

Accurate determination of the free carrier capture kinetics of deep traps by space-charge methods

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A detailed analysis of the pulsed bias techniques used to determine the capture kinetics of free carriers by deep traps in Schottky diodes or asymmetric bipolar junctions is presented. Both exact simulations, involving an exact integration of Poisson's equation and a self-consistent treatment in the case of large deep trap concentrations and simple analytical approximations are given. The usual depletion approximation for the distribution of free carriers in the Debye tail is demonstrated to yield erroneous results in some occasions and it is shown how to deal simply with the exact distribution. A novel experimental technique is proposed to rigorously extract the exponential capture kinetics in the neutral semiconductor, from the total capture kinetics, getting rid of the capture in the Debye tail; it is also shown how it is possible to obtain a correct estimation of the capture rate from the capture in the Debye tail, when the direct determination by the above mentioned method is impossible.

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I. INTRODUCTION

One of the most delicate experimental problems encountered in the study of deep traps in semiconductors is perhaps the accurate and rigorous determination of their kinetics for capturing free carriers. The more direct method is the "pulsed-bias" technique used for instance by Henry *et al.*¹ to measure the cross sections for capture of free carriers on the two energy levels of the substitutional oxygen in GaP. The technique consists of measuring the change ΔC of the capacitance of a reverse biased Schottky diode after the application of an electrical pulse of duration t_p . This pulse serves the purpose of shrinking the space-charge region of the diode and of refilling the deep trap in the neutralized semiconductor. If ΔC is entirely due to the refilling of this deep trap, one expects to obtain a functional dependence (corresponding to "purely exponential" refilling kinetics):

$$\Delta C(t_p) = \Delta C_{\max} [1 - \exp(-t_p/\tau_c)], \quad (1)$$

where τ_c is the capture time constant of the deep trap and ΔC_{\max} is the maximum change of the capacitance due to complete refilling.

In fact, it is usually observed that Eq. (1) only poorly fits the experimental data, and particularly that the saturation is only obtained after refilling pulses of duration several orders of magnitude longer than τ_c .

It is well known now that one reason for these apparent "nonexponential" capture kinetics is due to the refilling in the potential barrier remaining during the pulse. Zylbersztejn² showed that the kinetics could be described as the sum of a "fast part" ("exponential" part of the kinetics) and of a "slow part" ("nonexponential" part of the kinetics). The "fast part" is the contribution to the total kinetics of the capture in the neutral semiconductor with an homogeneous capture rate $c_n n$ where n is the density of free carriers (assumed to be equal to the dopant concentration N_D) and where the capture coefficient c_n is usually related to the capture cross section σ_n of the deep trap by the relationship

$$c_n = \sigma_n \bar{v}_n, \quad (2)$$

where \bar{v}_n is the mean thermal velocity.

The "slow part" corresponds to the capture in the remaining potential barrier during the pulse. There exists a distribution of capture rates $c_n n(x)$, since the density of free carriers $n(x)$ varies strongly in the space-charge region from N_D near the edge to zero some Debye lengths inside. This distribution of free carriers near the edge of the space-charge region is often called "Debye tail"; the "slow part" of the capture kinetics will be therefore called "capture in the Debye tail" in the following of this paper.

Usually one attempts to minimize the contribution of the refilling in the Debye tail by applying a forward bias as a refilling pulse and a large reverse bias after the pulse. However, one is left with a "slow part" of a least one tenth of the total kinetics and the exponential part is usually obtained by a delicate and more or less unjustified subtraction of a base line.

In addition, it must be recognized that the refilling of the deep trap in the neutral semiconductor itself can give rise to nonmonoexponential capture kinetics. For instance, Rees *et al.*³ showed that if capture by the deep trap occurs through one or more excited states, this implies as a general rule capture kinetics with a distribution of capture rates.

Therefore, in order to distinguish between these possible nonexponential kinetics due to the microscopic mechanism itself for the capture and the inevitable nonexponential kinetics due to the capture in the Debye tail, one should be able to eliminate the contribution of the capture in the Debye tail and extract the contribution of the capture in the neutral semiconductor from the total kinetics. It is the purpose of this paper to propose a general method to perform rigorously this extraction. This will proceed from a complete analysis of the refilling kinetics in a Schottky diode. It is well recognized now that one can take advantage of the slowing down of the capture rates in the potential barrier to manage the deter-

mination of the refilling kinetics in a more tractable time scale: the drawback being of course that one no longer deals with a well defined time constant but with a large distribution from which it is far more delicate and necessarily less accurate to extract the relevant parameters of the deep traps. Methods have been however proposed by Grimmeiss *et al.*⁴ and by the present author.⁵ Refilling in the Debye tail has been the matter of numerous publications. See for instance Noras,⁶ Noras and Szawelska,⁷ and Meijer *et al.*⁸ The more complete work is certainly that of Borsuk and Swanson⁹ who calculated the refilling kinetics for transient current experiments; their results can be easily modified to deal with capacitance experiments. In most of these papers, a partial modelization can be found. However, it is the opinion of the author that a complete model, treating the capture kinetics as a whole, both in the neutral semiconductor and in the Debye tail, and examining in detail the validity of certain approximations, such as the replacement of the distribution of filled traps by step functions, has not yet been given, and it is the scope of this paper to propose it.

One approximation which is often made (and in particular in Refs. 5–8) is the so-called depletion approximation for the distribution of free carriers in the space-charge region. However, since we are concerned here by the refilling of traps in the very close vicinity of the edge of the space-charge region, where this approximation obviously fails, its use is likely to give erroneous results. This has been also realized by Borsuk and Swanson.⁹

The organization of this paper will be the following: In Sec. II the basic equations for the calculation of the refilling kinetics will be recalled, but in a more rigorous manner than is usually done, since we will not make use of the depletion approximation. In Sec. III, we treat the simplest case, where the deep trap concentration can be assumed negligible with respect to the dopant concentration. As a result of this study, we will propose a novel experimental method which allows the refilling kinetics in the neutral semiconductor to be rigorously extracted from the total kinetics. We give also a detailed analysis of the method proposed previously by the author⁵ to deduce the bulk capture time constant from the refilling in the Debye tail. The importance of using the exact distribution of free carriers rather than the usual depletion approximation is illustrated at this occasion. In Sec. IV we study the more complicated case of large deep trap concentrations. In this case the exact calculations demand a self-consistent treatment with respect to the electrical potential. This has been performed and compared to simple approximations. The paper is ended by a short conclusion in Sec. V.

II. HYPOTHESIS OF THE MODEL AND STARTING EQUATIONS

The basic hypothesis of our analysis is that the distribution of majority free carriers (assumed to be electrons in the following) of the reverse biased Schottky diode is completely determined by the position of a quasi-Fermi level which will be assumed to be constant throughout all the space-charge region and equal to the bulk Fermi level. It will be considered that this steady state distribution of free electrons establishes itself after a change in the depth of the space-charge

region, instantaneously as compared to the time scale of the deep trap capture time constants τ_c . A justification for this can be found if we compare the dielectric Debye time constant τ_D with τ_c . The ratio

$$\tau_D/\tau_c = \epsilon \sigma_n \bar{v}_n / q \mu_n \quad (3)$$

is independent of the free electrons concentration. In Eq. (3), ϵ is the dielectric constant of the semiconductor, μ_n the electron mobility, and q the (positive) elementary charge. For a crystalline semiconductor with a high electronic mobility such as GaAs, this ratio is usually much less than one, even for very large capture cross sections. However, for poorly conductive materials, the ratio can approach or even be larger than one, so that it will be difficult in this case to unravel the capture kinetics of the trap and the dielectric response of the semiconductor.

Let us now consider a Schottky diode fabricated on a n -type semiconductor containing a completely ionized shallow donor with a concentration $N_D(x)$ and a deep trap with a concentration $N_T(x)$. The electronic mobility of the semiconductor will be assumed high enough so that the ratio τ_D/τ_c is much less than one. With these hypothesis and if, in addition, the semiconductor is not degenerate, the free electron concentration is given by

$$n(x,t) = N_D(l) \exp[qV(x,t)/kT], \quad (4)$$

where $V(x,t)$ is the electric potential, the origin of which is put at $x = l$, a point deep into the bulk of the semiconductor where the electric field can be assumed zero and where electrical neutrality prevails during the whole experiment.

If the deep trap is donorlike, the total density of charge is equal to

$$qN(x,t) = q\{N_D(x) - n(x,t) + N_T(x)[1 - f(x,t)]\}, \quad (5)$$

where $f(x,t)$ is the fraction of occupied deep traps. In these equations t is the time and x is a space coordinate in the semiconductor ($x = 0$ denotes the metal-semiconductor interface).

The same analysis is equally valid for acceptorlike deep traps; this case is indeed completely identical to the case of donorlike traps providing that one replaces N_D by the concentration of free electrons in the neutral material, which is equal to $N_D - N_T$ if the deep acceptor concentration N_T is less than N_D . It is noteworthy that, contrary to the case of a donorlike trap whose concentration can be considered arbitrarily large with respect to the shallow donor concentration, one should restrict the analysis to concentrations of acceptorlike deep traps significantly less than that of the shallow donors. Otherwise the neutral material is compensated and the concentration of free electrons is very weak and must be deduced from the resolution of a charge neutrality equation, with a Fermi level in the vicinity of the deep trap energy level. Consequently the Debye length and the resistivity are very large, rendering such a material usually unsuitable for the transient capacitance experiments such that concerned by the present study. However our calculations, and especially that developed in Sec. IV, remain formally valid, except that it is not obvious, first that one may still define a constant quasi-Fermi level in the space-charge region since diffusion lengths can be shorter than the width

of the space-charge region, and second that the dielectric time constant is shorter than the capture time constants [Eq. (3) is only valid for uncompensated materials]. In the following of the paper we will develop the calculations for a donorlike deep trap. They can be safely extended to the case of an acceptorlike deep trap (simply replace N_D by $N_D - N_T$ in the whole paper), but subject to the restrictive condition that $N_T < N_D$; some final results will be given for both donor and acceptorlike traps, with the above restrictive condition. We will no longer discuss the case of very large concentrations of deep acceptors, that is the case of compensated materials. For simplicity we will assume that the deep trap acts only as an electron trap so that its emission rate (e_n) for electrons is much larger than for holes; also we will not consider the case of minority carrier injection and the density of free holes will be neglected everywhere in the semiconductor, and in particular near the interface. In these conditions the fraction of occupied deep traps is given by the detailed balance equation

$$\frac{df}{dt} = c_n n(x,t) [1 - f(x,t)] - e_n f(x,t). \quad (6)$$

With these hypothesis, the instantaneous free and trapped electron concentrations are obtained by solving Poisson's equation for the electric potential $V(x,t)$:

$$\frac{\partial^2 V(x,t)}{\partial x^2} = -\frac{q}{\epsilon} N(x,t). \quad (7)$$

