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Depletion width and capacitance transient formulas for deep traps of high concentration

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We derive expressions for the depletion width and capacitance transient applicable to traps which may be deep and of high concentration. The new results are compared with those obtained from the commonly used formulas, and also from an exact analysis. Experimental deep level transient spectroscopic data for EL2 in GaAs are in good agreement. © *1995 American Institute of Physics.*

It is well known that the accurate determination of concentrations and profiles of deep centers in semiconductors, as measured by deep level transient spectroscopy (DLTS)[1] or other capacitance techniques, must take account of the so-called λ effect,[2,3] which arises from a difference between the free-carrier depletion width w_r and the deep-donor depletion width $w_r-\lambda$. As can be surmised from the band bending illustrated in Fig. 1, the free carriers fall off rapidly to the left of w_r, a distance which is conveniently (but only approximately) measured by capacitance, $C \simeq \epsilon/w_r$. When the reverse-bias voltage V_r (-1.5 V, in the figure) is pulsed to a more forward-bias voltage V_f (-1.0 V) for a time period t_p, the free-electron concentration moves toward the surface to w_f, and fills the empty donor traps N_T^+ in the region between $w_f-\lambda$ and $w_r-\lambda$. Upon returning to the reverse bias V_r, the capacitance will instantaneously decrease by an amount ΔC (compared to the original reverse-bias capacitance C) because of the decrease in positive donor charge (from the trap filling) and the subsequent decrease in negative (free-electron) charge necessary to hold the surface at $\phi_B - V_r$, where ϕ_B is the Schottky barrier potential. Then, as the donor traps in the $\Delta\lambda$ region ($\Delta\lambda = w_r - w_f$) emit their electrons, ΔC will return to zero. If $N_T/N_D \ll 1$, where N_D is the net shallow donor concentration (not shown in Fig. 1), then the simplest and most frequently used analysis[1] gives $\Delta C/C \simeq N_T/2N_D$. The value of N_D can be found from the slope of a C^{-2} vs V_r plot, so that N_T can be calculated from the above formula.

There are several problems with this simple picture:

(1) the relationship $N_T/N_D \ll 1$ may not hold;

(2) even if it does, the λ effect must, in general, be included, i.e., $\Delta C/C \simeq f_\lambda N_T/2N_D$;

(3) the depletion-approximation solution to the Poisson equation, which is assumed in the relationship $C=\epsilon/w_r$ as well as in the use of the usual simple formulas[3] for w_r, λ, and $\Delta\lambda$, may cause substantial errors; and

(4) the forward-bias pulse of length t_p may not be long enough to fill all of the traps in the region $\Delta\lambda$, mainly because at small values of $(V_f - V_r)$ the filling is largely dependent upon the small concentration of free electrons in the Debye tail of the distribution.

The exact, or nearly exact, solution for $\Delta C/C$ is given by[2]

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

where it is assumed that N_T is constant in the region $w_r-\lambda-\Delta\lambda < z \lesssim w_r-\lambda$, and N_D is constant in the region $w_r < z < w_r + \Delta w_r$, where Δw_r is the increase in w_r immediately after the V_f pulse (i.e., at t_{p+}). The quantity f_λ obeys[4]

$$f_\lambda = \frac{2K_{CV}}{w_r^2 N_T} \int_0^\infty z[N_T^+(z,V_r,0_-) - N_T^+(z,V_f,t_{p-})]dz, \tag{2}$$

where $N_T^+(z,V_r,0_-)$ and $N_T^+(z,V_f,t_{p-})$ are determined from solutions of the Poisson equation immediately before the beginning and before the end of the pulse, respectively. The pulse-length dependence of N_T^+ can be found from Eq. (4.2.2) of Ref. 2; however, in the present communication we will be concerned only with the equilibrium case, i.e., $t_p=\infty$. Also, K_{CV} (a capacitance correction) and w_r^2 must in general be expressed in terms of integrals (to be published elsewhere); however, in the depletion approximation, $K_{CV}=1$, and for $N_T/N_D \ll 1$, w_r becomes the well-known expression

$$w_r^2(V) = \frac{2\epsilon(V_{\mathrm{bi}} - V_r - kT/e)}{eN_D}, \tag{3}$$

where $V_{\mathrm{bi}} = \phi_B - E_{C\infty}/e$, the built-in voltage. To a good approximation, $E_{C\infty} = kT[\ln(N_C/N_D) - N_D/N_C\sqrt{8}]$, where N_C is the effective density of states in the conduction band.[2]

