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One-Carrier Free Space Charge Motion under Applied Voltage*

L. E. CARRANO DE ALMEIDA** and G. F. LEAL FERREIRA

*Departamento de Física e Ciência dos Materiais, Instituto de Física e Química de São Carlos, USP, São Carlos****

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The article shows how to transform the system of partial differential equations, describing the free one-carrier space charge motion in solid dielectrics under a given applied voltage and while the charge distribution touches only one of the electrodes, into a first order ordinary differential equation from whose solution all the interesting quantities may be easily derived. It was found that some charge distributions can display current reversal.

O artigo mostra como transformar o sistema de equações diferenciais parciais que descrevem o movimento de carga espacial unipolar sob voltagem aplicada e enquanto a distribuição de carga toca somente um dos eletródios, em uma equação diferencial ordinária de primeira ordem, de cuja solução todas as grandezas pertinentes ao problema podem ser facilmente derivadas. Verificou-se que algumas distribuições de carga podem produzir a chamada inversão de corrente.

1. Introduction

Exact solutions of the problem of one-carrier space charge motion in solid dielectrics, in planar geometry, have received increasing attention recently. The problem can be divided according to:

a) the external conditions applied to the charged system;
b) the complexity assumed for the kinetics of the carriers.

Within a, we include the charge mode (open circuit) and the current mode (voltage applied). Within b, there are several possibilities, starting with the simplest – free space charge motion (hereafter FSCM) – and allowing increasing complexity with deep trap kinematics and further with trapping and de-trapping mechanisms simultaneously present. The FSCM itself can be considered to take place in an insulating or in a conducting dielectrics.

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**Presend address: *Universidade Federal do Paraná, 80000* – Curitiba PR.

***Postal address: 13560 – São Carlos, SP.

In general, the charge mode is a simpler problem to solve. Exact solutions have been found even for the deep trap case[1,2] and there is no special difficulty involving the solution of FSCM under this mode.

The pattern looks different in the current mode. Here, aside from those works dealing with SCL current injection[3,4], exact solutions are restricted to the FSCM for the box distribution[5,6,7,8] and for those charge distributions whose carriers have not yet reached the electrodes[9,10] (which will be called floating space charge). We include here the small signal case, extensively used in photoinjection experiments[11,12]. The numerical integration of the partial equations performed by J. Van Turnhout[8] should also be mentioned.

The aim of this article is to show how to reduce the problem of FSCM under the current mode, with the charge distribution touching only one of the electrodes, to a first order ordinary differential equation, from whose solution the external current can be easily derived. We leave to a forthcoming article the consideration of the completely charged filled case. It is assumed that the electrodes do not inject free space charge even under favorable conditions (that is, even when the electric field in an electrode points in the direction of the dielectrics). They can, however, supply current for the normal conductivity of a conducting material. On the other hand, it is assumed that the electrodes receive all the current the dielectric tends to deliver according to the electrical conditions prevailing on the dielectric side of the boundary: metal-dielectric.

The method of solution to be developed below can be applied as long as the system displays FSCM and is under the current mode, that is, under an applied voltage, which can be a function of time. We, however, will restrict numerical applications to the more interesting situation of short circuit. Here, we have found that some charge distributions may exhibit current reversal, as suggested by B. Gross[8,13], although not splitting themselves in two bumps.

The external current will be found from the initial charge distribution. In this respect, it can be argued that exact solutions are not needed since the external current is a gross measure of the process going inside the dielectric. We agree with this statement, inasmuch as, in the current mode, the external current is, rigorously, the average of the conduction current taken inside the dielectric. We cannot, however, agree any further, since only knowledge of the exact solutions will allow us to find which features of the charge distribution are most responsible for the behavíour of the external current.