A double integration of this equation yields

$$V(0,t) = -\frac{q}{\epsilon} \int_0^l x N(x,t) dx, \quad (8)$$

where $V(0,t)$ is the electric potential at the interface, equal to the sum of the externally applied reverse gate bias and of the constant built-in potential V_b . Since the reverse gate bias is kept constant during the refilling pulse [$V(0,t) = V_v$] or after it [$V(0,t) = V_v$], the time derivative of Eq. (8) gives

$$\frac{d}{dt} \left[\int_0^l x n(x,t) dx \right] = - \int_0^l x N_T(x) \frac{df(x,t)}{dt} dx. \quad (9)$$

The left-hand side of this equation is directly related to the rate of change of the depth $W(t)$ of the space-charge region. In the simplest model where $n(x)$ is assumed zero inside the space-charge region (that is $x < W$) and $N_D(x)$ outside ($x > W$), we obtain

$$\frac{d}{dt} \left[\int_0^l x n(x,t) dx \right] = - W N_D(W) \frac{dW}{dt}. \quad (10)$$

A rigorous calculation of this term can be done, accounting for the exact distribution of free carriers, if N_D can be assumed constant over several Debye lengths around W . It is shown in the appendix that the density of free electrons $n(x)$ is implicitly given by the equation

$$\frac{W-x}{L_D \sqrt{2}} = \Psi[v(x)] = - \int_{v(W)}^{v(x)} \frac{dv}{2v(v-1-\ln v)^{1/2}}, \quad (11)$$

where the reduced free electron concentration $v(x)$ is equal to $n(x)/N_D(W)$, and where the Debye length L_D is equal to

$$L_D = [\epsilon k T / q^2 N_D(W)]^{1/2} \quad (12)$$

(in the case of an acceptorlike deep trap, N_D must be re-

placed by $N_D - N_T$ in the expression of L_D , which therefore depends on N_T), where T is the temperature and k the Boltzmann constant.

Since we do not use the usual depletion approximation, the depth W of the space-charge region must be rigorously defined. It is shown in the appendix that a correct definition for W is

$$W = \epsilon / C, \quad (13)$$

where C is the high frequency capacitance per unit area of the Schottky diode.

From Eq. (11), straightforward algebra yields

$$\frac{d}{dt} \left[\int_0^l x n(x,t) dx \right] = - N_D \frac{dW}{dt} \left[W - L_D \sqrt{2} \int_0^1 \Psi(v) dv \right]. \quad (14)$$

However, it is also shown in the Appendix that the definition (13) of the depth of the space-charge region implies that

$$\int_0^1 \Psi(v) dv \equiv 0, \quad (15)$$

so that

$$\frac{d}{dt} \left[\int_0^l x n(x,t) dx \right] = - W N_D(W) \frac{dW}{dt}, \quad (16)$$

which reduces exactly to Eq. (10).

With the help of Eq. (16) an integration of Eq. (9) yields

$$\int_{W_0}^{W(t)} W N_D(W) dW = \int_0^l N_T(x) \Delta f(x,t) x dx, \quad (17)$$

with

$$\Delta f(x,t) = f(x,t) - f_0(x), \quad (18)$$

where $f_0(x)$ and W_0 are, respectively, the steady state fraction of occupied deep traps and depth of the space-charge region. With the definition (13) of W , we obtain

$$\begin{aligned} \int_{W_0}^{W(t)} W N_D(W) dW &= \frac{1}{2} \bar{N}_D(W_0) [W^2(t) + W_0^2] \\ &= \frac{1}{2} \bar{N}_D(W_0) W^2 \left(\frac{C_0^2}{C^2(t)} - 1 \right), \end{aligned} \quad (19)$$

where C_0 is the steady state capacitance per unit area of the diode and where $\bar{N}_D(W_0)$ is an average of the dopant concentration, identical with $N_D(W_0)$ if the concentration of the dopant is uniform in the semiconductor, or if the integral in the right-hand side of Eq. (17) is small (that is, if the deep trap concentration is negligible with respect to the dopant concentration).

Also in this case

$$\frac{1}{2} \left(\frac{C_0^2}{C^2(t)} - 1 \right) \simeq - \frac{C(t) - C_0}{C_0} = - \frac{\Delta C(t)}{C_0}. \quad (20)$$

We obtain therefore the relationship between the instantaneous high frequency capacitance of the diode and the distribution of occupied deep traps:

$$\frac{1}{2} \left(\frac{C_0^2}{C^2(t)} - 1 \right) = \frac{1}{\bar{N}_D(W_0)} \int_0^l N_T(x) \Delta f(x,t) \frac{x dx}{W_0^2}. \quad (21)$$

III. THE CASE OF NEGLIGIBLE DEEP TRAP CONCENTRATIONS

In this part of the paper we will assume that the concentration of the deep trap is negligible with respect to the dopant concentration and consequently it is not necessary in this section to precise the donor or acceptor character of the trap.

A. Calculation of the instantaneous distribution of occupied deep traps

We are now going to determine $\Delta f(x, t)$ in the following conditions. Let V_0 and V_1 be the electrical potential at the interface (equal to the sum of the externally applied bias on the gate with the constant built-in potential) respectively after (or before) and during the refilling pulse of amplitude $\Delta V = |V_0 - V_1|$, of duration t_p and applied at $t = 0$ (see Fig. 1). The amplitudes of the transients are now currently determined by differential techniques such as DLTS, which demands that the refilling pulses be repeated with a period t_f which has to be accounted for, since in these conditions, a steady state is not necessarily reached just before the application of the refilling pulse. In the case of a one shot refilling experiment, t_f will be made to go to infinity. If the deep trap concentration is negligible with respect to the dopant concentration, changes in the depth of the space-charge region at constant bias are negligible, so that the free electron concentrations can be replaced by their equilibrium values $n_0(x)$ and $n_1(x)$ for, respectively, $V(0, t) = V_0$ and V_1 . Let $f_0(x)$ and $f_1(x)$ be also the corresponding steady-state distributions of trapped electrons, equal to the Fermi-Dirac probability of occupation of the deep trap, assuming a constant quasi-Fermi level in the space-charge region.

The instantaneous distribution $f(x, t)$ is given by an integration of the detailed balance equation [Eq. (6)], which gives the two coupled relations:

$$f(x, t_p) - f_1(x) = [f(x, 0) - f_1(x)] \exp(-e_n t_p) \times \exp[-c_n n_1(x) t_p] \quad (22)$$

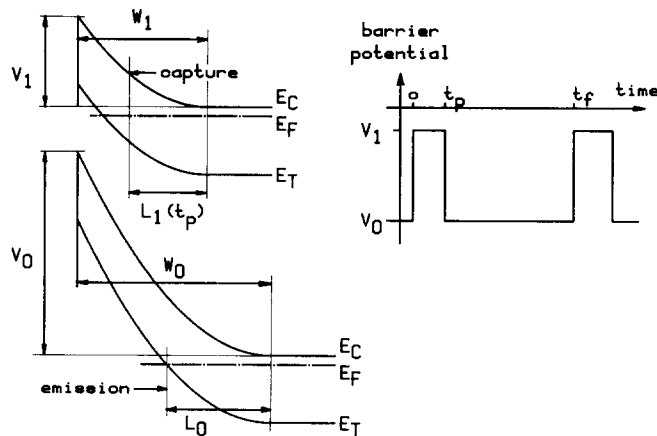


FIG. 1. Schematics of a Schottky barrier under barrier potential V_1 during the refilling pulse and under barrier potential V_0 after the refilling pulse. For clarity the top of the valence band has not been represented. The right hand side of the figure shows the sequence of barrier potentials (equal to the sum of a constant built-in potential and of the applied reverse bias) used in the trap filling experiments considered in this paper.

and

$$f(x, t) - f_0(x) = [f(x, t_p) - f_0(x)] \exp[-e_n(t - t_p)] \times \exp[-c_n n_0(x)(t - t_p)] \quad (23)$$

for $t > t_p$.

At a regulated temperature, or if the heating rate in the DLTS experiment is low enough, a constant regime can be assumed to be established so that

$$f(x, 0) = f(x, t_f); \quad (24)$$

with this last condition, the instantaneous distribution of occupied deep traps can be obtained from the two coupled Eqs. (22) and (23):

$$\Delta f(x, t) = f(x, t) - f_0(x) = [f_1(x) - f_0(x)] \frac{1 - A_1(x, t_p)}{1 - A_1(x, t_p)A_0(x, t_f)} A_0(x, t), \quad (25)$$

with

$$A_1(x, t_p) = \exp\{-[e_n + c_n n_1(x)]t_p\} \quad (26)$$

and

$$A_0(x, t) = \exp\{-[e_n + c_n n_0(x)](t - t_p)\}. \quad (27)$$

The amplitude of the transient after the refilling pulse is obtained by calculating the integral in Eq. (21) with $\Delta f(x, t)$ evaluated for $t = t_p$:

$$\Delta f(x, t_p) = [f_1(x) - f_0(x)] \frac{1 - A_1(x, t_p)}{1 - A_1(x, t_p)A_0(x, t_f)}. \quad (28)$$

B. Analytical approximations

In this section and in the two next sections, we will assume that the concentrations of the shallow dopant impurity and of the deep trap are both uniform, respectively equal to N_D and N_T . Using Eq. (28), the distribution of occupied deep traps can be calculated at every point of the space-charge region. The numerical results for a typical case are shown in Fig. 2 as a function of the pulse duration t_p . Roughly speaking, refilling of the traps occurs in two successive stages. The deep traps in the neutralized semiconductor ($x > W_1$) are first rapidly refilled with the well-defined bulk capture time constant τ_c ; secondly the refilling occurs further into the space-charge region [up to $W_1 - L_1(t_p)$] for longer pulse durations, on a typical logarithmic scale in time. It can be seen that an excellent approximation will be to replace $\Delta f(x, t_p)$ with a rectangular function $\tilde{\Delta f}(x, t_p)$, with a zero value outside a region defined by $x = W_1 - L_1(t_p)$ and $x = W_0 - L_0$. $W_0 - L_0$ is the point where $f_0(W_0 - L_0) = 1/2$, i.e.,

$$e_n = c_n n_0(W_0 - L_0). \quad (29)$$

Therefore, if we ignore the degeneracy factor g_n of the energy level of the deep trap in the detailed balance relation:

$$e_n = g_n c_n n_0(x) \exp\left(-\frac{E_F - E_T}{kT}\right). \quad (30)$$

$W_0 - L_0$ is the point where the quasi-Fermi level E_F coincides with the energy level of the trap E_T (see Fig. 1). Assuming a uniform dopant concentration N_D and that the trap is deep enough so that L_0 is much larger than L_D , it follows from Eq. (29) that¹⁰ (see Appendix A)

$$L_0 = L_D \sqrt{2} \left(\frac{E_F - E_T}{kT} - 1 \right)^{1/2} \\ = L_D \sqrt{2} \left[\ln \left(\frac{\tau_e}{\tau_c} \right) - 1 \right]^{1/2}. \quad (31)$$

$W_1 - L_1(t_p)$ is a point which depends on the pulse duration t_p . Inspection of Fig. 2 shows that $L_1(t_p)$ is zero for pulse durations less than the capture time constant in the neutral region $\tau_c = (c_n N_D)^{-1}$, and that $L_1(t_p)$ tends towards L_0 for t_p longer than the emission time constant $\tau_e = e_n^{-1}$. To replace $\Delta f(x, t_p)$ with the rectangular function $\Delta f(x, t_p)$ is equivalent to saying that the traps are refilled up to $W_1 - L_1(t_p)$ at the end of the pulse.

