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Deep Traps in Molecular-Beam-Epitaxial GaAs Grown at Low Temperatures

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Deep-level transient spectroscopy has been performed on Si-doped GaAs layers grown by molecular-beam epitaxy at substrate temperatures of 400–450 °C. The λ effect is taken into account and overlapping peaks are analyzed numerically. An 0.65 eV electron trap of concentration 2×10^{16} cm^{-3} is believed to be related to the As_{Ga}-associated 0.65 eV Hall-effect center, and also to the trap EB4 found in electron-irradiated GaAs.

I. INTRODUCTION

Molecular-beam-epitaxial (MBE) GaAs grown at temperatures T_G well below the normal growth temperatures, 580–600 °C, has unique properties because of high concentrations of point defects, such as As antisites (As_{Ga}) and Ga vacancies (see reviews in Refs. 1, 2, and 3). These defects have been studied by many different types of experiments, such as electron paramagnetic resonance,[4–6] absorption,[7,8] Hall effect,[9,10] photoluminescence,[11,12] thermally stimulated current,[13] and positron annihilation.[14] However, one of the most common forms of defect studies, namely deep-level transient spectroscopy (DLTS), has been applied sparingly,[15,16] because the creation of a conductive layer by doping is difficult for $T_G \leq 400$ °C, and also because Schottky barriers tend to be leaky in the presence of high quantities of deep-level defects. Thus, e.g., DLTS cannot be used to study 200–250 °C material, which is commonly used for low-temperature (LT) GaAs device fabrication.[17]

In this investigation we have used DLTS to analyze samples grown at 400, 450, and 560 °C. Because our apparatus, a BioRad DL4600, obtains and analyzes data by means of the simple, dual-gate, boxcar technique, it was necessary to use a numerical approach to get accurate results for two of the strong peaks which were overlapping. Also, because the energy levels were deep, the so-called λ effect was included in the analysis.[18–20] Two of the observed DLTS levels have concentrations greater than 10^{16} cm^{-3} and there is evidence that at least one of them is related to As_{Ga}.

II. ANALYSIS

We assume a semiconductor sample which contains shallow (fully ionized) donors of concentration N_D, acceptors of concentration N_A all with transition energies below that of the shallow donor, and a deep donor trap with a (0/+) transition energy E_T and concentration N_T. In the DLTS experiment, the sample is subjected to a reverse bias V_r (a negative number) for a long time, then a trap-filling forward bias V_f is applied for a short time (pulse), and finally the reverse bias is reapplied. The reverse bias depletes the free carriers to a depth w_r below the surface, and the deep trap to a depth $w_r-\lambda$, where[19,20]

$$\lambda=\left(\frac{2\epsilon(E_T-E_{C\infty}-2kT)}{e^2(N_D-N_A)}\right). \tag{1}$$

where $E_{C\infty}$ is the conduction band energy with respect to the Fermi level at $z=\infty$. Here ϵ is the dielectric constant and it is assumed that the depletion approximation is valid. The depletion capacitance at reverse bias is $C_0=\epsilon A/w_r$, where A is the Schottky barrier area. The forward bias pulse will decrease the depletion depth to w_f and will fill the deep traps in an additional region (toward the surface) of width $\Delta\lambda$, where $\Delta\lambda=w_r-w_f$. Immediately after the pulse, the depletion depth will be increased from its original value (w_r) by Δw_r, because more positive charge is needed from the shallow donors to balance the positive charge lost from the deep traps which were neutralized during the pulse. Then, the capacitance will decrease by an amount ΔC, which can be shown to obey[19]

$$\frac{\Delta C}{C_0}=-\frac{\{1+f_\lambda[N_T(w_r-\lambda)/N_D^{\rm net}(w_r)]\}^{1/2}-1}{\{1+f_\lambda[N_T(w_r-\lambda)/N_D^{\rm net}(w_r)]\}^{1/2}}, \tag{2}$$

where $N_D^{\rm net}=N_D-N_A$ and

$$\begin{aligned} f_\lambda&=\left(1-\frac{\lambda}{w_r}\right)^2-\left(1-\frac{\lambda}{w_r}-\frac{\Delta\lambda}{w_r}\right)^2 \\ &\simeq\left[1-\left(\frac{(E_T-E_{C\infty}-2kT)/e}{V_B-V_r}\right)^{1/2}\right]^2-\left[\left(\frac{V_B-V_f}{V_B-V_r}\right)^{1/2}\right. \\ &\quad\left.-\left(\frac{(E_T-E_{C\infty}-2kT)/e}{V_B-V_r}\right)^{1/2}\right]^2. \end{aligned} \tag{3}$$

