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On non-dispersive multiple-trapping transient currents in non-homogeneous layers

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Abstract. Non-dispersive transient currents in non-homogeneous films with a single discrete trap level have been calculated, the non-homogeneity consisting in spatial variations of trap depths or the presence of constant built-in electric fields in the limit cases of shallow and deep traps. Both kinds of spatial non-homogeneity may result in identical shapes of transients. Methods for determination of the spatial variations of trap depth and internal built-in electric field on the basis of experimental data are discussed.

1. Introduction

In recent years, non-homogeneous thin film structures of low-conductivity materials have become of increasing experimental and theoretical interest (Grung 1981, Chatterjee and Marshak 1983, Klose *et al* 1983). By applying a suitable preparation procedure (e.g. various epitaxial technologies, ion implantation and high-dose irradiation) it is possible to produce thin layers with a complicated position-dependent change in the band gap or layers with a very intricate shape (spatial and energetic) of localised states (Henniger and Keiper 1985, Osinskii *et al* 1985). Variations in these physical parameters across the layer affect the dynamics and distribution of charge carriers and must be taken into account when analysing the form of the transient currents. It has been shown experimentally that the spatial variations of the trap density have a pronounced effect on transient currents (Thomas *et al* 1968, Silnish 1970, Brodribb *et al* 1975, Samoć and Zboiński 1978). This case of a layer non-homogeneity has been described analytically by Rybicki and Chybicki (1989). In the present paper we deal with some spatial variations of discrete trap depth and the internal quasi-electric field which is assumed to be caused by the band-gap gradient only. Calculations are based on the conventional concepts of the multiple-trapping model for homogeneous layers (Zanio *et al* 1968, Schmidlin 1977, Noolandi 1977, Arkchipov and Rudenko 1982, Rudenko and Arkchipov 1982a, b, Baginskii and Kostsov 1985a, b). We give formulae for determining the spatial variations of the trap depths and internal built-in field from current–time characteristics.

2. General formulation

In the case of small-signal monopolar injection into a thin non-homogeneous insulating layer, the continuity equations for the concentration $n(x, t)$ of the free charge and the concentration $n_t(x, t)$ of the trapped charge, assuming multiple-trapping band transport, may be written as follows (Zanio *et al* 1968):

$$\partial n(x,t)/\partial t = -(\partial/\partial x)[\mu E(x)n(x,t)] - \partial n_t(x,t)/\partial t \tag{1}$$

$$\partial n_t(x,t)/\partial t = n(x,t)/\tau(x) - n_t(x,t)/\tau_d(x) \tag{2}$$

with initial conditions

$$n(x,0) = n_0\delta(x) \tag{3}$$

and

$$n_t(x,0) = 0 \tag{4}$$

where μ is the microscopic mobility, t the time ($t \geqslant 0$), x the spatial coordinate ($0 \leqslant x \leqslant L$), L the layer thickness, $E(x)$ the x-dependent electric field, $\tau(x)$ the x-dependent average trapping time, $\tau_d(x)$ the x-dependent average detrapping time, $\delta(x)$ the Dirac function and n_0 the surface density of the injected charge. $E(x)$, $\tau(x)$ and $\tau_d(x)$ are assumed to be time independent. In equation (1) the diffusion term as usual has been neglected, and in equation (2) a low trap occupation has been assumed. Equations (1)–(4) may be solved with the aid of the Laplace transform technique. The Laplace time-transform $\tilde{n}(x, s)$ of the free-charge concentration $n(x, t)$ is

$$\tilde{n}(x,s) = \frac{n_0\theta(x)}{\mu E(x)}\exp\left[-\int_0^x \frac{s\,d\xi}{\mu E(\xi)}\left(1 + \frac{1}{\tau(\xi)[s + 1/\tau_d(\xi)]}\right)\right] \tag{5}$$

where $\theta(x)$ is the unit-step function. Inverting the Laplace transform (5) and substituting the resultant free-carrier concentration $n(x, t)$ into

$$j(t) = \frac{q\mu}{L}\int_0^L E(x)n(x,t)\,dx \tag{6}$$

where q is the elementary charge, one gets the current $j(t)$ induced in the external circuit. In the following we shall discuss transient currents in non-homogeneous layers for pure cases of x-dependent trap depths and an x-dependent internal electrical field.

