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Transient States of Electric Conduction in Solid Dielectric Including Carrier Recombination. I. Ideal Dielectric Without Traps

by

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Summary. A model of a dielectric in which the charge carriers are electrons and holes is considered. The flow of charge is described by the Gauss equation, the continuity equation and an equation for the kinetics of carrier recombination. The boundary conditions are determined on the basis of the investigated mechanisms of injections of charge carriers from the electrode into the dielectric. The effect of injection mechanisms, carrier mobility and recombination coefficient on time curves of absorption intensity is investigated. The problem is solved numerically.

1. Introduction. Two groups of problems should be distinguished in the macroscopic theory of space charge in solid dielectric [3]:

— problems of dielectric interior description, and

— problem of the description of the electrode-dielectric contact.

The interior of a dielectric may be described by magnitudes such as electric field intensity, space charge density, electric permeability, charge carrier mobility, etc. The electrode-dielectric contact is characterized by the mechanism of charge injection from the electrode into the dielectric. One of the aims of space charge theory is the provision of criteria for verifying the electrode-dielectric contact and the dielectric interior. For example, given the time course of absorption current density, one could determine the presence of positive charge carriers and negative charge carriers, and also determine the mechanism of charge injection into the dielectric.

In the present work we consider a model of dielectric featuring density ${}^{+}q_v$ of the positive charge and density ${}^{-}q_v$ of the negative charge. The dielectric interior is described by the Gauss equation, the continuity equation, and the given voltage condition

$$\varepsilon\frac{\partial E(x,t)}{\partial x} = {}^{+}q_v(x,t) + {}^{-}q_v(x,t) \tag{1}$$

$$\frac{\partial}{\partial x}\{\mu_p\, {}^{+}q_v(x,t)\, E(x,t) - \mu_n\, {}^{-}q_v\, E(x,t)\} + \frac{\partial\, {}^{+}q_v(x,t)}{\partial t} + \frac{\partial\, {}^{-}q_v(x,t)}{\partial t} = 0 \tag{2}$$

$$\int_0^L E(x,t)\,dx = U \tag{3}$$

with $\mu_p > 0$ and $\mu_n > 0$, where x — distance of the point from the electrode, t — time, ε — immediate electric permeability; μ_p, μ_n — mobility of the positive and the negative charge, respectively; E — intensity of electric field, L — distance between electrodes, U — voltage applied to the electrodes.

The problem of electric conductivity in dielectric thus formulated, requires the introduction of an additional equation. Considered hitherto was a model of dielectric in which the densities ${}^{+}q_v(x,t)$ and ${}^{-}q_v(x,t)$ satisfied the law of mass action ${}^{+}q_v\,{}^{-}q_v = \text{const}$. Note that the law of mass action does not contain members characterizing the transient state, such as $\frac{\partial\, {}^{+}q^v}{\partial t}$ or $\frac{\partial\, {}^{-}q^v}{\partial t}$. There are tenets in solid state theory, such as carrier recombination, which indicate that the equation complementing Eqs (1)–(3) may be written in the form

$$F\left(\frac{\partial\, {}^{-}q_v}{\partial t};\ \frac{\partial\, {}^{-}q_v}{\partial x};\quad {}^{-}q_v;\ \frac{\partial E}{\partial x};\quad E;\ {}^{+}q_v\right) = 0. \tag{4}$$

Eqs (1)–(4) fully describe the transient state of electric conductivity in a dielectric. In what follows it will be demonstrated that the solution of transient state will require additional information about boundary and initial conditions. The aim of the present work is the determination of the time course of absorption current density $j_a(t)$

$$j_a(t) = \varepsilon\frac{\partial E(x,t)}{\partial t} + \mu_p\, {}^{+}q_v(x,t)\, E(x,t) - \mu_n\, {}^{-}q_v(x,t)\, E(x,t) \tag{5}$$

for given function F and for given mechanisms of charge injection and initial values.