Here $V_B\equiv\phi_B-E_{C\infty}/e-kT/e$, where ϕ_B is the Schottky barrier potential, about 0.7 V, and $E_{C\infty}$ is 0.034 eV for $T=296$ K and $N_D-N_A=1\times10^{17}$ cm^{-3}. Typically, $V_r=-1.0$ V and $V_f=0$. To derive Eqs. (2) and (3), it must be assumed that N_T is constant in the region $w_r-\lambda-\Delta\lambda<z<w_r-\lambda$, and N_D constant in $w_r<z<w_r+\Delta w_r$. If $f_\lambda N_T(w_r-\lambda)\ll N_D^{\rm net}(w_r)$, then Eq. (2) can be written

$$\frac{\Delta C}{C_0}\simeq f_\lambda\frac{N_T(w_r-\lambda)}{2N_D^{\rm net}(w_r)}. \tag{4}$$

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In most analyses of DLTS spectra it is assumed that $f_\lambda=1$, and therefore that the criterion for the validity of Eq. (4) is $N_T \ll N_D$; however, this criterion is often far too strong, since values of $f_\lambda \simeq 0.1$ are not unusual for deep centers. Note also that in such cases the calculated trap concentration N_T will be severely underestimated if f_λ is assumed to be unity.

The criterion $f_\lambda N_T \ll N_D^{\rm net}$ holds for the sample studied here and, thus, Eq. (4) applies. The time dependence of ΔC after the pulse will be given by

$$\frac{\Delta C}{C_0} \simeq f_\lambda \frac{N_T}{2N_D^{\rm net}} e^{-e_n t}, \tag{5}$$

where we have assumed that N_D and N_T are constant and where e_n, the emission rate, is given by[19]

$$e_n = G \frac{g_0}{g_1} e^{\alpha/k} T^2 \sigma_{n0} e^{-(E_{T0}+E_\sigma)/kT}. \tag{6}$$

Here, $G \simeq 2.0\times10^{20}\ \mathrm{s^{-1}\,cm^{-2}\,K^{-2}}$ for GaAs, g_0/g_1 is the trap degeneracy ratio, α is a temperature coefficient satisfying $E_T = E_{T0} - \alpha T$, and the capture cross section σ_n obeys $\sigma_n = \sigma_{n0} \exp(-E_\sigma/kT)$.

Our DLTS apparatus, a BioRad DL4600, uses the common, dual-gate boxcar technique[21] to determine E_{T0} and σ_n. That is, the transient $\Delta C(t)$ is sampled at two times, t_1 and t_2, and then the function

$$F(t_1,t_2,T) = C(t_1) - C(t_2) = \Delta C(t_1) - \Delta C(t_2) \tag{7}$$

is plotted versus temperature. From Eqs. (5), (6), and (7), it is seen that if f_λ is only a weak function of temperature, then $F(T)$ will go through a maximum at a temperature T_m satisfying the condition

$$\exp(-e_n^* t_2) = (t_1/t_2)\exp(-e_n^* t_1),$$

where $e_n^* = e_n(T_m)$. By using different values of t_1 and t_2, the peaks will shift and different values of $e_n(T_m)$ can be calculated. Therefore, the parameters $E_{T0}+E_\sigma$ and $(g_0/g_1)\sigma_{n0} \exp(\alpha/k) = \sigma_{n0}^{\rm eff}$ can be determined from an Arrhenius plot $\ln(e_n/T_m^2)$ vs T_m^{-1} of the data.

