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Convenient determination of concentration and energy in deep-level transient spectroscopy

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For defects or impurities with deep energy levels, such as the commonly observed EL2, EL3, and EL6 in GaAs, it is very important to take account of the so-called λ effect in order to deduce the correct concentrations of these centers when using capacitance techniques. By measuring capacitance at several forward bias voltages for a given reverse bias voltage it is possible to determine concentration N_T and energy E_T without requiring the usual emission rate analysis. Convenient formulas for N_T and E_T are given, although only N_T can be determined with a high degree of precision. The results for an n -type horizontal Bridgman wafer ($n \approx 2.8 \times 10^{16} \text{ cm}^{-3}$) are: $N_{\text{EL2}} = (1.14 \pm 0.02) \times 10^{16} \text{ cm}^{-3}$, $E_{\text{EL2}}(377 \text{ K}) = 0.71 \pm 0.06 \text{ eV}$; $N_{\text{EL6}} = (8.0 \pm 0.5) \times 10^{15} \text{ cm}^{-3}$, $E_{\text{EL6}}(167 \text{ K}) = 0.42 \pm 0.09 \text{ eV}$. © 1995 American Institute of Physics.

I. INTRODUCTION

Deep-level transient spectroscopy (DLTS) is a popular technique for determining transition energy E , capture cross section σ , and concentration N of various defect and impurity traps in semiconductors;¹ however, the usual DLTS analysis gives only effective values for all of these quantities.² For example, the calculated energy E includes not only the trap energy E_T (actually E_{T0} , the value at $T=0$), but also E_σ , a contribution from the temperature dependence of σ . Also, σ includes a degeneracy factor g_0/g_1 and a term $\exp(\alpha/k)$, where α is given by $E_T = E_{T0} - \alpha T$. Finally, the calculated N is related to the true trap concentration N_T by $N_T = N/f_\lambda$, where f_λ takes account of the fact that a certain fraction of the traps in the depletion region are already filled, even before the filling pulse is applied.²⁻⁴ In this article we present a simple formulation of f_λ which allows an accurate determination of N_T and a value of E_T that is less accurate but free of the ambiguity discussed above.

II. λ EFFECT

Consider a reverse-biased, n -type Schottky diode as shown in Fig. 1. A barrier $\phi_B - V_r$ exists between the metal Fermi level and the semiconductor conduction band where ϕ_B (a positive number) is the Schottky barrier potential and V_r (a negative number) is the reverse bias potential. Suppose the Fermi level in the semiconductor is controlled by shallow donors of concentration N_D , compensated by acceptors of concentration N_A . Then, in the depletion approximation, a region w_r will be depleted of free carriers, where

$$w_r = \left(\frac{2\epsilon(V_{\text{bi}} - V_r - kT/e)}{eN_D^{\text{net}}} \right)^{1/2} \times \left(\frac{[1 + (N_T/N_D^{\text{net}})(1 - \beta)]^{1/2} + (N_T/N_D^{\text{net}})\beta^{1/2}}{1 + N_T/N_D^{\text{net}}} \right). \quad (1)$$

Here $N_D^{\text{net}} = N_D - N_A$, $V_{\text{bi}} = \phi_B - E_{C\infty}/e$, $E_{C\infty} = E_C - E_F$ at $z = \infty$, and

$$\beta = (E_T - E_{C\infty} - kT)/e(V_{\text{bi}} - V_r - kT/e),$$

V_{bi} is known as the built-in voltage. The first factor in Eq. (1) is well known;² the second, which is a correction for large N_T/N_D^{net} , results from a rather involved analysis which will be published elsewhere. In the region $z < w_r$ all of the shallow donors are ionized, but only a fraction $(w_r - \lambda)/w_r$ of any deep donors is ionized, where²⁻⁴

$$\lambda = \left(\frac{2\epsilon(E_T - E_{C\infty} - kT)/e}{eN_D^{\text{net}}} \right)^{1/2}. \quad (2)$$