To conveniently use this approximation for $\Delta f(x, t_p)$, two quantities have to be obtained, the amplitude $R(t_p)$ of the rectangular function and $L_1(t_p)$. The amplitude is easily obtained, if we consider that, for x between W_1 and $W_0 - L_0$, we can write $f_1(x) = 1$ and $f_0(x) = 0$ and

$$A_1(x, t_p) = \exp[-(e_n + c_n N_D)t_p] = \alpha_p, \quad (32)$$

$$A_0(x, t_p) = \exp[-e_n(t_f - t_p)] = \alpha_f. \quad (33)$$

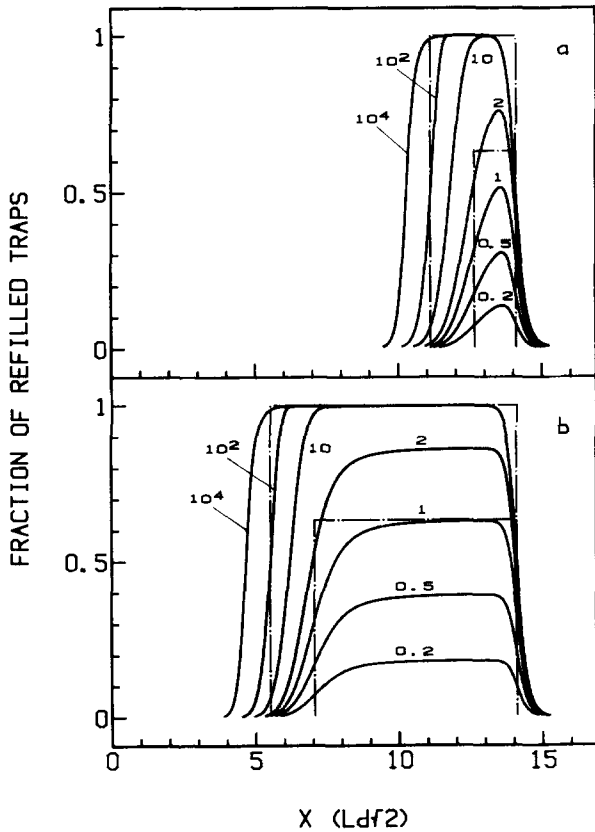


FIG. 2. Fraction of refilled traps $\Delta f(x, t_p)$ as a function of the distance from the metal-semiconductor interface (in units of $L_D/2$) after refilling pulses of different durations t_p indicated in units of τ_c in the figure. The typical case considered here is $V_0 = -5$ V, $T = 200$ K, $N_D = 1 \times 10^{15}$ cm $^{-3}$, $\tau_e = 10^{-2}$ s, $\tau_c = 10^{-6}$ s, and a negligible concentration of the trap. These time constants correspond to a trap with an energy level approximately 0.25 eV below the conduction band in GaAs. Calculations gives $W_0 \approx 17.0$ and $L_0 = 2.87$ in units of $L_D/2$. Case a corresponds to refilling pulses of amplitude $\Delta V = 2$ V and case b to $\Delta V = 4$ V. In case a, $W_1 = 13.16$ and in case b, $W_1 = 7.55$. The solid lines are exact numerical calculations of $\Delta f(x, t_p)$, while the dashed lines are the rectangular functions used as approximations for $\Delta f(x, t_p)$ for $t_p \approx \tau_c$ and $t_p = 10^2 \times \tau_c$.

Hence the amplitude of the rectangular function is

$$R(t_p) = \frac{1 - \alpha_p}{1 - \alpha_p \alpha_f}. \quad (34)$$

$L_1(t_p)$ is obtained by looking for the point where

$$\Delta f[W_1 - L_1(t_p), t_p] = \frac{1}{2} R(t_p). \quad (35)$$

At this point, the approximations $f_0[W_1 - L_1(t_p)] = 0$ and $A_0[W_1 - L_1(t_p), t_p] = \alpha_f$ are still valid. Therefore, from Eq. (28) we deduce the transcendental equation to be solved:

$$A_1[W_1 - L_1(t_p), t_p] \\ = \frac{f_1[W_1 - L_1(t_p)] - R(t_p)/2}{f_1[W_1 - L_1(t_p)] - \alpha_f R(t_p)/2}. \quad (36)$$

This equation can be solved by successive iterations with the starting value $f_1[W_1 - L_1(t_p)] = 1$ in the right-hand side. After the first iteration we find

$$\frac{n_1[W_1 - L_1(t_p)]}{N_D} = \frac{\tau_c}{\beta(t_p) t_p}, \quad (37)$$

with

$$\beta(t_p) = 1/\ln \left(\frac{1 - \alpha_f R(t_p)/2}{1 - R(t_p)/2} \right), \quad (38)$$

which allows us to calculate $L_1(t_p)$ from the known distribution of free carriers:

$$L_1(t_p) = L_D \sqrt{2} \Psi \left(\frac{\tau_c}{t_p \beta(t_p)} \right). \quad (39)$$

This value gives for $f_1[W_1 - L_1(t_p)]$ a value very close to the starting value if t_p is short with respect to the emission time constant $\tau_e = e_n^{-1}$, therefore one iteration is enough in this case; otherwise more iterations are needed.¹¹ Of course, if t_p is of the order of magnitude, or larger than τ_e , then $L_1(t_p)$ tends towards L_0 . In the intermediate case $\tau_c \ll t_p \ll \tau_e$, the use of the asymptotic approximation for $\Psi(\nu)$ is allowed, which yields

$$L_1(t_p) \approx L_D \sqrt{2} [\ln(\beta_0 t_p / \tau_c) - 1]^{1/2}, \quad (40)$$

where β_0 is a constant

$$\beta_0 = 1/\ln(2 - \alpha_f). \quad (41)$$

With the approximation of the rectangular function for $\Delta f(x, t_p)$, it is now straightforward to derive an analytical approximation for the maximum amplitude $\Delta C(t_p)$ of the transient capacitance after the refilling pulse:

$$\frac{\Delta C(t_p)}{C_0} = -\frac{N_T}{N_D} F(t_p) \\ \approx -\frac{N_T}{N_D} R(t_p) \int_{W_1 - L_1(t_p)}^{W_1 - L_0} \times \frac{d_x}{W_0^2}. \quad (42)$$

Traps are refilled up to $W_1 - L_1(t_p)$ at the end of the pulse and only those traps lying between $W_1 - L_1(t_p)$ and $W_0 - L_0$ can emit an electron after the pulse. This is only possible if the pulse amplitude is large enough so that $W_0 - L_0 > W_1 - L_1(t_p)$.

This inequality yields an expression of a threshold $\Delta V_{th}(t_p)$ for the refilling pulse amplitude:

$$\frac{\Delta V_{th}(t_p)}{|V_0| - \frac{kT}{q}} = 1 - \left(1 - \frac{L_0}{W_0} + \frac{L_1(t_p)}{W_0}\right)^2. \quad (43)$$

The analytical approximation for $\Delta C(t_p)$ is therefore

$$\begin{aligned} \frac{\Delta C(t_p)}{C_0} &= 0, \quad \text{for } \Delta V < \Delta V_{th}, \\ \frac{\Delta C(t_p)}{C_0} &= \frac{1}{2} \frac{N_T}{N_D} R(t_p) \\ &\times \left[\left(1 - \frac{L_0}{W_0}\right)^2 - \left(\sqrt{1 - \frac{\Delta V}{|V_0| - \frac{kT}{q}}} - \frac{L_1(t_p)}{W_0} \right)^2 \right] \quad (44) \end{aligned}$$

for $\Delta V > \Delta V_{th}$.

We give in Fig. 3 the results for a typical case of the exact calculation [numerical integration of Eq. (21), using Eq. (28) for $\Delta f(x, t_p)$] and of the analytical approximation [Eq. (44)]. Note that the exact analytical calculation predicts also the existence of a marked threshold. One can appreciate the good agreement between the exact calculation and the analytical approximation and particularly the ability of the analytical approximation to give a correct value, first for the

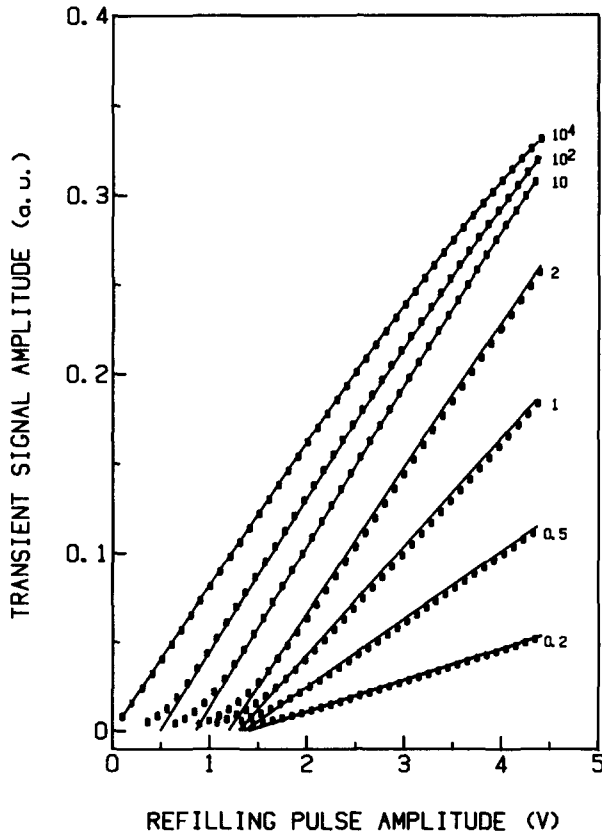


FIG. 3. Plot of $F(t_p)$ as a function of the refilling pulse amplitude ΔV , for different values of the refilling pulse duration t_p , indicated in the figure in units of τ_c . (•) exact numerical calculations. Solid lines: analytical approximation (see text). The same typical case as for Fig. 2 has been considered here.

threshold, and second for the slope of the curves for refilling pulse amplitudes larger than the threshold.