3. Spatial variations of the trap depths

3.1. Equations for transient currents

In the case of spatial variations of the depth $\mathscr{E}(x)$ of a single locally discrete trap level, the x-dependent average detrapping time $\tau_d(x)$ is given by

$$\tau_d(x) = [1/\nu(x)]\exp[\mathscr{E}(x)/kT] \tag{7}$$

where $\nu(x)$ is an x-dependent frequency factor, given by the number of phonons absorbed per second by a trapped carrier multiplied by the probability of transition to the conduction band, k the Boltzmann constant and T the temperature. The x-dependent trapping time $\tau(x)$ assumes the explicit form

$$\tau(x) = [N_0\sigma(x)v_{th}]^{-1} \tag{8}$$

where N_0 is the x-independent trap concentration, v_{th} the thermal velocity and $\sigma(x)$ the x-dependent trapping cross section. The electric field is assumed to be position independent and equal to the applied external field $E_0 = V/L$, where V is the applied voltage. In such a case, (5) simplifies to

$$\tilde{n}(x, s) = \frac{n_0\theta(x)}{\mu E_0} \exp\left[-\frac{s}{\mu E_0}\left(x + \int_0^x \frac{1/\tau(\xi)}{s + 1/\tau_d(\xi)}\,d\xi\right)\right] \tag{9}$$

and may be immediately inverted in the two limit cases of shallow and deep traps. Assuming $s\tau_d(x) \ll 1$ for shallow traps (the formal condition $s\tau_d(x) \ll 1$ being further referred to as the shallow-trapping case, even if it is fulfilled for somewhat deeper traps), one gets

$$n(x, t) = \frac{n_0\theta(x)}{\mu E_0}\,\delta\left[t - \frac{1}{\mu E_0}\left(x + \int_0^x \frac{\tau_d(\xi)}{\tau(\xi)}\,d\xi\right)\right] \tag{10}$$

which on substitution into equation (6) for the electric current induced in the external circuit leads to

$$j(t) = (qn_0\mu E_0/L)\{1 + \tau_d[x^*(t)]/\tau[x^*(t)]\}^{-1} \tag{11}$$

where $x^*(t)$ is the solution of

$$t = \frac{1}{\mu E_0}\left(x + \int_0^x \frac{\tau_d(\xi)}{\tau(\xi)}\,d\xi\right) \tag{12}$$

and is the actual position of the centroid of the drifting carriers.

In the limit case of deep trapping, i.e. for $s\tau_d(x) \gg 1$ for all x-values, the traps act as absorbing centres, and the currents will be influenced only through the variations in the trapping cross section $\sigma(x)$, which enters $\tau(x)$ according to (8). In particular, for deep traps the free-carrier concentration is

$$n(x, t) = \frac{n_0\theta(x)}{\mu E_0} \exp\left(-\frac{1}{\mu E_0}\int_0^x \frac{d\xi}{\tau(\xi)}\right)\delta\left(t - \frac{x}{\mu E_0}\right). \tag{13}$$

Substituting (13) into (6) with $E(x) = E_0 = \text{constant}$, one gets

$$j(t) = \frac{qn_0\mu E_0}{L} \exp\left(-\frac{1}{\mu E_0}\int_0^{\mu E_0 t} \frac{d\xi}{\tau(\xi)}\right). \tag{14}$$

