text{ cm}^{-2}$). N'_T is not the true value of N_T , even at the peak of each curve. The solid lines are simply drawn through the points.

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FIG. 2. DLTS fitting of trap E ($e_n = 400 \text{ s}^{-1}$, fluence $\phi_3 = 2.5 \times 10^{15} \text{ cm}^{-2}$, $t_p = 5 \text{ ms}$). The dashed and solid lines are theoretical fits.

the preexisting trap D signal is masked by the increasing signal of trap E. Capacitance–voltage ($C-V$) measurements, performed after each irradiation, show that the free-carrier concentration n remains nearly constant with irradiation at 300 K, but decreases slightly between 200 and 80 K. These findings suggest that the irradiation influences the low-temperature transport properties of the material.

The usual means to analyze DLTS spectra is the Arrhenius plot, i.e., $\ln(T^2/e_n)$ vs $1/T$, where e_n is the emission rate and T is the temperature at the signal peak.¹⁴ However, for trap E, due to an anomalous dependence of the peak position on emission rate, the Arrhenius plot gives only approximate values of the energy and capture cross section: $E = E_C - 0.14 \text{ eV}$ and $\sigma = 7 \times 10^{-17} \text{ cm}^2$. Moreover, the peak height increases with emission rate, a peculiar feature which often results from a temperature dependence of the capture cross section.¹⁵ In this letter, we have adopted an exact fitting procedure of the spectra in order to improve the accuracy of our analysis.

The general expression for e_n is¹⁶

$$e_n = C \frac{g_0}{g_1} \sigma_n(\infty) T^2 e^{\alpha/k} e^{-(E_{T0} + E_\sigma)/kT}, \quad (1)$$

where k is the Boltzmann constant, $C = 16\pi m_n^* k^2/h^3 = 6.57 \times 10^{20} \text{ cm}^{-2} \text{ s}^{-1} \text{ K}^{-2}$ for n -type GaN, $\sigma_n(\infty)$ is the capture cross section at $T = \infty$, E_{T0} is the thermal energy at $T = 0$ (the energy also determined from Hall-effect measurements⁷), E_σ is the barrier energy for the capture cross section, g_0/g_1 is the unoccupied (occupied) state degeneracy, and α is a parameter indicating the temperature dependence of the thermal energy ($E_T = E_{T0} - \alpha T$). We assume that $\alpha \approx 0$, for a level close to the conduction band, and we also assume that $g_0/g_1 = 1/2$, appropriate for V_N . The measurements taken at different pulse widths allow us to distinguish at least two levels, with different emission kinetics; as evidenced in Fig. 1, for pulse widths lower than $50 \mu\text{s}$, the component at low temperature does not appear. This observation suggests that this trap should have a very small capture cross section, as also observed by Goodman *et al.*¹⁷

To reduce the uncertainty, fitting has been carried out simultaneously over six spectra, including emission rates from 20 to 1000 s^{-1} . The parameters determined by the fitting are then: $E_{\text{TOT}} = E_{T0} + E_\sigma$, $\sigma(\infty)$, and N_T' , where N_T' is the apparent concentration. A typical fitted spectrum is

TABLE I. Overall fitting parameters for data averaged over several emission rates.

Parameter	ED1	ED2	D
Energy (eV)	0.060 ± 0.005	0.110 ± 0.010	0.25 ± 0.1
$\sigma_n(\infty)$ (cm^2)	$1-3 \times 10^{-20}$	$5-8 \times 10^{-19}$	$1-2 \times 10^{-14}$

shown in Fig. 2. The peak-height variation with temperature (or emission rate) is mainly due to the second component ED2, while the first component ED1, lower in concentration, is nearly independent of temperature. The fitted parameters are given in Table I. To obtain the true values of N_T , we must take into account two other effects: (i) the incomplete filling of the traps, due to the low capture cross section,¹⁶ and (ii) the so-called λ effect, which involves a correction due to traps already filled before the forward-bias pulse is even applied.¹⁸ Using small pulse widths, to display just ED2, we observe that the capture cross section of this trap exhibits a temperature dependence. Peak-height versus pulse-width experiments at different emission rates (temperatures) give values of E_σ on the order of 30–50 meV,¹⁴ however, the temperature dependence of the peak height allows us to determine more accurately these values, as discussed below.