Equation (44) shows that, strictly speaking, $\Delta C(t_p)$ is not linear with the refilling pulse amplitude ΔV , except for short refilling pulses for which $L_1(t_p) \approx 0$. However, the examination of Fig. 3 shows that the dependence is quasilinear on a large range for ΔV , which renders easy the determination of the threshold ΔV_{th} . This threshold diminishes from the maximum value

$$(\Delta V_{th})_{\max} = \left(|V_0| - \frac{kT}{q}\right) \left[1 - \left(1 - \frac{L_0}{W_0}\right)^2\right] \quad (45)$$

for $t_p \lesssim \tau_c$ down to zero for $t_p \gtrsim \tau_c$.

In Fig. 4 we give the refilling kinetics for the same typical case, as a function of the logarithm of the refilling pulse duration for different values of the amplitude of the refilling pulse. Observe that the fast part of the kinetics is completely cancelled for $\Delta V = 1$ V, a value lower than the threshold for $t_p < 5 \tau_c$; in this case the refilling kinetics are entirely constituted by the slow part which goes on up to $t_p \approx \tau_c$.

From a practical point of view it is interesting to know the relative importance of the fast exponential part in the total amplitude of the refilling kinetics as a function of the amplitude ΔV of the refilling pulse. This is given in Fig. 5 where the amplitude of the fast part of the kinetics, expressed as a fraction of the total amplitude, has been plotted as a function of ΔV , expressed as a fraction of the total barrier potential $|V_0|$ for different values of the ratio L_0/W_0 . This can be written as

$$L_0/W_0 = \left(\frac{E_F - E_T - kT}{q|V_0| - kT}\right)^{1/2} \quad (46)$$

and which varies therefore as the depth of the trap. Note once again that the fast exponential part for the refilling kinetics is completely eliminated if the amplitude of the refilling pulse is lower than a threshold value, which can represent an appreciable fraction of the barrier potential, in particular for very deep traps.

C. Experimental determination of the capture kinetics

The dependence of $\Delta C(t_p)$ with the refilling pulse duration t_p can be considered to be composed of two parts: first $R(t_p)$, which describes the refilling in the neutralized semiconductor and which is the desired quantity, and second the term between the brackets in Eq. (44), which depends on t_p only through $L_1(t_p)$. This second term describes the capture in the Debye tail which adds to the fast exponential kinetics $R(t_p)$ a slow contribution, varying typically with the logarithm of t_p . We are going to profit from the quasilinear dependence of $\Delta C(t_p)$ with ΔV to derive a simple method to extract $R(t_p)$ from the total kinetics. Let us consider the derivative of $\Delta C(t_p)$ with respect to ΔV , extrapolated for $\Delta V = \Delta V_{th}$:

$$\begin{aligned} \frac{\partial |\Delta C(t_p)|}{\partial \Delta V} \Big|_{\Delta V_{th}} &= \frac{1}{2} R(t_p) \\ &\times \frac{N_T C_0 (1 - L_0/W_0)}{N_D \left(|V_0| - \frac{kT}{q}\right) \left[1 - \Delta V_{th} / \left(|V_0| - \frac{kT}{q}\right)\right]^{1/2}}. \quad (47) \end{aligned}$$

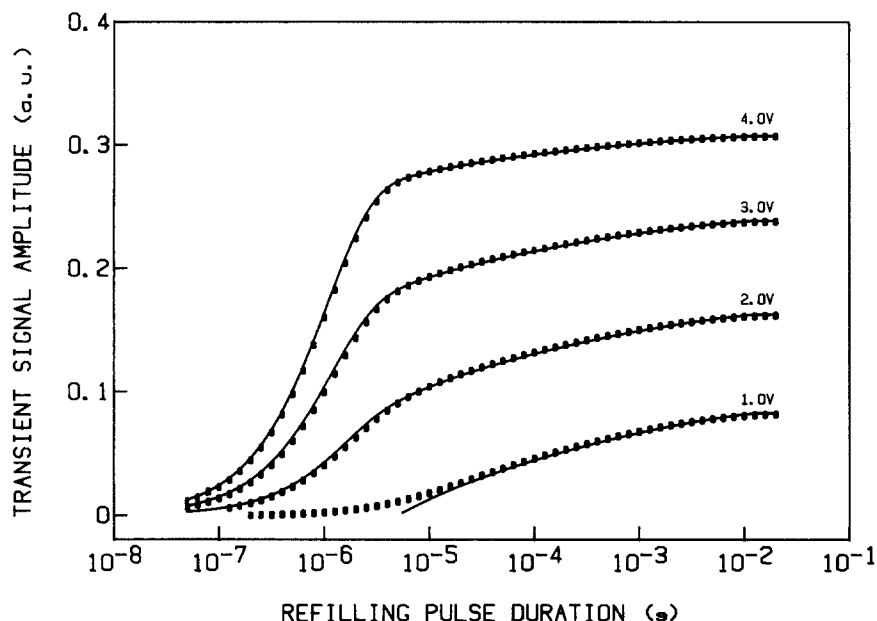


FIG. 4. Plot of $F(t_p)$ as a function of the refilling pulse duration t_p for different values of the refilling pulse amplitude ΔV , indicated in the figure. Same typical case as for Fig. 2. (●) exact numerical calculations. Solid lines: analytical approximation (see text).

Therefore, forming the product $S(t_p)$

$$S(t_p) = \left(1 - \frac{\Delta V_{th}(t_p)}{|V_0| - \frac{kT}{q}}\right)^{1/2} \frac{\partial |\Delta C(t_p)|}{\partial \Delta V} \Big|_{\Delta V_{th}} \\ = \frac{1}{2} R(t_p) \frac{N_T C_0}{N_D \left(|V_0| - \frac{kT}{q}\right)} \left(1 - \frac{L_0}{W_0}\right), \quad (48)$$

eliminates the slow contribution of the capture kinetics in the Debye tail and keeps only the contribution of the capture kinetics into the bulk.

The expression Eq. (39) for $L_1(t_p)$ has been obtained by assuming that the capture in the bulk can be described by exponential kinetics with a well-defined capture time constant τ_c . However, the analytical approximation Eq. (42) is

of the widest generality; all that is in fact needed is that the capture rates vary linearly with the free carrier concentration. The fact that this free carrier concentration changes very rapidly in the space-charge region renders valid the approximation of $\Delta f(x, t_p)$ by a rectangular function and therefore Eq. (42). In turn, this expression for $\Delta C(t_p)/C_0$ implies the apparition of a threshold ΔV_{th} decreasing for increasing refilling pulse durations t_p and a quasilinear dependence of $\Delta C(t_p)$ with respect to ΔV larger than ΔV_{th} , the slope of these curves being proportional to the bulk refilling of the trap $R(t_p)$. Therefore a plot of the experimentally determined product $S(t_p)$ [Eq. (48)] vs t_p will constitute an accurate check of the exponential character of the capture kinetics of the trap, the contribution of the capture kinetics in the Debye tail being completely eliminated.

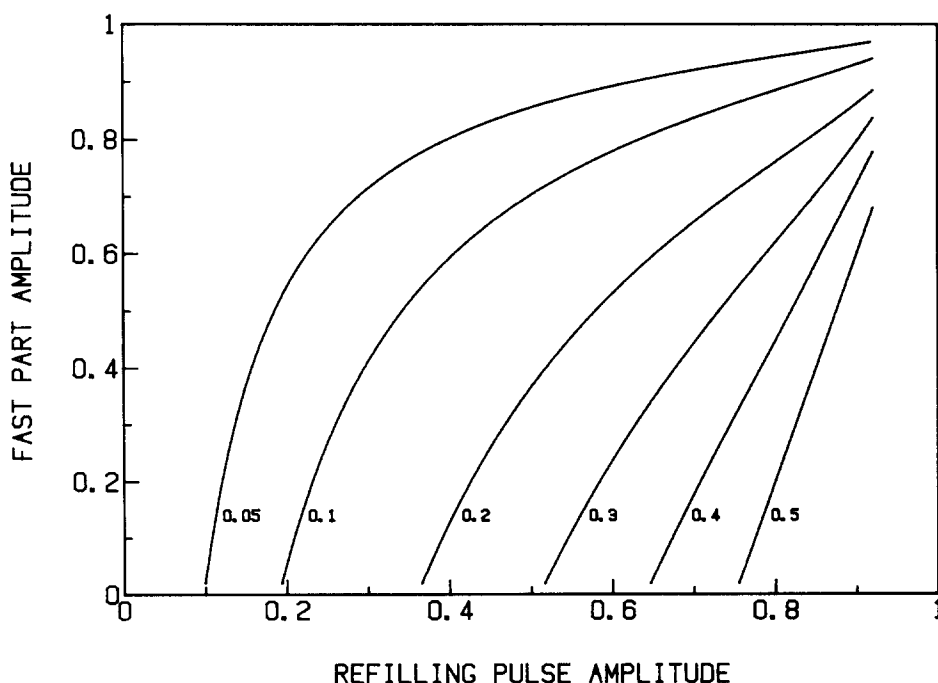


FIG. 5. Total refilling kinetics are equal to the sum of a fast part which corresponds to the refilling in the neutral semiconductor and of a slow part which corresponds to the refilling in the Debye tail. This figure gives the fraction of the fast part with respect to the total refilling kinetics as a function of the ratio of the refilling pulse amplitude by the barrier potential V_0 , for different values of L_0/W_0 , indicated in the figure. $L_0/W_0 = 0.05$ (resp. 0.5) corresponds to a trap depth of approximately 0.1 eV for $V_0 = -5$ V and $T = 200$ K in GaAs (resp. 0.6 eV for $V_0 = -2$ V).