The "peak" analysis described above is probably the most common technique used to analyze DLTS results, and indeed is the method employed in our commercial spectrometer. Another method is to digitize and analyze the whole emission transient, $\exp(-e_n t)$ in Eq. (5), but for this technique specialized equipment is necessary. A third option, evidently used very seldom, is to analyze the whole $F(T)$ curve rather than just the peak. Let the electronically amplified and plotted signal be $S(T) = \gamma F(T)$, where γ is a constant. The software sets $S(T) = f_\lambda N_T$ at its maximum which leads to

$$f_\lambda N_T = S(T_m) = \gamma F(T_m) = \gamma C_0 \frac{f_\lambda N_T}{2N_D} e^{-e_n^* t_1}\left(1 - \frac{t_1}{t_2}\right), \tag{8}$$

so that

$$S(T) = f_\lambda N_T \frac{e^{\ln(t_2/t_1)/(t_2/t_1-1)}}{(1-t_1/t_2)} (e^{-e_n t_1} - e^{-e_n t_2})$$
$$= 3.07 f_\lambda N_T (e^{-e_n t_1} - e^{-e_n t_2}). \tag{9}$$

The factor 3.07 results from the fact that all of the pairs t_1 and t_2 used in the BioRad system satisfy the condition $t_2/t_1 = 2.5$. For example, one pair of times is $t_1 = 7.63$ ms, $t_2 = 19.07$ ms so that the maximum in $S(T)$ will occur at an emission rate

$$e_n^* = \ln(t_2/t_1)/(t_2-t_1) = 80\ \mathrm{s^{-1}}.$$

At this maximum, from Eq. (9), $S = f_\lambda N_T$, as it should. Of course, the software in our spectrometer includes the assumption $f_\lambda = 1$, which will underestimate N_T for a deep trap.

In principle, an "exact" analysis can be carried out by fitting the complete line shape $S(T)$ from a single t_1, t_2 pair, with fitting parameters $\sigma_{n0}^{\rm eff}$ and $E_{T0}+E_\sigma$; however, we have found much better accuracy by simultaneously fitting to two line shapes resulting from two different t_1, t_2 pairs, or rate windows. A big advantage of using the full line shape instead of just the peak is that overlapping lines, which shift the peaks, can be analyzed in a straightforward manner. For two traps, A and B,

$$S(T) = 3.07[f_{\lambda A} N_{TA}(e^{-e_{nA} t_1} - e^{-e_{nA} t_2})$$
$$+ f_{\lambda B} N_{TB}(e^{-e_{nB} t_1} - e^{-e_{nB} t_2})]. \tag{10}$$

Equation (10) has been used in the results which follow.

III. SAMPLES AND DISCUSSION

Three samples, H37, H38, and G593, are discussed in this study. Samples H37 and H38 were grown to thicknesses of 5 μm at substrate temperatures of 560 and 450 °C, respectively, in a Varian 360 apparatus with the substrates In bonded to the sample holder; thus, the temperatures, measured by a thermocouple attached to the holder, can be considered to be fairly accurate. The carrier concentration was $1\times10^{17}\ \mathrm{cm^{-3}}$, from Si doping, in both cases. Sample G593 was grown to a thickness of 2 μm, and a concentration $2\times10^{17}\ \mathrm{cm^{-3}}$, in a Varian Gen II apparatus at a substrate temperature of 400 °C; however, in this case the substrate was not In bonded so that the temperature, measured by a thermocouple near to but not touching the sample, is not as accurate. In all cases, the As_4/Ga beam equivalent pressure ratio was about 20.

As mentioned earlier, our DLTS apparatus is a commercial BioRad DL4600 instrument which employs the dual-gate boxcar technique. A spectrum for H38, using a rate window $e_n \simeq 50\ \mathrm{s^{-1}}$ and a reverse bias of -1 V, is shown in Fig. 1. As seen, there are at least four peaks, A, B, C, and D, with characteristics given in Tables I and II. Sample H37 (not shown) displayed only peak A, and at a much lower concentration, about $4\times10^{14}\ \mathrm{cm^{-3}}$. (Note that the concentrations in Fig. 1 are not corrected for the λ effect, and thus are much too small. The values in Table I are corrected.) Because peaks A and D are small and somewhat overlapping with larger peaks, we have not studied them in detail but have performed only the usual Arrhenius analysis of the peak emission rates, with results given in Tables I and II. Thus, we do not consider the A and D parameters to be accurate. Peaks B and C, on the other hand, are better defined because the concentrations are much higher. However, because of the overlap complications, we have carried out a simultaneous

