Convenient Determination of Concentration and Energy in Deep-Level Transient Spectroscopy

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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 X 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 \((n=2.8 \times 10^{16} \text{ cm}^{-3})\) are:

\[
N_{\text{EL2}} = (1.14 \pm 0.02) \times 10^{16} \text{ cm}^{-3}, \quad E_{\text{EL2}}(377 \text{ K}) = 0.71 \pm 0.06 \text{ eV}; \quad N_{\text{EL6}} = (8.0 \pm 0.5) \times 10^{15} \text{ cm}^{-3}, \quad E_{\text{EL6}}(167 \text{ K}) = 0.42 \pm 0.09 \text{ eV}.
\]

I. INTRODUCTION

Deep-level transient spectroscopy (DLTS) is a popular technique for determining transition energy \(E\), capture cross section \(\sigma\), 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 \(E_{\sigma}\), a contribution from the temperature dependence of \(\sigma\). Also, \(\sigma\) includes a degeneracy factor \(g_0/g_1\) and a term \(\exp(\alpha T/K)\), where \(\alpha\) is given by \(E_T = E_{T0} - \alpha T\). Finally, the calculated \(N\) is related to the true trap concentration \(N_T\) by \(N_T = NF/\tau_T\), where \(\tau_T\) 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.\(^3,4\) In this article we present a simple formulation of \(\tau_T\) 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. \(\lambda\) 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 \(\phi_B\) (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. 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

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

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

\[
\beta = (E_T - E_{\text{Cov}} - kT/e)(V_{bi} - V_r - kT/e).
\]

\(V_{bi}\) is known as the built-in voltage. The first factor in Eq. (1) is well known;\(^5\) the second, which is a correction for large \(N_T/N_D^{\text{net}}\), 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 \((w_r - \omega)/w_r\) of any deep donors is ionized, where\(^3,4\)

\[
\lambda = \left(\frac{2e(E_T - E_{\text{Cov}} - kT/e)}{eN_D^{\text{net}}}\right)^{1/2}.
\]

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 evidence\(^5\) 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 \(\Delta w\) are filled, where \(\Delta w = w_r - w_f\). Before the filling pulse, the capacitance per unit area will be \(C_0 = e/w_r\), whereas immediately after the pulse, \(w_r\) will be increased by \(\Delta w\) and \(C\) will be decreased by \(\Delta C\). It can be shown that\(^2\)

\[
\frac{\Delta C}{C} = -\frac{1}{\left\{1 + f_N[N_T(w_r - \lambda)/N_D^{\text{net}}(w_f)]\right\}^{1/2}} - \frac{1}{\left\{1 + f_N[N_T(w_r - \lambda)/N_D^{\text{net}}(w_f)]\right\}^{1/2}},
\]

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

\[
f_N = \frac{\left(1 - \frac{\lambda}{w_f}\right)^2}{\left(1 - \frac{\lambda}{w_r} - \Delta \lambda\right)^2}.
\]

If \(f_N N_T \ll N_D^{\text{net}}\), which is often true, then

\[
\frac{\Delta C}{C} = -\frac{f_N N_T(w_r - \lambda)}{2 N_D^{\text{net}}(w_r)}.
\]

After the pulse, the \(f_N N_T\) traps will begin to lose their electrons at a rate \(\exp(-e_{ni}t)\), 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 $\phi_b - V_s = 1.3$ V on the surface.

\[ e_n = 2 \times 10^{20} (g_0 / g_1) \sigma_n e^{-e / kT} = e^{-\left[(E_f - E_C)/e + \alpha N_T\right] / kT}. \]  

(6)

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

\[ S = Af\lambda N_T (e^{-\alpha t_1} - e^{-\alpha t_2}), \]  

(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 $\Delta = w_r - w_f$, we can write

\[ f\lambda = \frac{1}{V_{bi} - V_f} \left[ (V_f - V_r) - 2 \sqrt{(E_f - E_C)/e} (\sqrt{V_{bi} - V_f}) \right], \]  

(8)

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

\[ f\lambda = \frac{\Delta}{V_{bi} - V_f} - 2 \left( \frac{(E_f - E_C)/e}{V_{bi} - V_f} \right)^{1/2} \left[ 1 - \left( 1 - \frac{\Delta}{V_{bi} - V_f} \right)^{1/2} \right]. \]  

(9)

First note that

\[ \frac{df\lambda}{dV_f} = \frac{df\lambda}{d\Delta} = \frac{1}{V_{bi} - V_f} \left[ 1 - \left( \frac{(E_f - E_C)/e}{V_{bi} - V_f} \right)^{1/2} \right] \times \frac{1}{\left( 1 - \frac{\Delta}{V_{bi} - V_f} \right)^{1/2}}, \]  

(10)

or

\[ f_{\lambda 0} = \frac{df\lambda}{dV_f} \Bigg|_{V_f - V_r} = \frac{df\lambda}{d\Delta} \Bigg|_{\Delta = 0} = \frac{1}{V_{bi} - V_f} \left[ 1 - \left( \frac{(E_f - E_C)/e}{V_{bi} - V_f} \right)^{1/2} \right]. \]  

(11)

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

\[ f_{\lambda \text{max}} = \frac{1}{V_{bi} - V_f} \left[ 1 - \left( \frac{(E_f - E_C)/e}{V_{bi} - V_f} \right)^{1/2} \right]. \]  

(12)