D. Large capture cross sections

In the case of a deep trap with a very large capture cross section, yielding capture time constants too short to be directly measured, it is however possible to get a good evaluation of the capture time constant by studying the capture kinetics in the Debye tail. One possible experimental method (which has been proposed recently by the author⁵) consists of determining the threshold ΔV_{th} as a function of the refilling pulse duration. If the bulk capture kinetics is well described by monoexponential kinetics with a capture time constant τ_c , then a fit of the experimentally determined ΔV_{th} with the theoretical value [from Eqs. (31), (39), (43)] valid for $t_p \ll \tau_e$

$$\frac{\Delta V_{th}(t_p)}{|V_0| - \frac{kT}{q}} = 1 - \left(1 - \frac{[\ln(\tau_e/\tau_c) - 1]^{1/2} - \Psi[\tau_c/t_p \beta(t_p)]}{(q|V_0|/kT - 1)^{1/2}} \right)^2, \quad (49)$$

will determine the only unknown parameter τ_c .

We give in Fig. 6 the curves of ΔV_{th} vs t_p , for a typical case, using the bulk capture time constant τ_c as a parameter. The importance of using the actual distribution of free carriers [Eq. (11)] rather than the usual depletion approximation [Eq. (A1)] is also illustrated in this figure. These examples show that this method allows the capture time constant τ_c to be currently determined within a factor of two; also obvious in this figure is the fact that the shorter the refilling pulses used, the better is the accuracy obtained.

IV. LARGE DEEP TRAP CONCENTRATION

The case of large deep trap concentrations is complicated since refilling or emptying of these traps causes non-negligible changes in the charge density in the space-charge region, which modify the shape of the potential. As a consequence, Eqs. (22) and (23) for instance are no longer valid, since the instantaneous free carrier concentrations $n_0(x, t)$ and $n_1(x, t)$ can no longer be replaced by their equilibrium values $n_0(x)$ and $n_1(x)$. An exact calculation of the refill-

ing kinetics therefore demands a self-consistent treatment. This has been performed in the following way.

We assume the same situation as for Sec. III A, where t_f is taken equal to infinity for simplicity: in this case steady state is assumed to be reached just before the application of the refilling pulse ($t = 0$), and we compute first the shape of the potential $V(x)$ just before the pulse by numerically integrating Poisson's equation¹² [Eq. (7)] where the density of charge $N(x)$ is again given by Eq. (5) but where the fraction of occupied deep traps $f(x)$ is equal to the equilibrium value $f_0(x)$:

$$f(x) = f_0(x) = \frac{c_n n_0(x)}{e_n + c_n n_0(x)}, \quad (50)$$

and which is also a function of the potential $V(x)$ (the shape of the potential can also be analytically deduced in this equilibrium state; see appendix B). Then, we change abruptly the total barrier potential from $V(0, 0_-) = V_0$ to $V(0, 0_+) = V_1$ and we compute again the potential shape by a numerical integration of Poisson's equation by letting the free carrier concentration follow immediately the potential changes [Eq. (4)] but where the fraction of occupied traps is taken as quenched to its initial value $f(x, 0_+) = f_0(x)$.

The evolution of the fraction of occupied deep traps $f(x, t)$ is then iteratively calculated. After an increment of time Δt_k , $f(x, t_k + \Delta t_k)$ is obtained from $f(x, t_k)$ by assuming that the free carrier concentration $n(x, t)$ has remained equal to $n(x, t_k)$:

$$f(x, t_k + \Delta t_k) = f_k(x) + [f(x, t_k) - f_k(x)] \times \exp\{-[e_n + c_n(x, t_k)]\Delta t_k\}, \quad (51)$$

where

$$f_k(x) = c_n n(x, t_k) / [c_n n(x, t_k) + e_n], \quad (52)$$

and from which we can compute the new free carrier concentration $n(x, t_k + \Delta t_k)$ by a further integration of Poisson's equation.

Results for typical examples are given in Figs. 7 and 8. In Fig. 7 we show the fraction of refilled traps after refilling

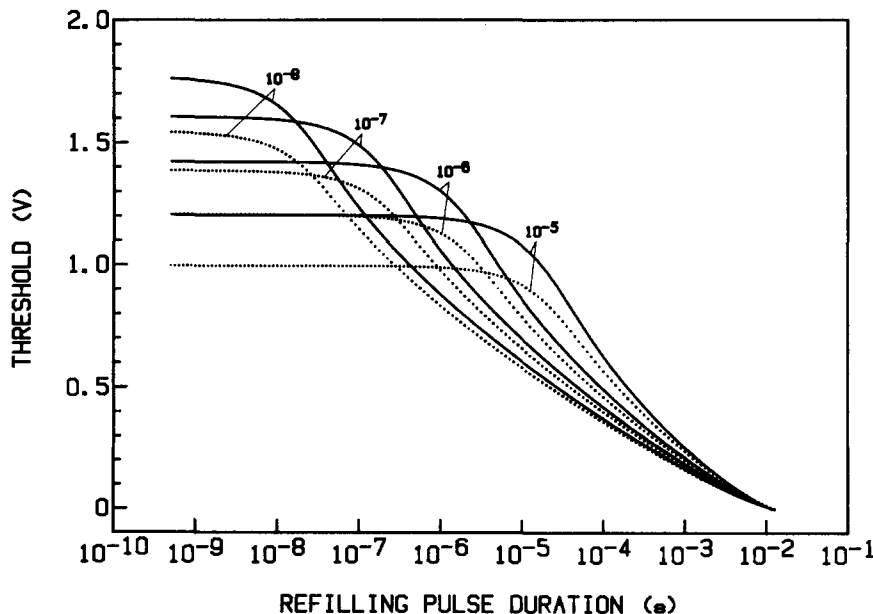


FIG. 6. Plot of the threshold ΔV_{th} for the refilling pulse amplitude (see text) as a function of the refilling pulse duration t_p for different values of the capture time constant τ_c indicated in seconds in the figure, for the same typical case as in Fig. 2 (except for τ_c). In these conditions $\tau_c = 10^{-5}$ s (resp. 10^{-8} s) corresponds to a trap depth of approximately 0.22 eV (resp. 0.38 eV). The solid lines correspond to a correct calculation of ΔV_{th} using the exact free carrier distribution and the dotted lines correspond to a noncorrect calculation of ΔV_{th} using the usual depletion approximation for the distribution of free carriers.

pulses of different durations. Figure 8 gives the resulting refilling kinetics, or more exactly the integral.

$$F(t_p) = \int_0^{t_p} \Delta f(x, t_p) \frac{xdx}{W_0^2}, \quad (53)$$

from which we can deduce the amplitude of the emptying kinetics, $\Delta C_{\max} = C(0) - C_0$, with the help of Eq. (21):

$$\frac{\Delta C_{\max}(t_p)}{C_0} = \left[1 + \frac{2N_T}{N_D} F(t_p) \right]^{-1/2} - 1. \quad (54)$$

Of course $\Delta C_{\max}/C_0$ is no longer linear with N_T/N_D , but since $F(t_p)$ is always less than 1/2, if $N_T < N_D$ then we can expand $\Delta C_{\max}/C_0$ in powers of N_T/N_D :

$$\begin{aligned} \frac{\Delta C_{\max}}{C_0}(t_p) = & -\frac{N_T}{N_D} F(t_p) \left\{ 1 - \frac{3}{2} \frac{N_T}{N_D} F(t_p) \right. \\ & \left. + \frac{5}{2} \left[\frac{N_T}{N_D} F(t_p) \right]^2 + \dots \right\}. \end{aligned} \quad (55)$$

At this point, it is important to recall that N_D must be replaced by $N_D - N_T$ in the case of an acceptorlike trap. One must notice that even if the deep donor (resp. acceptor) trap concentration is as large as (resp. half as large as) the shallow donor concentration, the complete refilling of the trap will provoke less than about 30% change in the capacitance of the diode.

Figures 7 and 8 are the equivalent of Figs. 2 and 4 except that we have assumed a deep donor concentration equal to the shallow donor concentration. Two important facts are noteworthy.

(a) The free carrier density at the beginning of the refilling pulse differs markedly from the equilibrium density. See for instance the calculated free carrier concentration just after the application of the refilling pulse in Fig. 9. One can see a strong enhancement of the free carrier concentration in the region $W_1 < x < W_0 - L_0$. In order to insure electrical neutrality, the free electrons compensate the initially unoccupied traps, so that the initial free carrier concentration is equal to $N_D + N_T$ in this region, whereas it is equal to N_D deeper in the bulk.

As a direct consequence, the refilling kinetics are strongly affected by this out-of-equilibrium free carrier distribution. The increased free carrier concentration at the beginning of the pulse provokes an acceleration of the refilling kinetics with an initial capture time constant reduced by a factor $(N_D + N_T)/N_D$ for a deep donor trap or $N_D/(N_D - N_T)$ for a deep acceptor.