2. Theory

The equations describing the FSCM in an insulating dielectric, in planar geometry, will be written in dimensionless variables

$$\frac{\partial E}{\partial x} = \rho, \qquad \frac{\partial i}{\partial x} = -\frac{\partial \rho}{\partial t}, \qquad i = \rho E. \tag{1}$$

The relation between the dimension variable E' (electric field), ρ' (charge density), conduction current density i', time t', and coordinate x' and the corresponding dimensionless ones, E, p, i, t and x, may be taken the same as those defined by Many-Rakavy[3] when the applied voltage is not zero, or may chosen as

$$x' = xd, \quad \rho' = \rho_0\rho, \quad E' = \frac{\rho_0 dE}{\varepsilon}, \quad i = \frac{\mu d\rho_0^2 i}{\varepsilon}, \quad t' = \frac{\varepsilon t}{\mu\rho_0},$$

whether or not the applied voltage is zero. In the above relations, d is the distance between the electrodes, ε the dielectric permitivity, μ the constant mobility of the carriers and ρ_0 may have any desired value. The applied voltage V'_0 and its corresponding dimensionless voltage V_0 are related according to:

$$V'_0 = \frac{d^2\rho_0 V_0}{\varepsilon}.$$

We note that the FSCM is completely specified by the expression defining the conduction current density i' $= \mu\rho' E'$ (or, in dimensionless variables i $= \rho E$). It is supposed that only a kind of carrier (here taken of positive polarity) can move. Traps are not considered, unless they are in so intimate contact with the conducting band that a drift mobility can be used[3]. In this case, p' is the total charge density (that is, trapped plus free charge).

The total current density j is known to be

$$j = \rho E + \frac{\partial E}{\partial t} \tag{2}$$

Using the method of characteristics[3], the following equations for the system[1] result:

$$\frac{dx}{dt} = E, \qquad \frac{dE}{dt} = j, \qquad \frac{d\rho}{dt} = -\rho^2.$$

The relation between position x and time t defines the flow lines, which can be labeled by the initial value of the position, x_0, and of the electric field $E(x_0)$:

$$x = x_0 + E(x_0)\,t + \int_0^t dt' \int_0^{t'} dt''\, j(t''). \tag{3}$$

In this notation, $E(x_0) = E(x, 0)$. The charge density along a flow line can be easily found, with the same simplified notation, as

$$\rho(x, t) = \frac{\rho(x_0)}{1 + \rho(x_0)\,t}\,. \tag{4}$$

In the charge mode, $(j = 0)$, Eqs. (3) and (4) give directly the desired solution of FSCM, in terms of the initial charge distribution and field. In the current mode, however, the density of the total current j must be found before the integral in (3) can be performed. In the floating space charge, it can indeed be found [9,10] and so the problem is soluble up to that time when one of the edges of the charge distribution reaches one of the electrodes. The corresponding time will be taken as the origin for the next stage of the problem, and charge distribution and field will be supposed to be known at that instant of time. So, we will take, for $\rho(x, 0)$,

$$\rho(x, 0) = \begin{cases} \rho(x_0), & 0 < x < s_0\,, \\ 0, & s_0 < x < 1, \end{cases}$$

s_0 denoting the position of the leading edge.

The electric field along a flow line can be found by differentiating Eq. (3) with respect to time:

$$E(x, t) = E(x_0) + \int_t^t j(t')\,dt'. \tag{5}$$

3. The Function y(t)

Those charges near the electrode at $x = 0$ are moving toward it and will reach it at increasing times according to their initial coordinates. So, we can define a function of time, $y = y(t)$, y being the initial coordinate of the carriers that reach the electrode at the time t. $y(t)$ will be a monotonically increasing function of time as long as the electric field remains negative at $x = 0$.

Obviously, $y(0) = 0$. Charge density and electric field, at time t, when those carriers, initially at y, are at $x = 0$, are by Eqs. (4) and (5),

$$\rho(0, t) = \frac{\rho(y)}{1 + \rho(y)\, t} \tag{6}$$

and

$$E(0, t) = E(y) + \int_0^t j(t')dt'. \tag{7}$$

The expression for the total current, Eq. (2), gives, at $x = 0$,

$$j(t) = \rho(0, t)\, E(0, t) + \frac{dE(0, t)}{dt}. \tag{8}$$

Differentiating (7) with respect to t, we find

$$\frac{dE(0, t)}{dt} = \frac{dE}{dy}\,\frac{dy}{dt} + j(t).$$

But $\frac{dE}{dy} = \rho(y)$ by Poisson's equation at $t = 0$, and substituting the above expression in Eq. (8), we find, taking notice of Eq. (6), that

$$E(0, t) = -\,[1 + \rho(y)\, t]\,\frac{dy}{dt}. \tag{9}$$

Let us call $s(t)$ the coordinate of the far edge of the charge distribution. We put $s(0) = s_0$. The amount of charge between the planes at y and s_0 (at $t = 0$) is conserved during their motion.