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

\[ N_T = \frac{S_{\text{max}}(V_{bi} - V_f)}{S_{\text{max}}} \left( 1 - \frac{S_{\text{max}}(V_{bi} - V_f) / S_{\text{max}}}{N_D} \right)^2, \]  

(13)

where $S_{\text{max}} = N_T f_{\lambda 0}$ [Eq. (11)] and we have assumed that $S$ is always measured at the peak of the $S$ vs $T$ spectrum, i.e., at

\[ A(\exp(-e / T) - \exp(-e / T)) = 1, \]  

the usual case in DLTS. We can also derive

\[ E_f - E_C = e(V_{bi} - V_f) \left( 1 - \frac{S_{\text{max}}}{S_{\text{max}}(V_{bi} - V_f)} \right)^2 \left( 1 + \frac{S_{\text{max}}}{N_D} \right), \]  

(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, $E_f$ 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., $E_T + E_C$. Further note that it is not necessary to have a precise value of $V_{bi}$ (typically about 1 V for GaAs) since $V_f$ can be made much larger (4 or 5 V). Finally, if $\Delta - V_f - V_s \ll V_m - V_f$, $S$ vs $V_f$ (or $\Delta$) will be linear over a large range, and $S_{\text{max}}$ will be easy to measure accurately. Near the maximum in $S$ vs $V_f$ (occurring at $V_f = \phi_b - E_C/e$), $S$ is varying slowly so that $S_{\text{max}}$ can also be determined with good precision; thus, the determination of $N_T$ [Eq. (13)] is very robust at large $V_f$.

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 obey
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 \( \tau = (2e_n)^{-1} = 10 \text{ ms} \). 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 \( z = w \). For example, simulations show that \( n \) increases an order of magnitude, i.e., from \( 6 \times 10^9 \) to \( 6 \times 10^{10} \text{ cm}^{-3} \) in only about 100 Å, a fraction of the Debye length (-290 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 \( z = w - \lambda \)) except for perhaps those in the first 100 Å beyond this point. Let the thickness of the "poor" trap filling region be designated by \( S \). Then, in Eq. (4), we should set \( \Delta \lambda = w_f - w - \delta \), and carry this change through the subsequent steps in the derivation. However, clearly the analysis is affected only for small \( \Delta \) (or \( V_f \) near \( V_r \)), as estimated by \( \Delta \approx 2(V_{bi} - V_f) \delta w_c \approx 0.2 \text{ V} \) if \( V_f = -4 \text{ V} \). Thus, we would expect the initial part of the \( S \) vs \( V_f \) curve to rise slowly with \( \Delta \), because of trap filling problems, if \( \tau \) 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 \( \tau \) can be used to calculate accurate values of \( \sigma_n \) 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 \( \Delta = 0.5 \text{ to } 4.5 \text{ V} \)), 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, \( E_{CC}=0.099 \text{ eV} \) 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 \( \Delta \) and then saturate at large \( \Delta \); 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 \( \phi_{bi} \) can be determined from \( C \text{ vs } V \) or \( I \text{ vs } V \) plots, such measurements can give spurious results if not carefully performed and interpreted. Thus, we prefer to use the value given by Missous and Rhoderick\(^3\) for Au on (100) GaAs: \( \phi_{bi} = 0.83 \text{ V} \) at 300 K with a temperature coefficient of \( -2.3 \times 10^{-4} \text{ eV/K} \). Therefore, \( \phi_{bi} = 0.81 \text{ V} \) 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:

- \( N_{EL2} = (1.14 \pm 0.02) \times 10^{16} \text{ cm}^{-3} \), \( E_{EL2} = 0.71 \pm 0.06 \text{ eV} \), \( N_{EL6} = (8.0 \pm 0.5) \times 10^{15} \text{ cm}^{-3} \), and \( E_{EL6} = 0.42 \pm 0.09 \text{ eV} \), where the errors are determined from the differences in the values determined from the data sets at \( V_r = -4.0 \text{ and } -1.5 \text{ V} \), 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 \( V_r \) 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 \( \lambda \) 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,
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 \( E_{\text{eff}} = E_T + E_\sigma = 0.75 + 0.075 = 0.825 \) eV, obtained from an Arrhenius plot of the emission data. Duncan and Westphal have obtained a value of \( E_{\text{EL2}} \) (296 K) = 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

\[ \alpha = (0.75 - 0.65) / 296 = 3.4 \times 10^{-4} \text{ eV/K} \]

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

The magnitude of \( E_{\text{EL6}} \) is also quite interesting. The temperature coefficient \( \alpha_{\text{EL6}} \) is not known, but many standard DLTS emission rate analyses have given \( E_{\text{EL2}} + E_\sigma \approx 0.35 \) eV. Zhao and co-workers have measured \( E_\sigma = 0.20 \) eV, which would then give \( E_{\text{EL2}} = 0.15 \) 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. However, our present result, \( E_{\text{EL6}} \) (167 K) = 0.42 ± 0.09 eV, is more consistent with a small value of \( E_\sigma \), 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 \( E_\sigma \) 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 \( N_T / N_{D\text{et}}^0 \ll 1 \),

\[ N_T = \frac{S_0^2 (V_{bi} - V_r)}{(E_T - E_C) / V_{bi}} \left( \frac{V_{bi} - V_r}{V_{bi} - V_T} \right)^{1/2}. \]

[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 \( E_T - E_C = 0.5 \) eV; then, for \( V_r = 4 \) V, \( N_T = 7.09 S_0^2 \). 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 \( S_0^2 \) 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 \( S_0^2 \), 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 \( S_0^2 \) 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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