Here $E_T = E_{T0} - \alpha T$ is the activation energy of the trap at temperature T , and the kT terms in Eqs. (1) and (2) are corrections for the Debye-tail free carriers. [Note that there is also some evidence⁴ for a $2kT$ correction in Eq. (2); however, this term is usually not significant anyway.] When a forward bias V_f (also usually a negative number or zero) is applied, then the traps in an additional region of width $\Delta\lambda$ are filled, where $\Delta\lambda = w_r - w_f$. Before the filling pulse, the capacitance per unit area will be $C_0 = \epsilon/w_r$, whereas immediately after the pulse, w_r will be increased by Δw and C will be decreased by ΔC . It can be shown that²

$$\frac{\Delta C}{C} = - \frac{\{1 + f_\lambda[N_T(w_r - \lambda)/N_D^{\text{net}}(w_r)]\}^{1/2} - 1}{\{1 + f_\lambda[N_T(w_r - \lambda)/N_D^{\text{net}}(w_r)]\}^{1/2}}, \quad (3)$$

where f_λ is the fraction of depletion-region ($z < w_r$) traps with energies above E_F under the initial reverse bias. If N_D^{net} is constant in the region Δw , and N_T in the region $\Delta\lambda$, then

$$f_\lambda = \left(1 - \frac{\lambda}{w_r} \right)^2 - \left(1 - \frac{\lambda}{w_r} - \frac{\Delta\lambda}{w_r} \right)^2. \quad (4)$$

If $f_\lambda N_T \ll N_D^{\text{net}}$, which is often true, then

$$\frac{\Delta C}{C} = - \frac{f_\lambda N_T(w_r - \lambda)}{2 N_D^{\text{net}}(w_r)}. \quad (5)$$

After the pulse, the $f_\lambda N_T$ traps will begin to lose their electrons at a rate $\exp(-e_n t)$, where the emission rate for GaAs is given by

FIG. 1. Band diagram illustrating some of the quantities used in this study. It is assumed that $\phi_B - V_r = 1.3$ V on the surface.

$$e_n = 2 \times 10^{20} (g_0/g_1) \sigma_{n0} e^{a/kT} e^{-(E_{T0} + E_\sigma)/kT}. \quad (6)$$

Note that the true capture cross section is $\sigma_n = \sigma_{n0} e^{-E_\sigma/kT}$. An Arrhenius plot of $\ln(e_n/T^2)$ vs T^{-1} gives a slope $-(E_{T0} + E_\sigma)/k$ and an intercept $2 \times 10^{20} \sigma_{\text{eff}}$, where $\sigma_{\text{eff}} = (g_0/g_1) e^{a/k} \sigma_{n0}$. In the boxcar technique,¹ the signal is given by

$$S = A f_\lambda N_T (e^{-e_n t_1} - e^{-e_n t_2}), \quad (7)$$

where $t_2/t_1 = 2.5$ and $A = 3.07$ for our commercial spectrometer, a BioRad DL4600. The constant A is chosen such that $S_{\text{peak}} = f_\lambda N_T$ at each peak of the S vs T spectrum.

By applying Eqs. (1) and (2) along with the relationship $\Delta\lambda = w_r - w_f$, we can write

$$f_\lambda = \frac{1}{V_{\text{bi}} - V_r} [(V_f - V_r) - 2\sqrt{(E_T - E_{C\infty})/e}(\sqrt{V_{\text{bi}} - V_r} - \sqrt{V_{\text{bi}} - V_f})], \quad (8)$$

where we have dropped the kT/e terms. Let $\Delta = V_f - V_r$. Then,

$$f_\lambda = \frac{\Delta}{V_{\text{bi}} - V_r} - 2 \left(\frac{(E_T - E_{C\infty})/e}{V_{\text{bi}} - V_r} \right)^{1/2} \left[1 - \left(1 - \frac{\Delta}{V_{\text{bi}} - V_r} \right)^{1/2} \right]. \quad (9)$$

First note that

$$\frac{df_\lambda}{dV_f} = \frac{df_\lambda}{d\Delta} = \frac{1}{V_{\text{bi}} - V_r} \left(1 - \left(\frac{(E_T - E_{C\infty})/e}{V_{\text{bi}} - V_r} \right)^{1/2} \right) \times \frac{1}{\left(1 - \frac{\Delta}{V_{\text{bi}} - V_r} \right)^{1/2}}, \quad (10)$$

or

$$f'_{\lambda 0} = \left. \frac{df_\lambda}{dV_f} \right|_{V_f \rightarrow V_r} = \left. \frac{df_\lambda}{d\Delta} \right|_{\Delta \rightarrow 0} = \frac{1}{V_{\text{bi}} - V_r} \left[1 - \left(\frac{(E_T - E_{C\infty})/e}{V_{\text{bi}} - V_r} \right)^{1/2} \right]. \quad (11)$$