We consider the general expression for trap filling:¹⁶

$$N_T^0(z, t_p) = N_T(z) \left(\frac{1}{1 + e_n/n(z)\sigma_n v} \right) (1 - e^{-(e_n + n(z)\sigma_n v)t_p}). \quad (2)$$

In Eq. (2), t_p is the filling pulse width, z is the distance from the surface into the depletion layer, $N_T^0(z, t_p)$ is the density of filled traps at the end of the pulse of width t_p , $N_T(z)$ is the total density of traps, $n(z)$ is the free-carrier concentration available for filling during the pulse, v is the thermal velocity of the carriers, equal to $\sqrt{8kT/\pi m^*}$, and σ_n is the actual capture cross section, i.e., $\sigma_n(\infty)e^{-E_\sigma/kT}$. Note that $(1/[1 + e_n/n(z)\sigma_n v])^{-1}$ is simply the equilibrium Fermi factor. $C-V$ measurements show that $n(z)$ is approximately constant with z , and we will tentatively assume that $N_T(z)$ is constant, also.

Equation (2) is applied as follows. In our type of DLTS apparatus (BioRad-DL4600), the capacitance (C) transients are sampled at two times, t_1 and t_2 . As temperature is swept, a peak occurs in the signal $\Delta C = C(t_1) - C(t_2)$ at temperature T_m , and at this temperature, $e_n(T_m) = \ln(t_2/t_1)/(t_2 - t_1)$. In our experiment, different combinations of t_1 and t_2 were chosen such that $e_n(T_m)$ varied from 20 to 1000 s^{-1} , giving e_n as a function of T_m . Thus, in Eq. (2), if N_T^0 is plotted as a function of T_m , the only unknowns are N_T , $\sigma_n(\infty)$, and E_σ , since e_n is known at each value of T_m . Also from Eq. (1), the knowledge of e_n as a function of T_m allows calculation of $(E_{T0} + E_\sigma)$ and $(g_0/g_1)\exp(\alpha/k)\sigma_n(\infty)$, by using the usual Arrhenius plot of $\ln(T^2/e_n)$ vs T^{-1} , mentioned earlier. Therefore, the use of both Eqs. (1) and (2) yields E_{T0} and E_σ , separately.

The values of N_T^0 (ED2) vs T_m , at three different irradiation fluences and for $t_p = 5 \text{ ms}$, are plotted in Fig. 3. Included are the theoretical plots of Eq. (2), which yield a fitting parameter $E_\sigma = 0.064 \text{ eV}$ for trap ED2. Thus, since $E_{T0} + E_\sigma$ was found to be around 0.11–0.12 eV, from the Arrhenius plot, it follows that $E_{T0} = 0.055 \text{ eV}$, about the

FIG. 3. Filling evolution of trap ED2 at $t_p = 5$ ms calculated from Eq. (2). Fitting parameters are $\sigma_n(\infty) = 5 \times 10^{-19} \text{ cm}^2$, $E_\sigma = 0.064 \text{ eV}$, and $N_T(\text{ED2}) = 5.2 \times 10^{14} \text{ cm}^{-3}$ at ϕ_3 ; $N_T(\text{ED2}) = 8.3 \times 10^{14} \text{ cm}^{-3}$ at ϕ_4 ; and $N_T(\text{ED2}) = 12.5 \times 10^{14} \text{ cm}^{-3}$ at ϕ_5 .