We may, therefore, write

$$E(s) - E(0, t) = E(s_0) - E(y).$$

There is no charge beneath the plane at s and this means that $E(s) = E(1, t)$. Rewriting the above expression, we have

$$E(0, t) = E(y) - E(s_0) + E(1, t). \tag{10}$$

4. The Differential Equation in y and t

In the current mode, the voltage is supposed to be given as a function of time:

$$V(t) = \int_0^1 E\, dx.$$

$V(t)$ is the potential of the electrode at $x = 0$, compared with the grounded electrode at $x = 1$. Integrating by parts, we obtain

$$E(1, t) = V(t) + \int_0^s x\, \rho(x, t)\, dx. \tag{11}$$

We want to write the integral in this expression in terms of quantities defined at $t = 0$. Once this is accomplished, use of $E(1, t)$ in Eq. (10) will allow us to turn Eq. (9) into a differential equation.

With this aim in mind, let us differentiate Eq. (3) with respect to x_0, keeping time fixed. Using Poisson's equation, we get:

$$dx = [1 + \rho(x_0)\, t]\, dx_0 . \tag{12}$$

We need also to express x in the integrand in Eq. (11) in terms of x_0. If we write the **Eq.** (3) foi. the leading edge s and substract it from Eq. **(3)** itself we get

$$x = s + x_0 - s_0 + [E(x_0) - E(s_0)]\, t. \tag{13}$$

s is an unknown function of time and must be related to quantities defined at $t = 0$ and perhaps to y. This can be done by taking the expression (13) for the point $x = 0$, when x_0 turns into y:

$$s = s_0 - y + [E(s_0) - E(y)]\, t. \tag{14}$$

The limits of the integral, in Eq. (11), go obviously in y and s_0, since the integral will be performed in the variable x_0.

Now, Eqs. (12)-(14) can be substituted in Eq. (11), giving

$$E(1,t) = V(t) - (y - s_0)\, E(s_0) + \int_{s_0}^{y} E(x_0)\, dx_0 + \frac{t}{2}\,[E(y) - E(s_0)]^2. \tag{15}$$

Using this equation, together with Eq. (10), in **Eq.** (9), we finally get a differential equation in y:

$$\frac{dy}{dt} = \frac{-1}{1 + \rho(y,t)\,t}\left\{V(t) + E(y) - E(s_0) - (y - s_0)\,E(s_0) + v(y) - v(s_0) + \frac{t}{2}\,[E(y) - E(s_0)]^2\right\}, \tag{16}$$

where

$$v(r) = \int_0^r E(x_0)\, dx_0\,.$$

5. Charge as a Function of Position and Time

Suppose that y has been found from Eq. (16) as a function of time. The motion of the leading edge may be found using Eq. (14) and, from it, the flow lines corresponding to any x_0 can be determined by Eq. (4). In this way, the whole pattern of the charge distribution as a function of position may be found for any time.

6. The Total Current j(t)

If we integrate Eq. (4) in x, from 0 to 1, we get

$$j(t) = \frac{1}{2}\,[E^Z(1, t) - E^Z(O, t)] + V(t). \tag{17}$$

Using Eqs. (15) and (10), together with the solution $y(t)$ of Eq. (16), $j(t)$ may be derived.

7. FSCM in Conducting Medium

We assume now that the dielectric in which FSCM takes place has an intrinsic conductivity τ'. This conductivity may be due either to an ionic process or to some carriers, with charge density ρ_0' – of the same kind as those giving rise to the FSCM – already present in the conduction band of the material. In this case, calling ρ' the density of free charge, we take the density of total charge ρ'' in Poisson's equation[3],

$$\varepsilon \frac{\partial E'}{\partial x'} = \rho' - \rho'_0 = \rho'',$$

as a new variable and use it in the expression of the conduction current density, obtaining