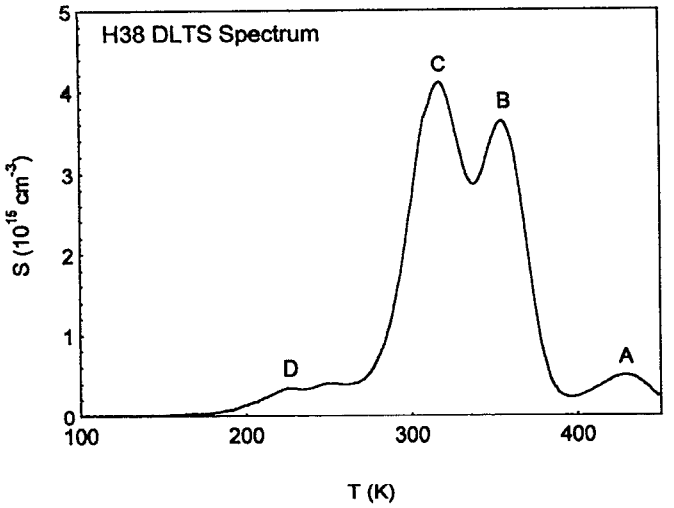

FIG. 1. The DLTS spectrum of sample H38 under the following conditions: $V_r=-1$ V, $V_f=0$ V, rate window=50 s^{-1}.

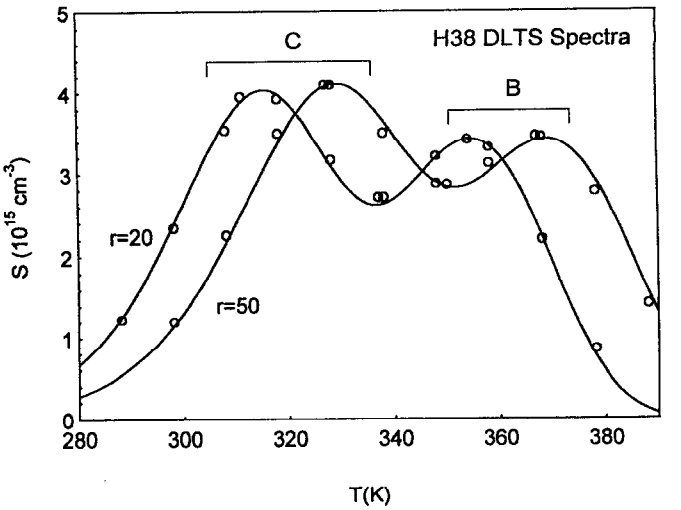

FIG. 2. A numerical fit (solid lines) to the H38 DLTS spectral region including traps B and C. The circles are selected experimental points to illustrate the goodness of fit.

least-squares fit of Eq. (10) for two rate windows, 20 and 50 s^{-1}. The results are shown in Fig. 2 and it is seen that the fits are very good. For sample G593, only one major peak (E) was found, and, again, a simple peak analysis was performed to get the parameters found in Tables I and II.

For comparison purposes, in Table II we have listed parameters $E(=E_{T0}+E_\sigma)$ and σ for certain electron traps which have values e_n(300 K) within a factor ~5 of our e_n(300 K) values for traps A–E. The actual magnitudes of e_n are important as a comparison because a small error in E can cause a larger error in σ. Thus, to be considered identical, traps should have nearly equal values of E and e_n (300 K), but not necessarily σ. Using these criteria, trap A might be the same as EB1, B the same as EF1 or EB4, and D the same as EL4. Because the concentrations of traps A–E ($>10^{15}$ cm^{-3}) are higher than any impurity concentrations other than that of the dopant Si, and because of the known high concentrations of defects in LT-MBE GaAs layers,[1–3,8] we believe that these traps are either pure defects or defect-Si complexes. Therefore, since EB4 is defect related (found in e-irradiated GaAs), and EL4 is MBE related, the equalities B≡EB4 and D≡EL4 seem to be the most likely of the possibilities proposed above.

We next compare with DLTS results from the earlier work of Wood and co-workers[15] and Stall *et al.*[16] They have identified traps in 430 °C Sn-doped material as EB7 (0.30 eV), EB5 (0.48 eV), and EB3 (0.90 eV), and in 380 °C Ge-doped material as EB6 (0.41 eV), EB5 (0.48 eV), and EB4 (0.71 eV). Although no information on actual emission rates is given, we evidently have agreement at least on EB4, which indeed was their dominant trap in the 380 °C layer. The fact that their layer was doped with Ge, and ours with Si suggests that the specific nature of the donor is irrelevant, although the possible involvement of the donor in a defect-donor complex cannot be ruled out. Much work on EB4 in electron-irradiated GaAs has been carried out in the past, and several workers have concluded that it is a complex,[22–24] but a defect-defect complex rather than a defect-donor complex. All of the suggested EB4 complexes involve As_{Ga}.