same energy as that found for trap ED1. In Fig. 3, the concentrations N_{T0} were calculated from the capacitance data by using the usual approximation, valid for $N_T \ll N_D$: $N_{T0} = 2n(\Delta C/C_0)$, where $n \approx N_D - N_A$ is determined from the $C-V$ data. However, a more accurate relationship is $N_{T0} = 2n(\Delta C/C_0)/f_\lambda$, where f_λ accounts for the λ effect.^{16,18} For the conditions here, the λ correction was about 20%, and was included in the N_{T0} data shown in Fig. 3. The fitted values of N_T , from Eq. (2), are: at ϕ_3 , $N_T(\text{ED1}) = 3.5 \times 10^{14} \text{ cm}^{-3}$ and $N_T(\text{ED2}) = 5.2 \times 10^{14} \text{ cm}^{-3}$; at ϕ_4 , $N_T(\text{ED1}) = 5.4 \times 10^{14} \text{ cm}^{-3}$ and $N_T(\text{ED2}) = 8.3 \times 10^{14} \text{ cm}^{-3}$; and at ϕ_5 , $N_T(\text{ED1}) = 8.1 \times 10^{14} \text{ cm}^{-3}$ and $N_T(\text{ED2}) = 12.5 \times 10^{14} \text{ cm}^{-3}$.

The conclusion that both ED1 and ED2 have a thermal energy of about 0.06 eV is significant, because it resolves the major discrepancy with the Hall-effect experiment,⁷ which also found an energy of 0.06 eV. Earlier DLTS analyses^{8,10,12,17} had found much higher energies, 0.14–0.20 eV; however, in these cases, a single peak was assumed, Arrhenius plots were used to determine the energies, and the E_σ contribution to the energies was not considered. In spite of this agreement between the Hall and DLTS energies one mystery remains; namely, the combined production rate of ED1+ED2, i.e., $[1.2 \times 10^{15} + 0.8 \times 10^{15}] \text{ cm}^{-3}/6.5 \times 10^{15} \text{ cm}^{-2} \approx 0.3 \text{ cm}^{-1}$, is much smaller than that measured by the Hall effect, which was about 1 cm^{-1} . One possible reason for this difference is that the Hall experiment samples the whole layer, whereas the DLTS experiment samples only the near-surface region, i.e., only the top $0.4 \mu\text{m}$, in this case. The near-surface region contains an electric field, due to the surface potential, and also will usually have a smaller strain and dislocation density than the lower region. It is possible that some of these factors could affect the room-temperature stability of some of the irradiation-induced defects. In fact, partial annealing ($\approx 20\%$) of the DLTS signal, over a period of about 1 day, has already been observed.¹⁹ If this effect is stronger in the near-surface region, then the effective DLTS production rate will be smaller than the Hall rate, as observed. These phenomena must be studied further.

The microscopic nature of the defects ED1 and ED2 has not been elucidated yet, but the 0.06 eV Hall defect was earlier assigned to the N vacancy, V_N .⁷ Now, a 1 MeV elec-

tron hitting either the Ga or N face in GaN would be expected to produce not only simple V_N-N_1 Frenkel pairs, but also defects composed of longer chains, such as $V_N-N_{\text{Ga}}-N_1$.²⁰ Such defects may have a common thermal energy, determined by V_N , but different capture cross sections. Plans are underway to carry out lower-energy irradiations, in an attempt to eliminate some of the higher-order chains. Also low-temperature irradiations would allow the systematic study of annealing in the room-temperature region.

In summary, we have conducted a detailed evaluation of the main DLTS spectral feature produced by 1 MeV electron irradiation. The DLTS peak was shown to have a contribution from two separate defects, having equal thermal energies of 0.06 eV, but different capture cross sections. Earlier DLTS results, which gave higher energies than those obtained from Hall-effect experiments, were shown to suffer from inaccurate analyses. In spite of this agreement between DLTS and Hall-defect energies, their respective defect production rates, 0.3 and 1 cm^{-1} , still differ.

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