$$i' = \mu\rho' E' = \mu\rho'' E' + \mu\rho'_0 E'.$$

The coefficient of E', in $\mu\rho'_0 E'$, simulates a conductivity with $\tau' = \mu\rho'_0$. In both cases, the conduction density i' may be written as

$$i' = \mu\rho' E' + \tau' E'.$$

Expressed in terms of dimensionless variables, this reads

$$i = \rho E + \tau E, \quad \text{with} \quad \tau' = \mu\rho_0\tau.$$

The equations deduced from the method of characteristics[3] are

$$\frac{dx}{dt} = E, \quad \frac{dE}{dt} = j - \tau E, \quad \frac{d\rho}{dt} = \rho^2 - \tau\rho.$$

We can now follow the same procedure as in the insulating case. The expressions are more involved and we restrict ourselves to those leading directly to the solution of the problem, e.g., Eqs. (4), (9), (10), (13), (14), (15), (16) and (17). They are

$$\rho(x, t) = \rho(x_0)\, e^{-\tau t}\left[1 + \frac{1 - e^{-\tau t}}{\tau}\rho(x_0)\right]^{-1}, \tag{4'}$$

$$E(0, t) = -\left[1 + \frac{1 - e^{-\tau t}}{\tau}\rho(y)\right]\frac{dy}{dt}, \tag{9'}$$

$$E(0, t) = E(1, t) + e^{-\tau t}\left[E(y) - E(s_0)\right] \tag{10'}$$

$$x = s + x_0 - s_0 + \frac{1 - e^{-\tau t}}{\tau}\left[E(x_0) - E(s_0)\right], \tag{13'}$$

$$s = s_0 - y + \frac{1 - e^{-\tau t}}{\tau}\left[E(s_0) - E(y)\right], \tag{14'}$$

$$E(1,\ t) = V(t) + e^{-\tau t}\left\{-(y - s_0)\,E(s_0) + \int_{s_0}^{y} E(x_0)dx_0 + \right.$$

$$\left. + \left[(1 - e^{-\tau t})/2\tau\right]\left[E(y) - E(s_0)\right]^2\right\}, \qquad (15')$$

$$\frac{dy}{dt} = -\left[1 + \frac{1 - e^{-\tau t}}{\tau}\rho(y)\right]^{-1}\left\{V(t) + e^{-\tau t}\left[E(y) - E(s_0) - (y - s_0) \times \right.\right.$$

$$\left.\left. \times\ E(s_0) + v(y) - v(s_0) + \frac{1 - e^{-\tau t}}{2\tau}(E(y) - E(s_0))^2\right]\right\}, \qquad (16')$$

$$j(t) = \frac{1}{2}\left[E^2(1,\ t) - E^2(0, t)\right] + V(t) + \tau V(t). \qquad (17')$$

The total current can be obtained following the procedure scheduled in parts 5 and 6, substituting there the unprimed numbered equations by the corresponding primed ones given above.

8. Application

Obviously the differential equation, Eq. (16) or Eq. (16'), can hardly be expected to be easily integrable, with the possible exception of the box distribution. It is straightforward to verify that in this case it leads to the correct solution for the motion of the front edge $s(t)$ (Refs. 6,7). In general, Eq. (16) or (16') must be handled by computer, a very easy task indeed, nowadays.

For the sake of illustration, we show the solution for the initial charge distribution, $\rho(x, 0) = 1 - 2x$ for $0 < x < 1/2$, in an insulating ($\tau = 0$) dielectrics and with $V(t) = 0$ (short circuit); we have $s_0 = 0.5$.

Fig. 1 shows x and $s(t) - s_0$ as a function of time t, $t_c = 30.9$, indicating the time when $s(t) = 1$. Fig. 2 shows the evolution of charge density as a function of position, for several times. It is seen that the charge distribution tends rapidly to the box distribution as has already been found by J. Van Turnhout[8].

Fig. 4 shows the negative of the total current as a function of time; it decreases monotonically to zero.