3.2. Comparison of the analytical results with Monte Carlo simulation and discussion

The expressions for transient currents (equations (11), (12) and equation (14)) have been obtained for two limit cases of shallow and deep trapping, respectively. The concentrations $n(x, t)$ of free carriers (equations (10) and (13)) are δ-like in those limits, which seems to be a very radical simplification. Thus the approximate results (11), (12) and (14) have been compared with the exact solutions obtained with the aid of Monte Carlo simulation. The algorithm applied was similar to that described by Rybicki and Chybicki (1988), extended by taking into account the x dependence of the detrapping time $\tau_d(x)$ originating from spatial dependence of the trap depth $\mathscr{E}(x)$. Illustrative

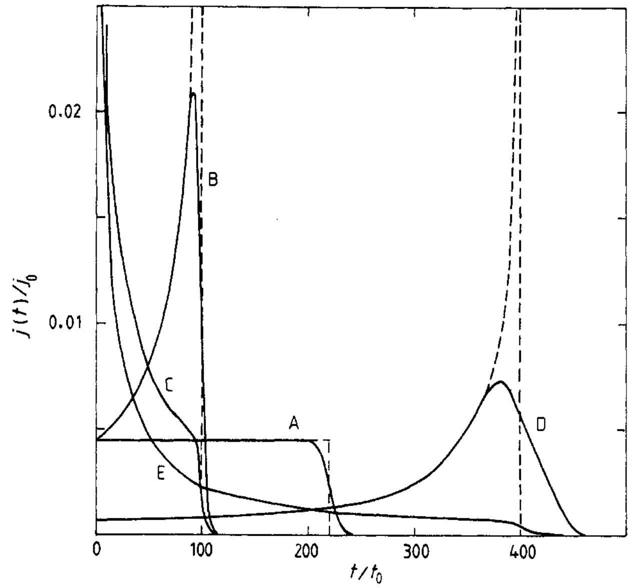

Figure 1. Shallow-trapping ($s\tau_d(x) \ll 1$) transient currents for x-dependent trap depths $\mathscr{E}(x) = \mathscr{E}_0 + \alpha x$ ($L = 10^{-2}$ cm; $\nu_0 = 10^{12}\,\mathrm{s}^{-1}$; $\tau_0 = 10^{-10}$ s; $t_0 = 10^{-5}$ s): curve A, $\mathscr{E}_0 = 10\,kT$, $\alpha = 0$; curve B, $\mathscr{E}_0 = 10\,kT$, $\alpha = -0.2 \times 10^3\,kT\,\mathrm{cm}^{-1}$; curve C, $\mathscr{E}_0 = 8\,kT$, $\alpha = 0.2 \times 10^3\,kT\,\mathrm{cm}^{-1}$; curve D, $\mathscr{E}_0 = 12\,kT$, $\alpha = -0.4 \times 10^3\,kT\,\mathrm{cm}^{-1}$; curve E, $\mathscr{E}_0 = 8\,kT$, $\alpha = 0.4 \times 10^3\,kT\,\mathrm{cm}^{-1}$; ——, Monte Carlo simulation; ---, approximate equations (11), (12).

shallow-trapping transients in figure 1 have been calculated for the linear dependence $\mathscr{E}(x) = \mathscr{E}_0 \pm \alpha x$, $\alpha > 0$. For simplicity, the parameters $\nu(x)$ and $\sigma(x)$ are assumed to be x independent, i.e. $\nu(x) = \nu_0 =$ constant and $\sigma(x) = \sigma_0 =$ constant. The full curves show the results obtained from the Monte Carlo simulation, and the broken curves correspond to the approximate equations (11), (12). The effective time t_{eff} of flight (position of the vertical fall in the current) is given by

$$t_{\mathrm{eff}} = \frac{1}{\mu E_0}\left(L + \int_0^L \frac{\tau_d(\xi)}{\tau(\xi)}\,\mathrm{d}\xi\right). \tag{15}$$

In particular, for the linear x dependence of trap depths assumed in figure 1;

$$t_{\mathrm{eff}} = (L/\mu E_0)\{1 + [\exp(\mathscr{E}_0)/\nu_0\tau_0\alpha L][\exp(\alpha L) - 1]\} \tag{16}$$

where $\tau_0 = (N_0\sigma_0 v_{\mathrm{th}})^{-1}$. As seen, the approximate formulae agree perfectly with the Monte Carlo simulation. In the case of deep trapping, equation (14) also satisfactorily agrees with the simulation. Thus, it is possible to use the analytical results in the previous section for determining the spatial variations of the trap depths from transient currents $j(t)$.