Next note that f_λ mathematically goes through a maximum at $\Delta = V_{\text{bi}} - V_r - (E_T - E_{C\infty})/e$, or $V_f = \phi_B - E_T/e$. Actually, f_λ saturates at this value of V_f , because it is unphysical for $\lambda + \Delta\lambda$ to be larger than w_r , which would occur at higher values of V_f . At this maximum, or saturation point,

$$f_\lambda^{\text{max}} = \left[1 - \left(\frac{(E_T - E_{C\infty})/e}{V_{\text{bi}} - V_r} \right)^{1/2} \right]^2. \quad (12)$$

Thus, from Eqs. (7), (11), and (12) we obtain the simple relationship $N_T = [S'_0(V_{\text{bi}} - V_r)]^2/S_{\text{max}}$, valid in the limit $N_T/N_D^{\text{net}} \ll 1$. A more complete analysis, to be presented elsewhere, gives a correction for large N_T/N_D^{net} , or actually large $[S'_0(V_{\text{bi}} - V_r) - S_{\text{max}}]/N_D^{\text{net}}$,

$$N_T = \frac{[S'_0(V_{\text{bi}} - V_r)]^2}{S_{\text{max}}} \left(1 - \frac{S'_0(V_{\text{bi}} - V_r) - S_{\text{max}}}{N_D^{\text{net}}} \right)^{-2}, \quad (13)$$

where $S'_0 = N_T f'_{\lambda 0}$ [Eq. (11)] and we have assumed that S is always measured at the peak of the S vs T spectrum, i.e., at

$$A[\exp(-e_n t_1) - \exp(-e_n t_2)] = 1,$$

the usual case in DLTS. We can also derive

$$E_T - E_{C\infty} = e(V_{\text{bi}} - V_r) \left(1 - \frac{S_{\text{max}}}{S'_0(V_{\text{bi}} - V_r)} \right)^2 \left(1 + \frac{S_{\text{max}}}{N_D^{\text{net}}} \right), \quad (14)$$

where, again, the last factor comes from a more complete analysis. It is important to note that neither of these relationships depends upon any parameters derived from e_n , Eq. (6). In particular, E_T in Eq. (14) is the true energy at the temperature of the peak in S vs T . (Note also that T_{peak} can be varied by changing the rate window, if desired.) In contrast, the usual Arrhenius analysis of e_n gives, in general, a much different quantity, i.e., $E_{T0} + E_\sigma$. Further note that it is not necessary to have a precise value of V_{bi} (typically about 1 V for GaAs) since $|V_r|$ can be made much larger (4 or 5 V). Finally, if $\Delta = V_f - V_r \ll V_{\text{bi}} - V_r$, S vs V_f (or Δ) will be linear over a large range, and S'_0 will be easy to measure accurately. Near the maximum in S vs V_f (occurring at $V_f = \phi_B - E_T/e$), S is varying slowly so that S_{max} can also be determined with good precision; thus, the determination of N_T [Eq. (13)] is very robust at large V_r .

In analyzing S vs T or S vs V_f data, we must consider trap filling phenomena. As can be surmised from the band bending shown in Fig. 1, the free electron concentration at $w_r - \lambda$ is very small, so that the trap filling time may be correspondingly large. If the traps at point z are empty at time zero [i.e., $N_T^+(z, t=0) = N_T$], then at time t_p (the pulse width) they will obey²

$$N_T^+(z, t_p) = \frac{N_T}{1 + n(z)\sigma_n v_n / e_n} \times \left(1 + \frac{n(z)\sigma_n v_n}{e_n} e^{-[e_n + n(z)\sigma_n v_n]t_p} \right), \quad (15)$$