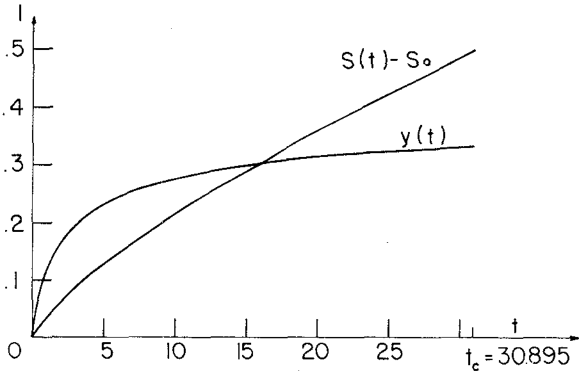

Fig. 1 - The function $y(t)$ and the motion of the leading edge of the charge distribution (minus its initial values, .5). The ordinate 1 represents linear dimension in reduced units. $t_c = 30.895$ is the time for which $s(t) = 1$. The corresponding value of y, $y(t_c)$, is 0.335.

9. Current Reversal

In the following discussion, we will suppose $V = 0$ and $\tau = 0$. Defining the center of mass of the charge distribution, $\bar{x}$, by

$$\bar{x} = q^{-1} \int_0^1 x\rho \, dx, \qquad q = \int_0^1 \rho \, dx,$$

it is **easy** to deduce the following relations

$$\begin{aligned} j(t) &= (3 - 1/2)\, q^2, \\ E(l,t) &= zq. \end{aligned} \tag{18}$$

Now, since $j = \dfrac{dE(1,t)}{dt}$, we have

$$j = q\frac{d\bar{x}}{dt} + \bar{x}\frac{dq}{dt}. \tag{19}$$

The time derivative of Eq. (18), gives

$$\frac{dj}{dt} = q^2\frac{d\bar{x}}{dt} + \frac{2j}{q}\frac{dq}{dt}. \tag{20}$$

Suppose that j(0) is small and negative. This happens if $-E(0,t) = E(1,t) + \delta$, δ being small (Eq. (17)). Therefore, Eqs. (19) and (20) give

$$\frac{d\bar{x}}{dt} \simeq -\frac{\bar{x}}{q}\frac{dq}{dt}, \quad \frac{dj}{dt} \simeq q^2\frac{d\bar{x}}{dt}.$$

Since $\frac{dq}{dt}$ is negative, and $\bar{x}$ is always positive, $\frac{d\bar{x}}{dt}$ is positive. This shows that $\frac{dj}{dt}$ is also positive. Therefore, if j were initially negative, it could reverse its sign in view of the positive value of its derivative. It is not

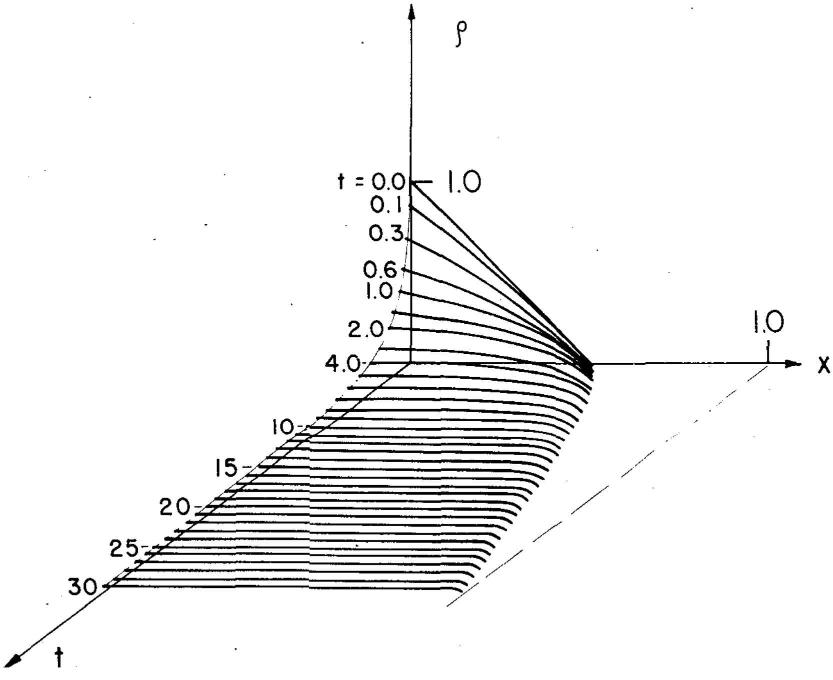

Fig. 2 - Three dimensional plot of the charge distribution as a function of the position, for several times. The $t = 0$ labeled curve represents the initial density, $\rho(x) = 1 - 2x$, $0 < x < s$. The axes correspond, in the usual xyz representation, to time, distance and charge density. (The time corresponding to the unlabeled curves can be found by regular interpolation from the times assigned to the labelled curves nearest to it).

surprising that even under a small negative applied voltage a system can show such a current reversal. In this case, the current would start negative, become positive for a while, returning finally to its more stable negative value.