To relate Eq. (2) to what has already been published we note that, in the depletion approximation, $N_T^+(z,V_r,0_-) = N_T$ for $0 < z \lesssim w_r - \lambda$, and is zero elsewhere, whereas $N_T^+(z,V_f,t_{p-}) = N_T$ for $0 < z \leqslant w_r - \lambda - \Delta\lambda$ (if $t_p=\infty$), and is zero elsewhere. Thus, Eq. (2) becomes

$$f_\lambda = \frac{2}{w_r^2}\left(\int_0^{w_r-\lambda} z\,dz - \int_0^{w_r-\lambda-\Delta\lambda} z\,dz\right)$$
$$= \left(1-\frac{\lambda}{w_r}\right)^2 - \left(1-\frac{\lambda}{w_r}-\frac{\Delta\lambda}{w_r}\right)^2. \tag{4}$$

Here w_r is given by Eq. (3), $\Delta\lambda = w_r - w_f$, and[2,5]

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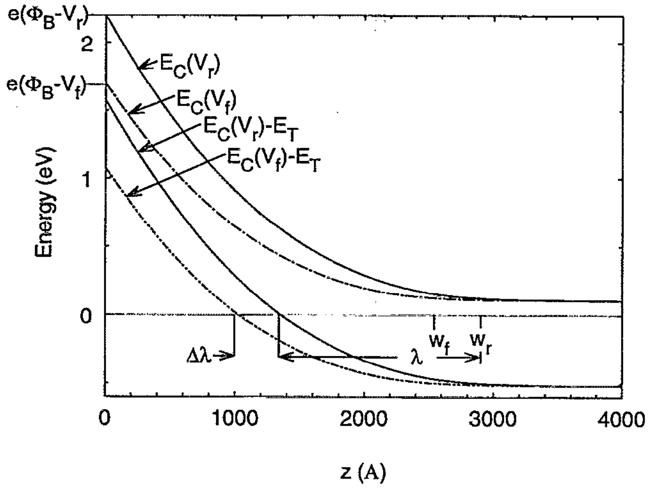

FIG. 1. A Poisson solution of the conduction band edge (E_C) and donor trap level (E_C-E_T) at two different applied voltages ($V_r=-1.5$ V and $V_f=-1.0$ V), for a sample with $N_D=2.8\times10^{16}$ cm^{-3} and $N_{\mathrm{EL2}}=1.2\times10^{16}$ cm^{-3}.

$$\lambda=\left(\frac{2\epsilon(E_T-E_{C\infty}-kT)}{e^2N_D}\right)^{1/2}, \tag{5}$$

where the kT term, due to Debye-tail free carriers, follows from an approximate analysis similar to that used to obtain the kT/e term in Eq. (3). It may be noted that Zhao *et al.* derive a formula for λ [Eq. (17) of Ref. 5] that contains a $2kT$ term, rather than kT. However, we find that our formula gives a slightly more accurate f_λ for the examples considered in this paper. Inserting Eqs. (3) and (5) into Eq. (4) gives the result

$$f_\lambda=\frac{V_f-V_r}{V_{\mathrm{bi}}-V_r-kT/e}-2\beta^{1/2}\left[1-\left(1-\frac{V_f-V_r}{V_{\mathrm{bi}}-V_r-kT/e}\right)^{1/2}\right], \tag{6}$$

where $\beta\equiv(E_T-E_{C\infty}-kT)/e(V_{\mathrm{bi}}-V_r-kT/e)$. Equation (6) corrects f_λ for large values of E_T, but not for large values of N_T. To correct for large N_T/N_D, we must modify the relationships for w_r [Eq. (3)] and $\Delta\lambda$, still of course retaining the depletion approximation. From Poisson's equation we can derive two expressions involving w_r and $\Delta\lambda$:

$$w_r^2-\frac{2\lambda N_T}{N_D+N_T}w_r+\lambda^2\frac{N_T}{N_D+N_T}\times\left(1-\frac{2\epsilon(V_{\mathrm{bi}}-V_r-kT/e)}{e\lambda^2N_T}\right)=0, \tag{7}$$

$$\Delta\lambda^2-2w_r\left[1-\frac{\lambda}{w_r}\frac{N_T}{N_D+N_T}\right]\Delta\lambda+\frac{2\epsilon(V_f-V_r)}{e(N_D+N_T)}=0. \tag{8}$$