It is possible to account for this in the simple following way: the fraction of filled traps is again governed by the detailed balance equation [Eq. (6)] but where the free carrier concentration $n(t)$ depends on the fraction of empty traps:

$$n(t) = N_D + N_T [1 - f(t)]. \quad (56)$$

The resolution of the detailed balance equation in this case is straightforward and gives the bulk refilling kinetics:

$$R(t_p) = 1 - \alpha_p / \left[1 + \frac{N_T}{N_D} (1 - \alpha_p) \right], \quad (57)$$

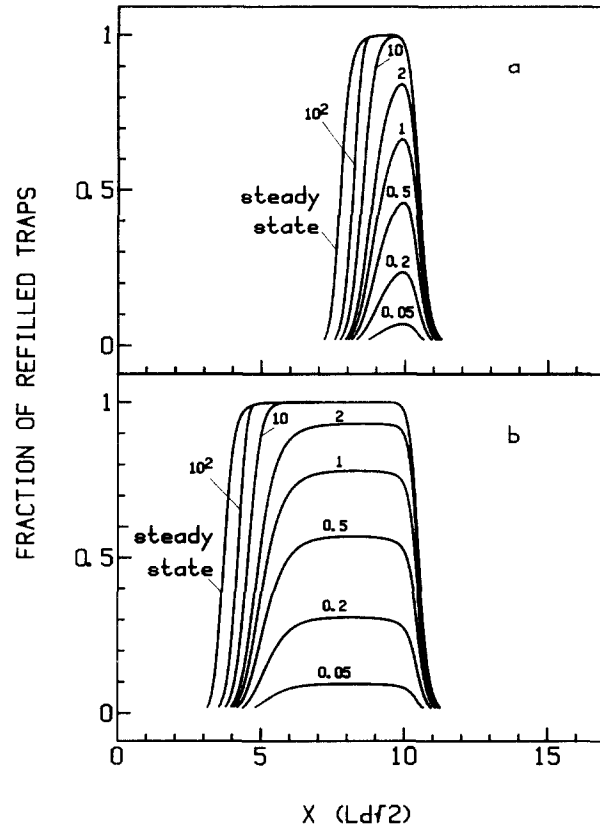


FIG. 7. Fraction of refilled traps $\Delta f(x, t_p)$ as a function of the distance from the metal semiconductor interface, after refilling pulses of different durations t_p indicated in units of τ_p in the figure. This is the same typical case as for Fig. 2 except that we have assumed that the concentration of the deep donor trap is equal to that of the shallow donor. Calculations give $W_0 = 13.4$ (in units of $L_D \sqrt{2}$) and $L_0 \approx 2.87$ (independent of the trap concentration). Case a corresponds to $\Delta V = 2$ V ($W_1 = 10.65$ at steady state) and case b to $\Delta V = 4$ V ($W_1 = 6.62$ at steady state).

where α_p is again given by Eq. (32). Of course, $R(t_p)$ reduces to Eq. (34) (with $\alpha_f = 0$) when N_T is negligible with respect to N_D . The corresponding result for an acceptorlike deep trap is

$$R(t_p) = (1 - \alpha_p) / [1 - \alpha_p N_T/N_D] \quad (57a)$$

(where $\alpha_p = \exp[-c_n(N_D - N_T)t_p]$). This result was also obtained by Borsuk and Swanson⁹ and also by Brotherton and Bicknell.¹³

(b) As can be appreciated from Fig. 7, replacing the refilled fraction of deep traps $\Delta f(x, t_p)$ by a rectangular function must remain perfectly justified, so that the same kind of approximation as developed in Sec. II C can be safely extended to the case of large deep trap concentrations.

We therefore obtain

$$F(t_p) \approx \frac{1}{2} \frac{R(t_p)}{W_0^2} \{ (W_0 - L_0)^2 - [W_1(t_p) - L_1(t_p)]^2 \} \quad (58)$$

subject to the same condition: $W_0 - L_0 > W_1(t_p) - L_1(t_p)$, and $F(t_p) \approx 0$ otherwise.

The steady-state quantities W_0 and L_0 are calculated in Appendix B.

$W_1(t_p)$ can be calculated by assuming that the fraction of occupied traps is zero for $x < W_1(t_p) - L_1(t_p)$ and $R(t_p)$ for $W_1(t_p) - L_1(t_p) < x < W_1(t_p)$. In this case:

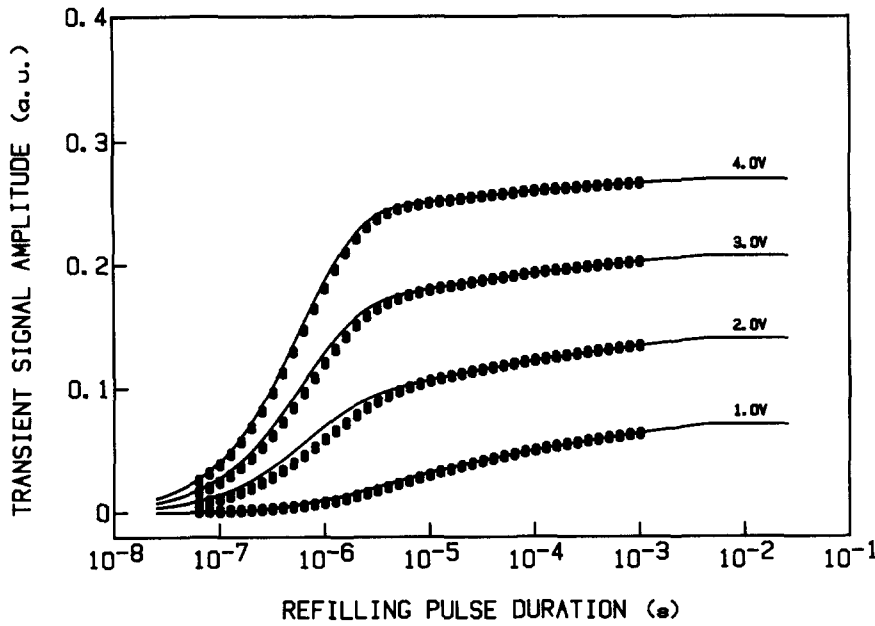


FIG. 8. Plot of $F(t_p)$ (see text) as a function of the refilling pulse duration t_p for different values of the refilling pulse amplitude ΔV (indicated in the figure). Same conditions as for Fig. 7, again with $N_T = N_D$ and a donorlike trap. (●) exact self-consistent calculation of the refilling kinetics. Solid lines: analytical approximation.

$$V_1 = -\frac{qN_D}{2\epsilon} \left\{ \left(1 + \frac{N_T}{N_D} \right) W_1^2 + 2L_D^2 - \frac{N_T}{N_D} R(t_p) [W_1^2 - (W_1 - L_1)^2] \right\} \quad (59)$$

(donorlike trap),

$$V_1 = -\frac{qN_D}{2\epsilon} \left\{ W_1^2 + 2 \left(1 - \frac{N_T}{N_D} \right) L_D^2 - \frac{N_T}{N_D} R(t_p) [W_1^2 - (W_1 - L_1)^2] \right\} \quad (59a)$$

(acceptorlike trap),

from which it is straightforward to deduce $W_1(t_p) - L_1(t_p)$ as a function of V_1 , N_T/N_D , $R(t_p)$ and $L_1(t_p)$, and from which it is possible to deduce a closed form formula for the threshold ΔV_{th} for the refilling pulse amplitude:

$$\Delta V_{th}(t_p) = \frac{kT}{q} \frac{W_0^2}{2L_D^2} \left[1 - \left(1 - \frac{L_0 - L_1(t_p)}{W_0} \right)^2 \right], \quad (60)$$

which is therefore explicitly identical to Eq. (43), except that $|V_0| - (kT/q)$ must be replaced by $kTW_0^2/2qL_D^2$. This expression for the threshold [Eq. (60)] is therefore preferable to Eq. (43) since it is of the widest generality.

In this expression, the ratio N_T/N_D appears only indirectly through W_0 . $L_1(t_p)$ remains to be calculated. It is however obvious that $L_1(t_p)$ must follow a law similar to Eq. (39) or Eq. (40), which expresses the fact that a refilling pulse of duration t_p refills the traps up to a point $W_1 - L_1$ in the potential barrier where the capture time constant $[c_n n(W_1 - L_1)]^{-1}$ is of the order of t_p . We compare in Fig. 8 the results of the calculation of $F(t_p)$ by the numerical computation and by the approximation (58). One can notice

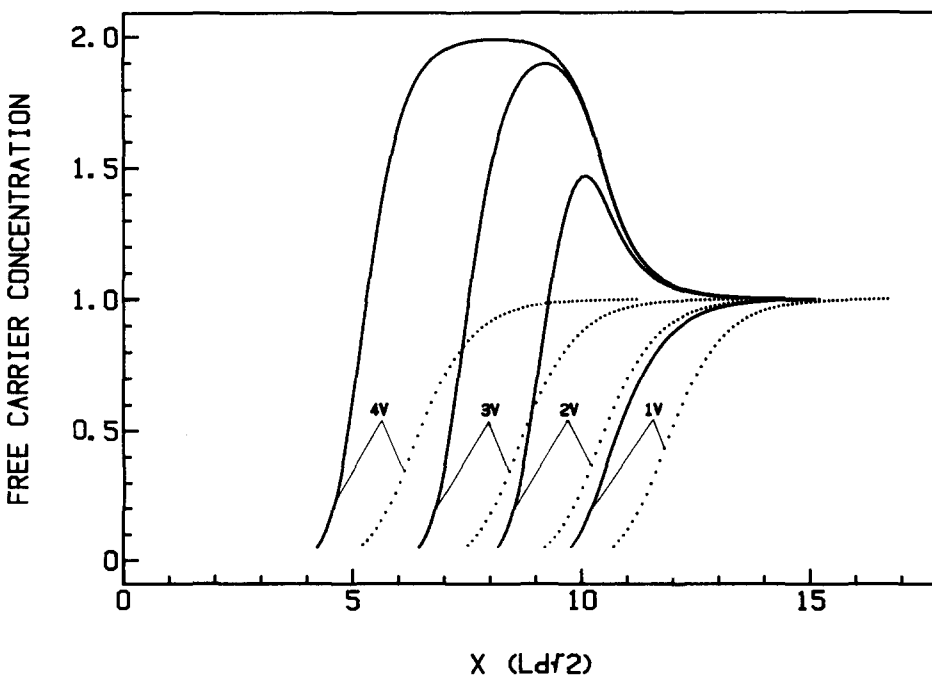


FIG. 9. Plot of the reduced free carrier concentration $n(x)/N_D$ as a function of the distance from the metal-semiconductor interface. Solid lines: just after the application of refilling pulses of different amplitudes (indicated in the figure). Dotted lines: after that steady state is reached. Same typical case as for Fig. 7, again with $N_T = N_D$, and a donorlike trap.

again the good agreement, which justifies again the use of step functions for the steady state or instantaneous distributions of trapped electrons.

V. CONCLUSION

A complete analysis of the refilling kinetics of deep traps in a Schottky diode has been presented, allowing us to deduce an experimental method to extract the refilling kinetics in the neutral semiconductor (which constitutes the physically important information to be obtained) from the total kinetics, getting rid of the obscuring contribution of the refilling in the potential barrier.

Emphasis has been given to the use of the exact distribution of free carriers in the vicinity of the edge of the space-charge region. It is shown that the renunciation of the usual depletion approximation, while giving appreciable corrections, does not necessarily yield severe complications in the calculations.

The approximation consisting in replacing the distributions of filled traps by step functions has been critically examined; it is demonstrated that the validity of these approximations can be safely extended from the equilibrium Fermi distributions to the transient distributions. As a consequence, we have shown that simple analytic approximations are able to describe accurately the refilling kinetics in most situations, even in the case of non-negligible concentration of deep traps with respect to the shallow dopant concentration. This has been demonstrated by a systematic confrontation of these approximations with numerical simulations.