2. Dielectric model. Charge carriers in the solid body are electrons and holes. Densities $^{+}q_v(x,t)$ of the positive charge and $^{-}q_v(x,t)$ of the negative charge are determined by excess carrier concentrations [5]

$$(6) \qquad ^{+}q_v(x,t) = e_0\left(p(x,t) - p_0\right); \qquad ^{-}q_v(x,t) = -e_0\left(n(x,t) - n_0\right)$$

where $e_0 = 1.6\ 10^{-19}\ C$; p, n — nonequilibrium concentrations of holes and electrons, respectively; p_0, n_0 — equilibrium concentrations of holes and electrones, respectively.

Carriers injected into the dielectric recombine. The assumed example of Eq. (4) is the equation describing the change of electron concentration due to recombination [1, 2, 4]

$$(7) \qquad \frac{\partial n(x,t)}{\partial t} - \frac{\partial}{\partial x}\{\mu_n n(x,t) E(x,t)\} + \beta\left(n(x,t) p(x,t) - n_0 p_0\right) = 0$$

where β is the recombination coefficient of constant value characteristic for the given mechanism of recombination. In what follows we consider an ideal dielectric $n_0 = p_0 = 0$. After taking into consideration Eqs (6) and (7), Eqs (1)–(4) take the form

$$(8) \qquad \varepsilon \frac{\partial E(x,t)}{\partial x} = e_0\left(p(x,t) - n(x,t)\right)$$

$$(9) \qquad \frac{\partial}{\partial x}\{\mu_p p(x,t) E(x,t) + \mu_n n(x,t) E(x,t)\} + \frac{\partial p(x,t)}{\partial t} - \frac{\partial n(x,t)}{\partial t} = 0$$

$$(10) \qquad \int_0^L E(x,t)\,dx = U; \qquad U = \text{const}; \qquad U > 0$$

$$(11) \qquad \frac{\partial n(x,t)}{\partial t} = \frac{\partial}{\partial x}\{\mu_n n(x,t) E(x,t)\} - \beta n(x,t) p(x,t).$$

Eqs (8)–(11) describe the transient state of electric conductivity in a dielectric, with carrier recombination taken into account. The density of absorption current $j_a(t)$ described by (5) takes the form

$$(12) \qquad j_a(t) = \varepsilon \frac{\partial E(x,t)}{\partial t} + e_0 \mu_p p(x,t) E(x,t) + e_0 \mu_n n(x,t) E(x,t).$$

The aim of this work is the investigation of the effect of the recombination coefficient and of carrier mobility on time courses of absorption current density $j_a(t)$.

3. Problem solution. The time courses of absorption current density were determined numerically. The considerations are performed in the system of dimensionless variables u, E', x', n', p', t', r, β_R and j_a described by the equations

$$u' = \frac{U}{U_0}; \quad E' = \frac{LE}{U_0}; \quad x' = \frac{x}{L}; \quad n' = \frac{e_0 L^2 n}{\varepsilon U_0}; \quad p' = \frac{e_0 L^2 p}{\varepsilon U_0} \tag{13}$$
$$t' = \frac{\mu_n U_0 t}{L^2}; \quad r = \frac{\mu_p}{\mu_n}; \quad \beta_R = \frac{e_0 \mu_n}{\varepsilon \beta}; \quad j'_a = \frac{L^3 j_a}{\varepsilon U_0^2 \mu_n}$$

where U_0 is the reference voltage.

After omitting the prim symbol in these quantities, the Eqs (8)–(11) in the system of dimensionless variables assume the following form

$$\frac{\partial E(x,t)}{\partial x} = p(x,t) - n(x,t) \tag{14}$$

$$\frac{\partial}{\partial x}\{rp(x,t)E(x,t) + n(x,t)E(x,t)\} + \frac{\partial p(x,t)}{\partial t} - \frac{\partial n(x,t)}{\partial t} = 0 \tag{15}$$

$$\int_0^1 E(x,t)\,dx = u \tag{16}$$

$$\frac{\partial n(x,t)}{\partial t} = \frac{\partial}{\partial x}\{n(x,t)E(x,t)\} - \frac{1}{\beta_R} n(x,t)p(x,t). \tag{17}$$