By substituting Eq. (5) for λ into Eq. (7) we can solve for w_r:

$$w_r=\frac{(1+\alpha-\alpha\beta)^{1/2}+\alpha\beta^{1/2}}{1+\alpha}\left(\frac{2\epsilon(V_{\mathrm{bi}}-V_r-kT/e)}{eN_D}\right)^{1/2}, \tag{9}$$

where $\alpha=N_T/N_D$. Equation (9), which is equivalent to Eq. (B20) in a work by Pons,[6] is a more accurate version of Eq. (3). Equations (5) and (9) can now be used with Eq. (8) to find $\Delta\lambda$, and finally f_λ [Eq. (4)] becomes

$$f_\lambda=1\Bigg/\left[1+\frac{\alpha\beta^{1/2}}{(1+\alpha-\alpha\beta)^{1/2}}\right]^2\times\left[\frac{1+\alpha}{1+\alpha-\alpha\beta}\frac{V_f-V_r}{V_{\mathrm{bi}}-V_r-kT/e}-2\frac{\beta^{1/2}}{(1+\alpha-\alpha\beta)^{1/2}}\times\left(1-\left(1-\frac{1+\alpha}{1+\alpha-\alpha\beta}\frac{V_f-V_r}{V_{\mathrm{bi}}-V_r-kT/e}\right)^{1/2}\right)\right]. \tag{10}$$

The various levels of approximation for f_λ (or actually f_λ/K_{CV}) are compared with each other and with experiment in Table I. The sample, which was cut from an n-type GaAs wafer grown by the horizontal Bridgman process, contained the deep donor EL2. From Hall-effect and C-V experiments it was determined that $N_D\simeq2.8\times10^{16}$, and, as it turns out, an excellent fit to both the $V_r=-1.5$ V data and the -4.0 V data is found with $N_T=N_{\mathrm{EL2}}=1.2\times10^{16}$ cm^{-3}; thus, $\alpha=0.43$. At $e_n=50$ s^{-1}, the DLTS peak for EL2 occurs at $T=377$ K; here E_T (or E_{EL2}) can be estimated to be 0.624 eV. Since $E_{C\infty}\simeq0.098$ eV, we can calculate $E_{\mathrm{EL2}}-E_{C\infty}-kT\simeq0.493$ eV. Also, $\phi_B\simeq0.9$ V for GaAs,[7] so that $V_{\mathrm{bi}}-V_r-kT/e=4.76$ V at $V_r=-4.0$ V, and 2.26 V at $V_r=-1.5$ V; thus, $\beta=0.103$ and 0.218, respectively. For the data in Table I we have set $V_f=0$ V in the experiment because it is the most commonly used V_f and also because it ensures that $n(z)$ is large enough everywhere to fill all of the

TABLE I. Approximate and exact calculations of f_λ and w_r compared with experiment.

V_r (V)	V_f (V)	α	β	Analysis	f_λ/K_{CV}	K_{CV}	f_λ	w_r (Å)
−1.5	0	0	0	approx.	0.662			3410
		0	0.218	approx.	0.271			3410
		0.430	0.218	approx.	0.245			3235
		0.430	0.218	exact	0.237	1.028	0.244	2885
				expt.			0.248	
−4.0	0	0	0	approx.	0.839			4950
		0	0.103	approx.	0.454			4950
		0.430	0.103	approx.	0.416			4550
		0.430	0.103	exact	0.412	1.016	0.419	4040
				expt.			0.420	

EL2 centers for the pulse length $t_p = 10$ ms; i.e., it ensures that $N_T^+(z, V_f, t_p-) \simeq 0$. For completeness it should be noted that the maximum value of f_λ in Eq. (10) occurs at $V_f = \phi_B - E_T/e \simeq 0.28$ V, so this is the value that must be used in Eq. (10) if the experimental V_f is larger than 0.28 V (not the case here).