ACKNOWLEDGMENTS

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APPENDIX: EXACT DISTRIBUTION OF FREE CARRIERS IN THE DEBYE TAIL AND STEADY STATE CALCULATION OF THE SPACE-CHARGE REGION

A. Ideal case: Uniform dopant concentration and negligible deep trap concentration

The usual depletion approximation for the distribution of free carriers in the Debye tail is obtained when it is assumed that the potential in the space-charge region has a parabolic shape

$$n(x) = N_D \exp\left(-\frac{(W-x)^2}{2L_D^2}\right) = N_D \nu(x). \quad (\text{A1})$$

This approximation is sufficient in most cases. However, it is not rigorously valid, especially close to the edge of the space-charge region. Since we are studying the electrical refilling of the trap in this region, this approximation, as shown in the paper, yields erroneous results, and an exact calculation is needed.

The free carrier concentration is given by

$$n(x) = N_D \nu(x) = N_D \exp\left(\frac{qV(x)}{kT}\right), \quad (\text{A2})$$

where the origin for the electric potential $V(x)$ has been put at $x = l$, a point deeper than the depth of the space charge region by several Debye lengths. With this expression for $n(x)$, the Poisson equation is integrated in a standard way [Eq. (14)] and we obtain

$$\frac{dv}{dx} = -\frac{\sqrt{2}}{L_D} \{v(x) - 1 + \exp[-v(x)]\}^{1/2}, \quad (\text{A3})$$

where the reduced (positive) potential v is equal to

$$v(x) = -qV(x)/kT. \quad (\text{A4})$$

By integrating Eq. (A3), we obtain

$$\frac{W-x}{L_D\sqrt{2}} = -\int_{v(W)}^{v(x)} \frac{dv}{2v(v-\ln v-1)^{1/2}} \equiv \Psi[v(x)]. \quad (\text{A5})$$

The concentration of free carriers is therefore implicitly obtained as a function of the position in the space charge region. Since we do not use the depletion approximation, W remains to be rigorously defined. Let W be defined by

$$W = \epsilon/C, \quad (\text{A6})$$

where C is the capacitance per unit area of the reverse biased diode, itself calculated as the derivative of the total charge Q in the semiconductor with respect to the barrier potential V_0 . Q is given by Gauss' law from the electric field at the metal-semiconductor interface:

$$Q = qN_D L_D \sqrt{2} [v(0) - 1 + e^{-v(0)}]^{1/2}, \quad (\text{A7})$$

from which we deduce

$$W = L_D \sqrt{2} [v(0) - 1 + e^{-v(0)}]^{1/2} / (1 - e^{-v(0)}). \quad (\text{A8})$$

In practical cases, Eqs. (A7) and (A8) reduce to

$$W = L_D \sqrt{2} [v(0) - 1]^{1/2}, \quad (\text{A9})$$

$$Q = qN_D W.$$

On the other hand, the total charge in the semiconductor and the barrier potential are given by

$$Q = qN_D \int_0^l [1 - \nu(x)] dx, \quad (\text{A10})$$

$$V(0) = -\frac{q}{\epsilon} N_D \int_0^l x [1 - \nu(x)] dx.$$

Integrating by parts both expressions, we get

$$Q = qN_D \int_0^1 [W - L_D \sqrt{2} \Psi(v)] dv$$

$$= qN_D (W - L_D \sqrt{2} I_1), \quad (\text{A11})$$

$$V(0) = -\frac{q}{\epsilon} N_D \int_0^1 \frac{1}{2} [W - L_D \sqrt{2} \Psi(v)]^2 dv$$

$$= -\frac{q}{\epsilon} N_D \left(\frac{W^2}{2} - W L_D \sqrt{2} I_1 + L_D^2 I_2 \right),$$

where

$$I_n = \int_0^1 \Psi^n(v) dv. \quad (\text{A12})$$

Comparison of Eqs. (A11) and (A9) yields immediately

$$I_1 = \int_0^1 \Psi(v) dv \equiv 0, \quad (\text{A13})$$

which is a direct consequence of the definition (A6) of W , and

$$I_2 = \int_0^1 \Psi(\nu)^2 d\nu \equiv 1. \quad (\text{A14})$$

Comparing Eq. (A5) for $x = 0$ and Eq. (A8), we obtain

$$\begin{aligned} - \int_{\nu(W)}^{\nu(0)} \frac{d\nu}{2\nu(\nu - \ln \nu - 1)^{1/2}} \\ = \frac{[-\ln \nu(0) - 1 + \nu(0)]^{1/2}}{1 - \nu(0)}, \end{aligned} \quad (\text{A15})$$

which allows us to deduce $\nu(W)$ as a function of $\nu(0)$. It can easily be shown that $\nu(W)$ tends towards a constant limit when $\nu(0)$ is made to go towards zero. A numerical calculation gives

$$\lim_{\nu(0) \rightarrow 0} \nu(W) = 0.55, \quad (\text{A16})$$

which completes the definition of the function $\Psi(\nu)$:

$$\frac{W-x}{L_D \sqrt{2}} = - \int_{0.55}^{\nu(x)} \frac{d\nu}{2\nu(\nu - \ln \nu - 1)^{1/2}} = \Psi[\nu(x)]. \quad (\text{A17})$$

The reduced free carrier concentration ν is therefore given by a universal law as a function of $(W-x)/L_D \sqrt{2}$, which needs to be calculated once.

An important quantity is the depth L_0 of the "edge region," defined by the length of semiconductor in the space-charge region where the energy level of the trap is below the quasi-Fermi level. If the energy level of the trap is deep enough and if the barrier potential is large enough so that

$$\nu(0) \gg (E_F - E_T)/kT \gg 1,$$

we obtain, for $0 < x < W - L_0$:

$$\frac{d\nu}{dx} \simeq - \frac{\sqrt{2}}{L_D} [\nu(x) - 1]^{1/2}. \quad (\text{A18})$$

integration of which, provides Eq. (10):

$$L_0 = L_D \sqrt{2} \left(\frac{E_F - E_T}{kT} - 1 \right)^{1/2}. \quad (\text{A19})$$

Finally, it is possible to get a good approximation for $\nu(x)$, valid for any x and especially near the edge of the space-charge region. The asymptotic behaviors [$\nu \sim 1$ for $x \gg W$, and $\nu(x) \simeq \exp\{-1 - [(W-x)^2/2L_D^2]\}$ for $x \ll W$, as deduced from Eq. (A18)] suggest the following relationship:

$$(\sqrt{\nu} - \Psi)\sqrt{\nu} = \alpha^2; \quad (\text{A20})$$

that is

$$n(x) \simeq N_D \exp \left[-\frac{1}{4} \left(\frac{W-x}{L_D \sqrt{2}} + \sqrt{\frac{(W-x)^2}{2L_D^2} + 4\alpha^2} \right)^2 \right]. \quad (\text{A21})$$

α^2 is a constant which can be chosen in order that relationship (A13) be still observed: we obtain $\alpha^2 = 1/2$. We compare in Fig. A1 the usual depletion approximation [Eq. (A1)], with the exact distribution [Eq. (A17)] and with the approximation given by Eq. (A21). Even more accurate analytical approximations have been derived by Jindal and Warner.¹⁵

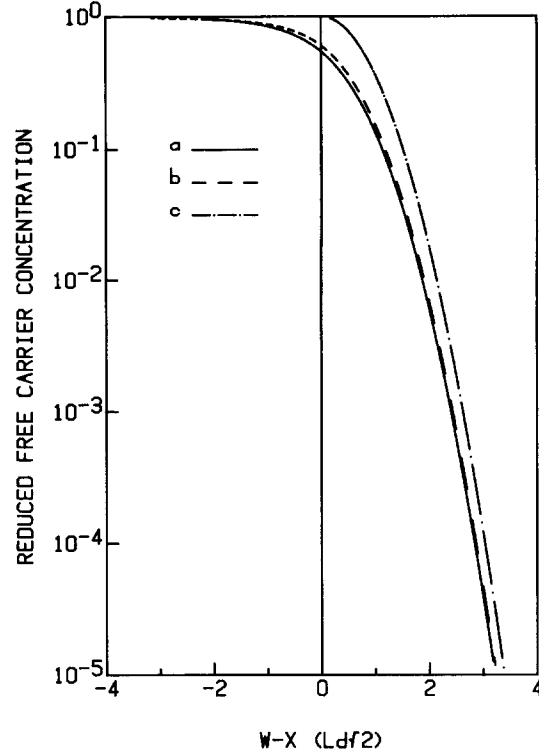


FIG. A1. Distribution of free carriers about the edge of the space-charge region W . The reduced free carrier concentration is the ratio $n(x)/N_D$ and distances are given in units of $L_D \sqrt{2}$. (a) Exact distribution [Eq. (A17)]. (b) The proposed simple analytical approximation [Eq. (A21)]. (c) The usual depletion approximation [Eq. (A1)].

B. Non-negligible deep trap concentration

We now calculate the equilibrium distribution of free carriers in the space-charge region in the presence of a deep trap whose concentration is not negligible with respect to the dopant concentration. We assume that the deep trap is donorlike, so that the total density of charge is given by Eq. (5). We will assume that the energy level of this trap in the neutral semiconductor is well below the Fermi level so that its equilibrium occupation is one and that the free electron concentration is equal to the shallow dopant concentration N_D . If we assumed that the deep trap has reached its steady state occupation, Poisson's equation can also be integrated exactly and the equivalent of Eq. (A3) is

$$\frac{d\nu}{dx} = - \frac{\sqrt{2}}{L_D} \left[\nu - 1 + e^{-\nu} + \frac{N_T}{N_D} \ln(e^{\nu - \nu_T} + 1) \right]^{1/2}, \quad (\text{B1})$$

where we have dropped terms proportional to $e^{-\nu_T}$ and where

$$\nu_T = (e_F - E_T)/kT. \quad (\text{B2})$$

The free carrier distribution is again implicitly obtained as a function of the position in the space-charge region:

$$\begin{aligned} \frac{W-x}{L_D \sqrt{2}} \\ = - \int_{\nu(W)}^{\nu(x)} \frac{d\nu}{2\nu \left[\nu - \ln \nu - 1 + \frac{N_T}{N_D} \ln(1 + \nu_T/\nu) \right]^{1/2}}, \\ = \Psi[\nu(x)] \end{aligned} \quad (\text{B3})$$

where

$$v_T = \exp(-v_T). \quad (\text{B4})$$

It is noteworthy that near the edge of the space-charge region, where $v(x) \gg v_T$, as it is shown in Fig. B1, Eq. (B3) reduces exactly to Eq. (A5) so that again $v(W) \simeq 0.55$, and the integrals $I_1 \simeq 0$ and $I_2 \simeq 1$ as for the case of negligible deep trap concentrations.