where $n(z)$ is the electron concentration at point z during the V_f pulse. The value of z at which the Fermi level crosses the trap level can be roughly determined by $N_T^+(z) = N_T/2$, or $n(z) \approx e_n / \sigma_n v_n$. For our case, $e_n \approx 50 \text{ s}^{-1}$, $\sigma_n(377 \text{ K}) \approx 2 \times 10^{-16} \text{ cm}^2$, and $v_n(377 \text{ K}) \approx 4 \times 10^7 \text{ cm/s}$, so that $n(z) \approx 6 \times 10^9 \text{ cm}^{-3}$. The time constant under these conditions is $\tau = (2e_n)^{-1} \approx 10 \text{ ms}$. Toward the interior of the sample, i.e., for $z > w - \lambda$, n increases rapidly until it reaches approximately $3 \times 10^{16} \text{ cm}^{-3}$ (in this case) at $z = w_r$. For example, simulations show that n increases an order of magnitude, i.e., from 6×10^9 to $6 \times 10^{10} \text{ cm}^{-3}$ in only about 100 Å, a fraction of the Debye length ($\sim 290 \text{ Å}$ at 377 K). Thus, in rough terms, a 10 ms pulse would be expected to easily fill all of the traps deeper than the Fermi level crossing point (at $z = w_f - \lambda$) except for perhaps those in the first 100 Å beyond this point. Let the thickness of the "poor" trap filling region be designated by δ . Then, in Eq. (4), we should set $\Delta\lambda = w_r - w_f - \delta$, and carry this change through the subsequent steps in the derivation. However, clearly the analysis is affected only for small Δ (or $V_f \sim V_r$), as estimated by $\Delta \lesssim 2(V_{bi} - V_r)\delta/w_r \approx 0.2 \text{ V}$, if $V_r \approx -4 \text{ V}$. Thus, we would expect the initial part of the S vs V_f curve to rise slowly with Δ , because of trap filling problems, if t_p is too short. In the work presented here, we have used 10 ms pulses, which lead to only a small error at $\Delta = 0.5 \text{ V}$, the lowest value used. In a future report, we will show how smaller values of t_p can be used to calculate accurate values of σ_n through the use of Eq. (15) and curve fitting.

III. RESULTS

In Fig. 2 we show S vs T spectra for $V_r = -4.0 \text{ V}$, and $V_f = -3.5$ to 0.5 V (or $\Delta = 0.5$ – 4.5 V), in 0.5 V increments. The sample was grown by the horizontal Bridgman (HB) technique and had a carrier concentration of $2.8 \times 10^{16} \text{ cm}^{-3}$ at 377 K and $2.1 \times 10^{16} \text{ cm}^{-3}$ at 167 K. Thus, $E_{C\infty} \approx 0.099 \text{ eV}$ at 377 K and 0.030 eV at 167 K, the respective peak temperatures of the two most prominent traps, EL2 and EL6. (Here, $e_n \approx 50 \text{ s}^{-1}$ at the peaks.) The S_{peak} vs V_f data are plotted in Fig. 3, and it is seen that they are quite linear at small Δ and then saturate at large Δ ; thus, good values of both S'_0 and S_{max} may be obtained.

To apply Eqs. (13) and (14), we also need a value of the built-in voltage V_{bi} . Although ϕ_b can be determined from C^{-2} vs V or I vs V plots, such measurements can give spurious results if not carefully performed and interpreted. Thus, we prefer to use the value given by Missous and Rhoderick⁵ for Au on (100) GaAs: $\phi = 0.83 \text{ V}$ at 300 K with a temperature coefficient of $-2.3 \times 10^{-4} \text{ eV/K}$. Therefore, $\phi_b = 0.81 \text{ V}$ at 377 K and 0.86 V at 167 K. Then, the application of Eqs. (13) and (14) to the data at both $V_r = -4.0 \text{ V}$ and $V_r = -1.5 \text{ V}$ gives: $N_{\text{EL2}} = (1.14 \pm 0.02) \times 10^{16} \text{ cm}^{-3}$, $E_{\text{EL2}} = 0.71 \pm 0.06 \text{ eV}$, $N_{\text{EL6}} = (8.0 \pm 0.5) \times 10^{15} \text{ cm}^{-3}$, and $E_{\text{EL6}} = 0.42 \pm 0.09 \text{ eV}$, where the errors are determined from the differences in the

FIG. 2. DLTS signal S [Eq. (7)] at a reverse bias $V_r = -4 \text{ V}$, pulse width $t_p = 10 \text{ ms}$, and rate window 50 s^{-1} . The forward biases are as follows: (a) -3.5 V ; (b) -3.0 V ; (c) -2.5 V ; (d) -2.0 V ; (e) -1.5 V ; (f) -1.0 V ; (g) -0.5 V .

values determined from the data sets at $V_r = -4.0$ and -1.5 V , respectively. The results for EL6 contain larger errors, most likely because of electric-field effects at $V_r = -4.0 \text{ V}$. (In Fig. 2, note the temperature shift in the EL6 peak as V_f increases.) More carefully designed experimental conditions can probably produce smaller uncertainties, but the goal of this article is mainly to establish the methodology.