In the case of shallow trapping and x-independent parameters ν_0 and σ_0, one gets the trap depth in the actual position of drifting carrier packet $\mathscr{E}(x^*(t))$ from (11) as

$$\mathscr{E}(x^*(t)) = kT\ln\{\nu_0\tau_0[j_0/j(t) - 1]\} \tag{17}$$

where $j_0 = qn_0\mu E_0/L$ and $j(t)$ is the measured current. In a more general case of x-dependent $\nu(x)$ and $\sigma(x)$, by inserting the explicit dependences of ν and σ on the trap depth $\mathscr{E}(x)$ into equation (11), one gets an algebraic equation from which one can calculate the trap depth $\mathscr{E}(x^*(t))$ in the actual position of the drifting charge centroid on the basis of the measured $j(t)$. The centroid position $x^*(t)$ may be found by measuring additionally the time dependence of the charge $Q(t)$ induced on the layer contacts and making use of the Ramo (1939) theorem:

$$Q(t) = qn_0x^*(t)/L. \tag{18}$$

This completes the determination of $\mathscr{E}(x)$.

In the case of deep trapping and x-independent σ the shape of the transient current does not depend on spatial variations of the trap depth which act simply as absorption centres. If the trapping cross section depends on the trap depth, i.e. $\sigma(x) = \sigma(\mathscr{E}(x))$, one can easily obtain $\tau(\mu E_0 t)$ from (14):

$$\tau(\mu E_0 t) = -\{[1/j(t)][\mathrm{d}j(t)/\mathrm{d}t]\}^{-1} \tag{19}$$

and then, from (8), $\sigma(\mu E_0 t) = \sigma(x) = \sigma(\mathscr{E}(x))$ up to the factor N_0. In this way the functional shape of $\mathscr{E}(x)$ can be estimated if only a reliable dependence of σ on $\mathscr{E}$ is assumed. For deep trapping in the considered sense the effective time of flight is simply $t_{\mathrm{eff}} = L/\mu E_0$.

In the cases of both shallow and deep traps the microscopic mobility μ is assumed to be known.

4. Built-in constant electric fields

4.1. Equations for transient currents

Because of the presence of a time-independent built-in electric field $\Delta E(x)$, due for example to the spatial variations in the band gap, the total electric field $E(x)$ causing the free-carrier drift is

$$E(x) = E_0 + \Delta E(x). \tag{20}$$

Assuming the trap depth $\mathscr{E}$ to be position independent, i.e. $\mathscr{E}(x) = \mathscr{E}_0 =$ constant (consequently $\nu(x) = \nu_0 =$ constant and $\sigma(x) = \sigma_0 =$ constant), the Laplace transform $\tilde{n}(x, s)$ of the free-charge concentration $n(x, t)$ is

$$\tilde{n}(x, s) = \frac{n_0\theta(x)}{\mu E(x)} \exp\left[-\left(s + \frac{s}{(s + 1/\tau_{\mathrm{d}0})\tau_0}\right)\int_0^x \frac{\mathrm{d}\xi}{\mu E(\xi)}\right] \tag{21}$$

where $\tau_{\mathrm{d}0} = (1/\nu_0)\exp(\mathscr{E}_0/kT)$ and $\tau_0 = (N_0\sigma_0 v_{\mathrm{th}})^{-1}$. Inverting (21) in the limit of shallow trapping ($s\tau_{\mathrm{d}} \ll 1$), one gets