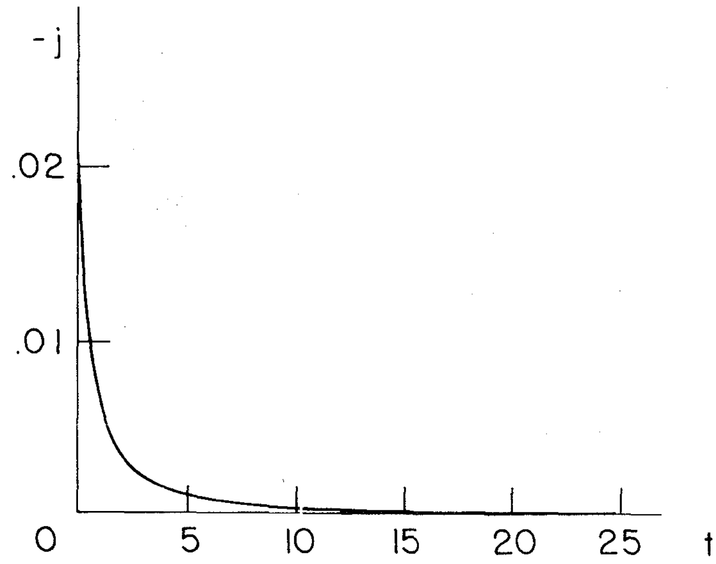

Fig. 3 - The negative of the total current as a function of time.

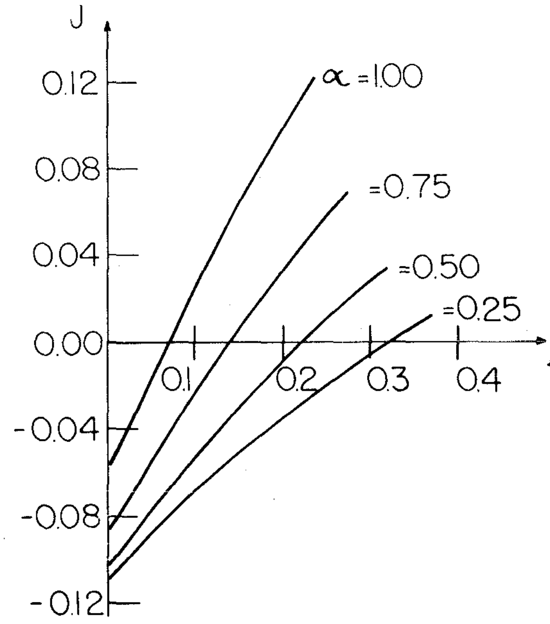

Fig. 4 - Current reversal for charge distribution of the form $\rho(x, 0) = e^{\alpha x}$, $0 \leq x \leq .85$. The parameter α labels the curves.

We have found that the condition for observing the current reversal is met for monotonically increasing charge distributions at $t = 0$, stopping at some point s_0, near the electrode at $x = 1$. Fig. 4 shows several discharges of an exponentially increasing charge distribution (e^{ax}), ending abruptly at $s_0 = .85$. These curves were obtained using the equations deduced in Section 4 and are shown for the time interval corresponding to s – giving the position of the shock front – between .85 and 1.

10. Final Remarks

This work is a step in the mathematical solution of the one carrier FSCM problem. Its theoretical importance lays in the method, which can be extended to cover the most general situation in which the space charge occupies the whole space. between the electrodes, as will be shown in a forthcoming article. On the other hand, providing an exact solution, the way now is open for trying approximate solutions carrying those most essential features leading to a reasonable correct description of the behavior of the externa1 current.

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