IV. DISCUSSION

The concentration results are quite reasonable. An EL2 concentration of $1 \times 10^{16} \text{ cm}^{-3}$ is typical in HB GaAs; note that the value that would normally have been obtained without consideration of the λ effect, i.e., $S(V_f = 0) \approx 4.2 \times 10^{15} \text{ cm}^{-3}$, is too low by almost a factor of 3, even at $V_r = -4 \text{ V}$. (The error is much worse at $V_r = -1.5 \text{ V}$.) Also, typically,

FIG. 3. DLTS peak EL2 signal $S = f_{\lambda \text{EL2}} N_{\text{EL2}}$ as a function of forward bias V_f for reverse biases $V_r = -4 \text{ V}$ and -1.5 V . The solid lines are theoretical fits.

N_{EL6} is somewhat lower than N_{EL2} , as we find here. Our method determines these concentrations with good (better than 10%) accuracy.

Of equal interest, although determined with less accuracy, are the energies. The calculated energy for EL2, 0.71 ± 0.06 eV, is the true energy at 377 K, not the effective energy

$$E_{\text{eff}} = E_{T0} + E_{\sigma} = 0.75 + 0.075 = 0.825 \text{ eV},$$

obtained from an Arrhenius plot of the emission data. Duncan and Westphal⁶ have obtained a value of $E_{EL2}(296 \text{ K}) \approx 0.65$ eV from a detailed study of a large number of semi-insulating GaAs wafers with varying EL2 and acceptor concentrations. Their data suggest a temperature coefficient

$$\alpha \approx (0.75 - 0.65)/296 \approx 3.4 \times 10^{-4} \text{ eV/K}$$

which would then predict $E_{EL2}(377 \text{ K}) \approx 0.62$ eV, a little outside the error of our value. Martin *et al.*⁷ have given a formula that predicts $E_{EL2}(377 \text{ K}) \approx 0.67$ eV, within the error of our value.

The magnitude of E_{EL6} is also quite interesting. The temperature coefficient α_{EL6} is not known, but many standard DLTS emission rate analyses have given⁸ $E_{T0} + E_{\sigma} \approx 0.35$ eV. Zhao and co-workers⁴ have measured $E_{\sigma} \approx 0.20$ eV, which would then give $E_{T0} \approx 0.15$ eV. It should be noted that Zhao and co-workers' results are consistent with the fact that an 0.15 eV donor is often observed by Hall effect in both electron-irradiated and bulk as-grown samples.^{9,10} However, our present result, $E_{EL6}(167 \text{ K}) \approx 0.42 \pm 0.09$ eV, is more consistent with a small value of E_{σ} , and may indicate that EL6 and the 0.15 eV donor are not identical. In any case, we feel that further studies are necessary to firmly establish E_T and E_{σ} for EL6.

It is clear that the maximum utility of the method suggested here is in the determination of N_T , rather than E_T . Since E_T and V_{bi} can be estimated, N_T can be found from Eq. (11), for the case $N_T/N_D^{\text{net}} \ll 1$,

$$N_T = \frac{S'_0(V_{bi} - V_r)}{1 - \left(\frac{(E_T - E_{C\infty})/e}{V_{bi} - V_r} \right)^{1/2}}. \quad (16)$$

[For the large N_T case, the appropriate expression can be found by combining Eqs. (13) and (14).] Suppose, without further knowledge, we simply set $V_{bi} = 0.8$ V and $E_T - E_{C\infty} = 0.5$ eV; then, for $V_r = -4$ V, $N_T = 7.09 S'_0$. Now if

we let V_{bi} vary over the wide range 0.6–1.2 V, and E_T vary over the wide range 0.2–0.8 eV, the coefficient of S'_0 in Eq. (16) does not change by more than 20% from the value 7.09; thus, N_T can be determined accurately even if E_T and V_{bi} are not well known. To find S'_0 , only a few (minimum of two) values of V_f slightly larger than V_r need to be used (say, $V_f = -3.5$, -3.0 , and -2.5 V for $V_r = -4$ V). An advantage of keeping V_f close to V_r is that the effective volume sampled is small so that, if N_T is not constant, a good profile can be obtained by varying V_r . Also, the electric field in the trap filling region will be smaller if V_f is restricted to values near V_r . Therefore, the use of Eq. (16), with a measured value of S'_0 and estimated values of V_{bi} and E_T , should prove to be useful in practice.

V. CONCLUSIONS

We have presented a new, convenient method for obtaining deep trap concentrations and energies without the use of emission-rate data. Results are given for EL2 and EL6 in GaAs and compared with data from the literature.

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