$$n(x, t) = \frac{n_0\theta(x)}{\mu E(x)}\,\delta\left[t - \left(1 + \frac{\tau_{\mathrm{d}0}}{\tau_0}\right)\int_0^x \frac{\mathrm{d}\xi}{\mu E(\xi)}\right] \tag{22}$$

and, with the aid of (6),

$$j(t) = (qn_0/L)\{\mu E[x^*(t)]/(1 + \tau_{\mathrm{d}0}/\tau_0)\} \tag{23}$$

where the actual position $x^*(t)$ of the drifting packet is the solution of

$$t = \int_0^x \frac{\mathrm{d}\xi}{\mu E(\xi)}\left(1 + \frac{\tau_{\mathrm{d}0}}{\tau_0}\right). \tag{24}$$

In the limit case of deep trapping ($s\tau_{\mathrm{d}} \gg 1$) the free-carrier concentration is

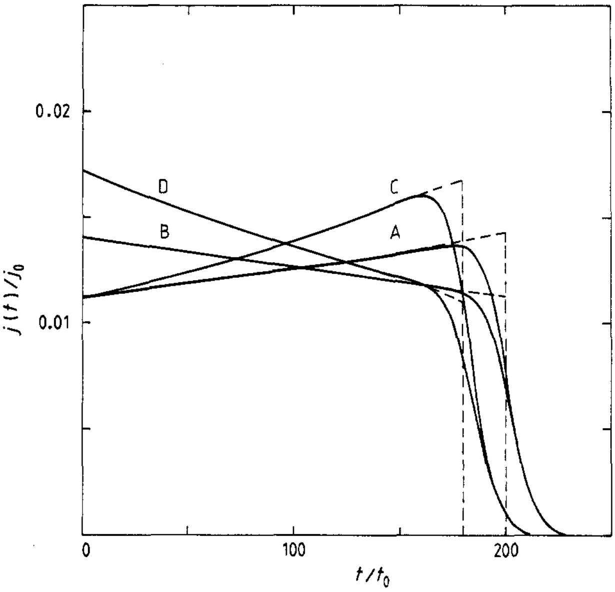

Figure 2. Shallow-trapping ($s\tau_d(x) \ll 1$) transient currents for x-dependent built-in electric field $\Delta E(x) = \beta + \gamma x$ ($L = 10^{-2}$ cm; $E_0 = 10^3$ V cm^{-1}; $\nu_0 = 10^{12}$ s^{-1}; $\tau_0 = 10^{-10}$ s; $t_0 = 10^{-5}$ s): curve A, $\beta = 0$ V m^{-1}, $\gamma = 0.25 \times 10^5$ V cm^{-2}; curve B, $\beta = 0.25 \times 10^3$ V m^{-1}, $\gamma = -0.25 \times 10^5$ V cm^{-2}; curve C, $\beta = 0$ V m^{-1}, $\gamma = 0.5 \times 10^5$ V cm^{-2}; curve D, $\beta = 0.5 \times 10^3$ V cm^{-1}, $\gamma = -0.5 \times 10^5$ V cm^{-2}; ——, Monte Carlo simulation; ---, approximate equations (23), (24).

$$n(x,t) = \frac{n_0\theta(x)}{\mu E(x)} \exp\left(-\frac{1}{\tau_0}\int_0^x \frac{\mathrm{d}\xi}{\mu E(\xi)}\right) \delta\left(t - \int_0^x \frac{\mathrm{d}\xi}{\mu E(\xi)}\right) \tag{25}$$

and thus, from (6),

$$j(t) = \frac{qn_0}{L}\mu E[x^*(t)] \exp\left(-\frac{1}{\tau_0}\int_0^{x^*(t)} \frac{\mathrm{d}\xi}{\mu E(\xi)}\right) \tag{26}$$

where

$$t = \int_0^{x^*(t)} \frac{\mathrm{d}\xi}{\mu E(\xi)} \tag{27}$$

relates time t with the actual position $x^*(t)$ of the drifting carrier packet.