Another interesting comparison can be made between the traps reported here and the 0.65 eV Hall-effect center[25] found in 350–450 °C GaAs and known to be related to As_{Ga}. Concentrations of the 0.65 eV center are about 2×10^{17} cm^{-3} in an undoped layer grown at 400 °C on a non-In-bonded substrate. Although this concentration is about an order of magnitude higher than that of traps B, C, or E in the present samples, it is important to note[26] that the concentration of another As_{Ga}-related center, EL2, is expected to fall rapidly for $n>10^{17}$ cm^{-3}. Thus, traps B, C, or E could possibly be associated with the 0.65 eV, As_{Ga}-related center, with trap B being the best candidate because of the closeness in energy.

TABLE I. Properties of major traps in this study ($V_r=-1.0$ V).

Trap	T_G	N_D-N_A (cm^{-3})	N_T (cm^{-3})	$E_{T0}+E_\sigma$ (eV)	σ_n^{eff} (cm^{-2})	Analysis
H38-A	450 °C	1×10^{17}	3.5×10^{15}	0.87	2.0×10^{-14}	peak
H38-B			2.5×10^{16}	0.65	1.5×10^{-15}	line shape fit
H38-C			2.1×10^{16}	0.56	9.0×10^{-16}	line shape fit
H38-D			1.1×10^{15}	0.55	6.1×10^{-12}	peak
[a]G593-E	400 °C	2×10^{17}	1.1×10^{16}	0.54	4.8×10^{-15}	peak

[a]Non-In-bonded substrate, so T_G not as accurate.

TABLE II. Comparison of LT-GaAs traps with those in the literature having similar values of e_n (300 K).

This study	Literature	E (eV)	σ (cm^2)	e_n(300 K) (s^{-1})	Association
H38-A		0.87	2×10^{-14}	8.7×10^{-4}	LT MBE
	EB1	0.86	3.5×10^{-14}	2.2×10^{-3}	Cr-doped LPE[a]
H38-B		0.65	1.5×10^{-15}	3.2×10^{-1}	LT MBE
	EF1	0.72	7.7×10^{-15}	1.1×10^{-1}	Cr-doped bulk
	EB3	0.90	3.0×10^{-11}	4.1×10^{-1}	e-irrad.
	EB4	0.71	8.3×10^{-13}	1.8×10^{1}	e-irrad.
H38-C		0.56	9.0×10^{-16}	6.3	LT MBE
	EL12	0.78	4.9×10^{-12}	6.9	VPE[b]
H38-D		0.55	6.1×10^{-12}	6.3×10^{4}	LT MBE
	EL4	0.51	1.0×10^{-12}	4.9×10^{4}	MBE
G593-E		0.54	4.8×10^{-15}	7.3×10^{1}	LT MBE
	EB4	0.71	8.3×10^{-13}	1.8×10^{1}	e-irrad.
	EL16	0.37	4.0×10^{-18}	4.4×10^{1}	VPE

[a]Liquid-phase epitaxy.
[b]Vapor-phase epitaxy.

Further work will be necessary for an absolute identification, but it seems probable that trap B in our LT-GaAs layers is the same as the 0.65 eV LT-GaAs Hall-effect center, and also the same as trap EB4 found in LT-GaAs and in e-irradiated GaAs.

IV. SUMMARY

Several DLTS traps, designated A, B, C, D, and E, have been characterized in MBE GaAs grown at 400 and 450 °C. Because these traps are all deep it was necessary to include the so-called λ effect in the analyses. Furthermore, because the signals for traps B and C were strongly overlapping, it was necessary to carry out a numerical analysis of the coupled line shapes. Three of the traps, B, C, and E, have concentrations greater than 10^{16} cm^{-3} and are probably either pure defects, or defect-Si complexes. One of these, trap B, has an energy of 0.65 eV and effective capture cross section of 1.5×10^{-15} cm^2, and may well be associated with both EB4, found in e-irradiated samples, and with the 0.65 eV Hall-effect center found in LT-MBE material and known to be related to As_{Ga}. From other DLTS results, many workers believe that EB4 is an As_{Ga}-defect complex.

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