In numerical calculations, use was made of the integral form of absorption current density

$$j_a(t) = \int_0^1 [rp(x,t) + n(x,t)]E(x,t)\,dx. \tag{18}$$

Next, the effect of the parameters r and β_R on the time courses of $j_a(t)$ were studied. After transforming Eqs (14), (15) and (17), we get

$$\frac{\partial n}{\partial t} - E\frac{\partial n}{\partial x} - \left\{n(p-n) - \frac{1}{\beta_R} np\right\} = 0 \tag{19}$$

$$\frac{\partial p}{\partial t} + rE\frac{\partial p}{\partial t} + rp(p-n) + \frac{1}{\beta_R} np = 0 \tag{20}$$

whence we obtain equations of characteristics

$$\frac{dx_n}{dt} = -E \quad \text{and} \quad \frac{dn}{dt} = n(p-n) - \frac{1}{\beta_R} np \tag{21}$$

and

$$\frac{dx_p}{dt} = rE \quad \text{and} \quad \frac{dp}{dt} = -rp(p-n) - \frac{1}{\beta_R} np. \tag{22}$$

On the basis of the voltage condition (10) it was assumed that there exist such conditions of charge flow for which the intensity of the electric field $E(x,t)$ is always positive. In the subsequent considerations we assume positive value of electric field intensity $E(x,t)>0$. Hence, from (21) and (22) it results that $\frac{dx_n}{dt}<0$ and $\frac{dx_p}{dt}>0$. From (21) and (22) we get

$$(23)\qquad x_n(t)=-\int_0^t E\,dt+x_n(0)\quad\text{or}\quad x_n(t)=-\int_\lambda^t E\,dt+x_n(\lambda),\qquad \lambda\geqslant 0$$

$$(24)\qquad x_p(t)=\int_0^t rE\,dt+x_p(0)\quad\text{or}\quad x_p(t)=\int_\lambda^t rE\,dt+x_p(\lambda);\qquad \lambda\geqslant 0$$

with $0\leqslant x_n(0)\leqslant 1$ and $0\leqslant x_p(0)\leqslant 1$. The values of concentrations $n(t)$ and $p(t)$ along the characteristics (23) and (24) at arbitrary time t have the form $n(t)=n(x_n(t),t)$ and $p(t)=p(x_p(t),t)$ with $n(0)=n(x_n(0),0)$ and $n(\lambda)=n(x_n(\lambda),\lambda)$ and $p(0)=p(x_p(0),0)$ and $p(\lambda)=p(x_p(\lambda),\lambda)$. Hence it results that if we assume $x_p(\lambda)=0$ and $x_n(\lambda)=1$, then to determine the values of concentrations $n(x,t)$ and $p(x,t)$ at any point in the dielectric we need information about the initial values $n(x,0)$ and $p(x,0)$ and information about the boundary values $p(0,t)$ and $n(1,t)$. The above reasoning is illustrated in Fig. 1.

In this work we consider the electric conductivity in an ideal dielectric $n_0=p_0=0$; accordingly, the initial values of carrier concentration are zero, $n(x,0)=p(x,0)=0$. The determination of boundary conditions $p(0,t)$ and $n(1,t)$ is one of the problems of the theory of the space charge in a dielectric. There are various mechanisms of charge carrier injection from the electrode into the dielectric [1, 5], e.g. the Schottky effect, the tunnel effect. These mechanisms are described by the function of

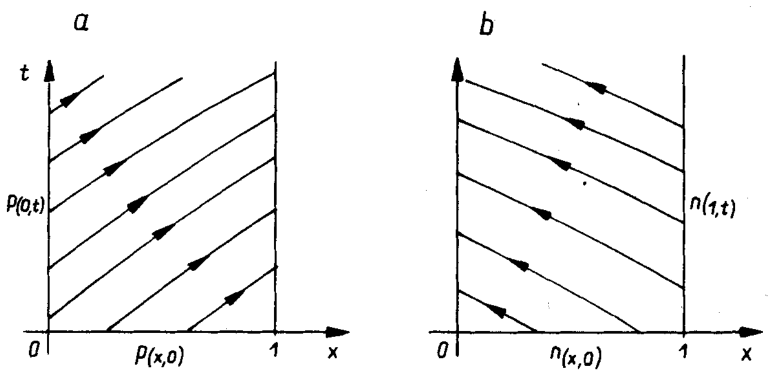


Fig. 1. Characteristics of absorption of: a — positive charge carriers, b — negative charge carriers

current density j_0 of the injected carrier and the electric field intensity E_0 at the injecting electrode