4.2. *Comparison of the analytical results with the Monte Carlo simulation and discussion*

In a similar way to § 3.2, we first compare the simplified analytical results with the Monte Carlo simulation. Illustrative shallow-trapping transients have been calculated for a linear x dependence of built-in electric field $\Delta E(x) = \beta \pm \gamma x$, $\gamma > 0$, corresponding to parabolic spatial changes of the band gap, for $\nu(x) = \nu_0 =$ constant and $\sigma(x) = \sigma_0 =$ constant (figure 2). The full curves correspond to Monte Carlo simulation, performed according to the algorithm modified to allow for x dependence of the band drift velocity

$\mu E(x)$, while the broken curves correspond to the approximate solutions (23), (24). The effective time $t_{\rm eff}$ of flight is given by

$$t_{\rm eff} = \int_0^L \frac{\mathrm{d}\xi}{\mu E(\xi)} \left(1 + \frac{\tau_{\rm d0}}{\tau_0}\right) \tag{28}$$

and thus, for $\Delta E(x)$ assumed in figure 2,

$$t_{\rm eff} = [(1 + \tau_{\rm d0}/\tau_0)/\gamma] \ln[1 + \gamma L/(E_0 + \beta)]. \tag{29}$$

Also in the case of deep trapping, equations (26), (27) recover the results of the Monte Carlo simulation despite the final portion of the current. Thus, the approximate formulae (23), (24) and (26), (27) should be accurate enough to estimate the internal built-in electric fields.

In the case of shallow trapping and x-independent parameters ν and σ, one immediately gets $E(x^*(t))$ from (23), and, in a similar way to § 3.2, by using the Ramo theorem, one completes the determination of $E(x)$.

In the case of deep trapping, from (26), (27) one gets

$$E(x^*(t)) = [j(t)L/qn_0\mu] \exp(t/\tau_0) \tag{30}$$

which, together with (18), gives $E(x)$.

5. Concluding remarks

In the previous paper (Rybicki and Chybicki 1989, section 2) we have described the influence of the spatial non-homogeneity of the trap concentration on non-dispersive transient currents flowing under the action of the uniform field $E_0 = V/L$, the traps being at x-independent depths. In the present paper we have discussed two other types of layer non-homogeneity: uniformly distributed traps of x-dependent depths (section 3) and uniformly distributed constant-depth traps in a layer with a non-uniform band structure (section 4). The analytical solution of the transport equations is possible because the diffusion term is neglected, and the description of current–time characteristics is especially simple in the two limit cases of shallow and deep trapping. The final formulae are suitable for determination of the non-homogeneity parameters. The shapes of transient currents obtained within all three non-homogeneity models are visually similar and do not have any features specific to a particular kind of the considered non-homogeneity (cf figures 1 and 3 of Rybicki and Chybicki (1989) with figures 1 and 2 of the present paper). A single transient current different from a typical rectangular type may be interpreted within all three types of non-homogeneity, i.e. the shape of such a characteristic may be explained by a spatial non-homogeneity of trap density, by a spatial non-homogeneity of trap depths or by the presence of internal built-in fields. Thus, in order to choose the proper interpretation, measurements at different temperatures and different external fields are necessary. When the experimental data are misinterpreted, the absolute values of the internal parameters describing the layer non-homogeneity depend on external conditions (temperature and applied field). On the other hand, if only the non-homogeneity model chosen for the data interpretation corresponds to the real situation in the layer, the absolute values of the parameters describing the non-homogeneity are temperature and field independent, at least if the field dependences of parameters such as μ, σ and $\tau_{\rm d}$ and the temperature dependences of μ, $\mathscr{E}_0$ and N_0 are neglected.

Thus, apart from showing the remarkable influence of the layer non-homogeneity on transient currents, we hope that the paper provides some formulae useful for the experimentalist to interpret his data.

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