From Gauss' law we again deduce the total charge in the semiconductor, when $v(0) - v_T \gg 1$:

$$Q = qN_D L_D \sqrt{2} \left\{ v(0) - 1 + \frac{N_T}{N_D} [v(0) - v_T] \right\}^{1/2}. \quad (\text{B5})$$

On the other hand the total charge Q and the barrier potential $V(0)$ are given by

$$\begin{aligned} Q &= Q_D + Q_T, \\ V(0) &= V_D + V_T, \end{aligned} \quad (\text{B6})$$

where Q_D and V_D (resp. Q_T and V_T) are the contribution of the shallow donors and of the free electrons (resp. deep traps and trapped electrons) to the total charge in the semiconductor and to the barrier potential:

$$Q_D = qN_D \int_0^l [1 - v(x)] dx, \quad Q_T = qN_T \int_0^l [1 - f_0(x)] dx,$$

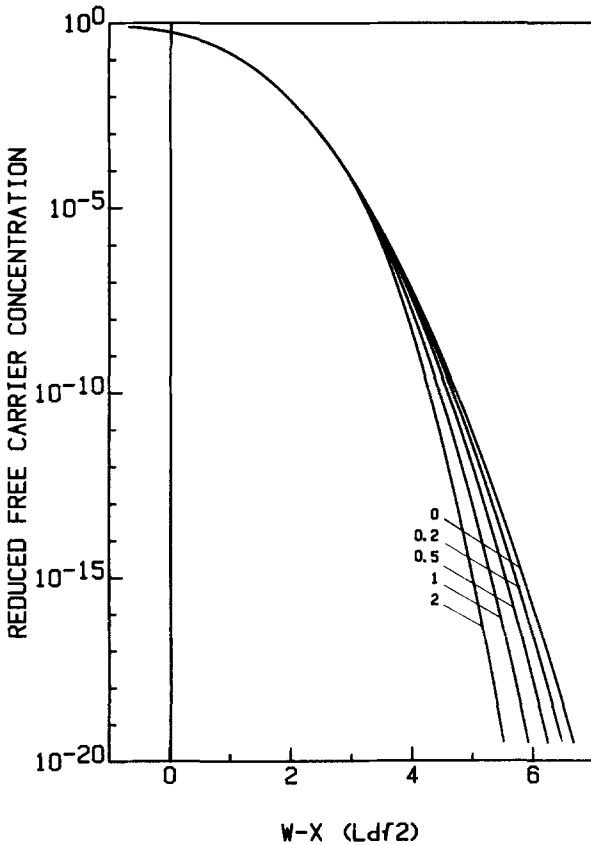


FIG. B1. Exact steady-state distribution of free carriers about the edge of the space-charge region W , for different values of the ratio N_T/N_D , indicated in the figure and assuming a donorlike trap. The reduced free carrier concentration is the ratio $n(x)/N_D$ and distances are given in units of $L_D \sqrt{2}$ (L_D is independent of N_T). Calculations are made using the same typical case as for Fig. 2 except for the trap concentration N_T . $L_0 \simeq 2.87$, independently of N_T . Note that about W , the steady-state distribution of free carriers is independent of N_T . However, W strongly depends on N_T and goes from 17.03 for $N_T \simeq 0$ to 11.65 for $N_T \simeq 2 N_D$.

$$\begin{aligned} V_D &= -\frac{qN_D}{\epsilon} \int_0^l x [1 - v(x)] dx, \\ V_T &= -\frac{qN_T}{\epsilon} \int_0^l x [1 - f_0(x)] dx, \end{aligned} \quad (\text{B7})$$

where $f_0(x)$ is the Fermi-Dirac distribution of occupied traps. Therefore if we consider the high frequency capacitance of the diode (that is measured at a frequency much higher than the emission rate of the trap), neither Q_T nor V_T follow the ac voltage so that

$$C_{\text{HF}} = \left| \frac{\delta Q}{\delta V} \right| = \left| \frac{dQ_D}{dV_D} \right|. \quad (\text{B8})$$

Integrating by parts Q_D and V_D as in Eq. (A11), we again deduce

$$C_{\text{HF}} = \frac{\epsilon}{W - L_D \sqrt{2} I_1}, \quad (\text{B9})$$

so that the definition of the depth of the space-charge region by

$$C_{\text{HF}} = \frac{\epsilon}{W} \quad (\text{B10})$$

is again equivalent to $I_1 \equiv 0$.

We integrate also Q_T and V_T by parts:

$$\begin{aligned} Q_T &= qN_T \int_0^l x df_0, \\ V_T &= -\frac{qN_T}{\epsilon} \int_0^l \frac{x^2}{2} df_0, \end{aligned} \quad (\text{B11})$$

and similarly to the function $\Psi(v)$, we introduce the function $\Phi(f_0)$

$$\Phi[f_0(x)] = \frac{W - L'_0 - x}{L_D \sqrt{2}}, \quad (\text{B12})$$

where L'_0 is defined by the condition

$$J_1 = \int_0^1 \Phi(f_0) df_0 = 0. \quad (\text{B13})$$

We obtain immediately

$$Q = qN_D \left[W + \frac{N_T}{N_D} (W - L'_0) \right], \quad (\text{B14})$$

and

$$\begin{aligned} V(0) &= -\frac{qN_D}{2\epsilon} \left[W^2 + \frac{N_T}{N_D} (W - L'_0)^2 \right. \\ &\quad \left. + 2L_D^2 \left(1 + \frac{N_T}{N_D} J_2 \right) \right], \end{aligned} \quad (\text{B15})$$

where

$$J_2 = \int_0^1 \Phi^2(f_0) df_0. \quad (\text{B16})$$

A comparison for Q between expressions (B14) and (B5) in which we inject Eq. (B15) for $v(0) = -[qV(0)/kT]$ yields

$$L'_0 = \sqrt{2} L_D \left[v_T - 1 - J_2 \left(1 + \frac{N_T}{N_D} \right) \right]^{1/2}, \quad (\text{B17})$$

which is independent of the applied gate bias.

The integral J_2 cannot be exactly determined. However, noting that f_0 is a Fermi distribution, an estimation of J_2 can

be obtained by standard methods (16). Expanding $\Phi(f_0)$ about the Fermi level, for $v \simeq v_T$, we get

$$\Phi(f_0) = \frac{v - v_T}{2 \left(v_T - 1 + \frac{N_T}{N_D} \ln 2 \right)^{1/2}}, \quad (\text{B18})$$

from which

$$J_2 \simeq \pi^2 / 12 \left(v_T - 1 + \frac{N_T}{N_D} \ln 2 \right). \quad (\text{B19})$$

Therefore, for reasonable values of V_T , J_2 is of the order or less than 0.1. Consequently, L'_0 can be replaced by L_0 in most cases, and W can be deduced from Eq. (B15):

$$W = \frac{\left(N_T/N_D L_0 + \left[2L_D^2 (1 + N_T/N_D) \left(\left| \frac{qV}{kT} \right| - 1 \right) - (N_T/N_D) L_0^2 \right]^{1/2} \right)}{1 + N_T/N_D}. \quad (\text{B20})$$

In the case of an acceptorlike deep trap the result is

$$W = \frac{N_T}{N_D} L_0 + \left[2L_D^2 \left(1 - \frac{N_T}{N_D} \right) \left(\left| \frac{qV}{kT} \right| - 1 \right) - L_0^2 \left(1 - \frac{N_T}{N_D} \right) \right]^{1/2}. \quad (\text{B20})$$

¹C. H. Henry, H. Kukimoto, G. L. Miller, and F. R. Merritt, Phys. Rev. B **7**, 2499 (1973).

²A. Zylbersztejn, Appl. Phys. Lett. **33**, 200 (1978).

³G. J. Rees, H. G. Grimmeiss, E. Janzen, and B. Skarstam, J. Phys. C **13**, 6157 (1980); see also R. M. Gibb, G. J. Rees, B. W. Thomas, B. L. H. Wilson, B. Hamilton, D. R. Wight, and N. F. Mott, Philos. Mag. **36**, 1021 (1977).

⁴H. G. Grimmeiss, L. A. Ledebø, and E. Meijer, Appl. Phys. Lett. **36**, 307 (1980).

⁵D. Pons, Appl. Phys. Lett. **37**, 423 (1980).

⁶See J. M. Noras, J. Phys. C **14**, 2341 (1981) for a modelization of Zylbersztejn's experiment (Ref. 2).

⁷J. M. Noras and H. R. Szawelska, J. Phys. C **15**, 2001 (1982).

⁸E. Meijer, L. A. Ledebø, and Zhan-Guo Wang, Solid State Commun. **46**, 255 (1983). See also H. G. Grimmeiss, L. A. Ledebø, and E. Meijer, in E. Meijer, Thesis Lund (1982), paper IV.

⁹J. A. Borsuk and R. M. Swanson, J. Appl. Phys. **52**, 6704 (1981).

¹⁰The usual depletion approximation gives the too large value $L_0 = L_D \sqrt{2} [\ln(\tau_e/\tau_c)]^{1/2}$.

¹¹An excellent approximation, valid for any t_p is

$$L_1(t_p) = L_D \sqrt{2} \Psi \left[\frac{\tau_c}{\tau_e} \left(\frac{\tau_e}{t_p \beta(t_p)} + \frac{\beta(t_p) R(t_p)/2}{1 - R(t_p)/2} \frac{1 - \alpha f}{1 - \alpha_f R(t_p)/2} - 1 \right) \right]$$

or $L_1(t_p) = L_0$, which one is the lowest.

¹²We use the same modification of the so-called Noumerov technique as in J. D. Cohen and D. V. Lang, Phys. Rev. B **25**, 5285 (1982).

¹³S. D. Brotherton and J. Bicknell, J. Appl. Phys. **49**, 667 (1978).

¹⁴See, for instance, E. H. Rhoderick, in *Metal Semiconductor Contacts* (Clarendon, Oxford, 1978), p. 184.

¹⁵R. M. Warner, Jr. and R. P. Jindal, Solid State Electron. **26**, 335 (1983).

¹⁶See, for instance, J. M. Ziman, in *Principles of the Theory of Solids* (Cambridge University, Cambridge, 1972), p. 138.