The first thing to note in Table I is that the λ correction is very large for EL2, more than a factor two for $V_r = -4.0$ V, $V_f = 0$ V, and more than a factor three for $V_r = -1.5$ V, $V_f = 0$ V. These are very common experimental conditions. The second thing to note is that the large-E_T (but still small-N_T) analysis of f_λ / K_{CV} [Eq. (6)] corrects for most of the error, in this case, and the large-E_T, large-N_T correction comes very close to the exact (Poisson) result. Of course, it must be remembered that the analytical formulas [Eqs. (6) and (10)] cannot be used unless the forward-bias pulses are long enough (10 ms in this case) to fill all of the traps in the $\Delta\lambda$ region; otherwise, Eq. (2) must be used with a numerical solution of $N_T(z)$. However, using a forward bias $V_f \gtrsim 0$ is usually sufficient to make the free carrier concentration $n(z)$ large enough everywhere to fill all the traps, although possible profile information is then lost. A third observation is that, fortunately, K_{CV} is close to unity for our conditions; future work will examine K_{CV} under more general conditions.

The approximate and exact values of w_r are also presented in Table I. For small N_T, the energy E_T does not matter, of course, because the traps do not provide significant charge compared to that of the shallow donors; thus, as long as $\alpha \simeq 0$, the value of β is inconsequential in the calculation of w_r. When N_T is large, Eq. (9) provides a significant correction toward the exact value of w_r, but still leaves a rather large error (~10%). This situation will be studied further in the future.

In general, the comparison with experiment is excellent. For $V_f = 0$, the exact (Poisson) f_λ's differ from the experimental f_λ's by less than 2% for both $V_r = -1.5$ V and $V_r = -4.0$ V. Furthermore, the approximate f_λ's determined by Eq. (10) differ from the exact f_λ's by less than 1% under our conditions; thus, Eq. (10) can be used with confidence if the filling pulses are long. At some point, however, the approximate theory [Eq. (10)] has to break down. In Table II, we compare the approximate and exact theoretical f_λ's with the experimental f_λ for $V_r = -1.5$ V. As seen in Table II, all three quantities are within 2% of each other for V_f down to −0.75 V. At $V_f = -1.00$ V, agreement is still within 11%, but at $V_f = -1.25$ V the error jumps to 50%. Similar results hold for the $V_r = -4.0$ V case (not shown), for which the error is 22% at $V_f = -3.5$ V, but very low for $V_f > -3.0$ V. Thus, our analysis of the results at $V_f = -1.5$ V and −4.0 V suggests that Eq. (10) begins to fail at low $V_f - V_r$, i.e., $V_f - V_r \lesssim 0.5$ V in the present cases. This is not surprising since the depletion approximation, on which Eq. (10) is based, must fail when $w_f - w_r$ is less than several Debye lengths (L_D's). At $V_r = -1.5$ V and $V_f = -1.0$ V, $w_r \simeq 3413$ Å and $w_f = 3014$ Å, respectively; also, for $N_D = 2.78 \times 10^{16}$ cm^{-3}, $L_D \simeq 289$ Å. Thus, the breakdown of Eq. (10) is clearly predictable, and the analysis of f_λ for small $(V_f - V_r)$, say to get deep profile information, must involve a numerical solution of the Poisson equation.

TABLE II. Comparison of approximate f_λ [Eq. (10)], exact f_λ [Eq. (2)], and experimental f_λ over a range of forward bias voltages V_f. The reverse bias is −1.5 V and the pulse length t_p is 10 ms. The approximate solution assumes $t_p = \infty$.

V_f (V)	Approx.	Exact	Experiment
−1.25	0.050	0.030	0.040
−1.00	0.098	0.088	0.094
−0.75	0.142	0.139	0.139
−0.50	0.182	0.182	0.184
−0.25	0.218	0.222	0.222
0.00	0.245	0.244	0.248
0.25	0.258	0.259	0.256

In summary, we have presented an exact formalism to calculate $\Delta C/C$, and derived an analytical approximation for cases in which the depletion approximation is valid and $t_p \to \infty$. Agreement between the analytical approximation, the exact theory, and experiment is excellent for the case of EL2 in GaAs, as long as the quantity $(V_f - V_r)$ is not too small. Future work will concentrate on fully numerical simulations at small t_p in order to get capture cross section information.

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