(25) $$j_0 = a \exp\left(b\sqrt{E_0}\right),$$

(26) $$j_0 = a_1 E_0^2 \exp\left(-b_1/E_0\right),$$

where a, b, a_1 and b_1 are material constants characteristic for the given electrode-dielectric contact at specific temperature. A major difficulty in determining the boundary values $p(0, t)$ and $n(1, t)$ is the determination of the value of current density j_0 of the injected carriers. According to the theory of electromagnetic field, the transport current density $j(x, t)$

(27) $$j(x, t) = \left[rp(x, t) + n(x, t)\right] E(x, t)$$

and current density j_0 satisfy the so called boundary equations

$$j(0, t) - j_0(0, t) = \pm \frac{dq_s}{dt}\bigg|_{x=0}; \quad j(1, t) - j_0(1, t) = \pm \frac{dq_s}{dt}\bigg|_{x=1}$$

where $q_s|_{x=0}$ and $q_s|_{x=1}$ denote the density of the surface charge on the surface of dielectric at electrodes $x = 0$ and $x = 1$, respectively.

We assumed zero value of the derivative of surface charge density at the electrodes $\frac{dq_s}{dt}\bigg|_{x=0} = 0$ and $\frac{dq_s}{dt}\bigg|_{x=L} = 0$, and on this basis we determined the boundary values $p(0, t)$ and $n(1, t)$ of charge carrier concentration at the electrodes

(28) $$\left[rp(0, t) + n(0, t)\right] E(0, t) = f_0\left[E(0, t)\right],$$

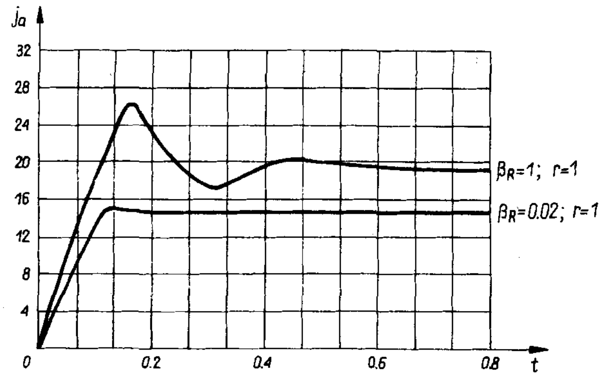
(29) $$\left[rp(1, t) + n(1, t)\right] E(1, t) = f_1\left[E(1, t)\right]$$

with the values of functions $f_0[E(0, t)]$ and $f_1[E(1, t)]$ being equal to the values of current density j_0 determined from either (25) or (26). The boundary values $n(0, t)$ and $p(1, t)$ are described by Eqs (21)–(24), while the values of the intensity of electric field at the electrodes are determined from the Gauss equation (14) and the voltage condition (16)

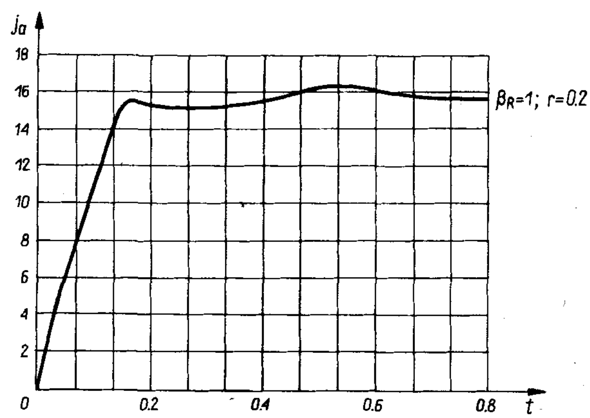
(30) $$E(1, t) = \int_0^1 \left[p(x, t) - n(x, t)\right] dx + E(0, t)$$

$$E(0, t) = u - \int_0^1 (1 - x)\left[p(x, t) - n(x, t)\right] dx.$$

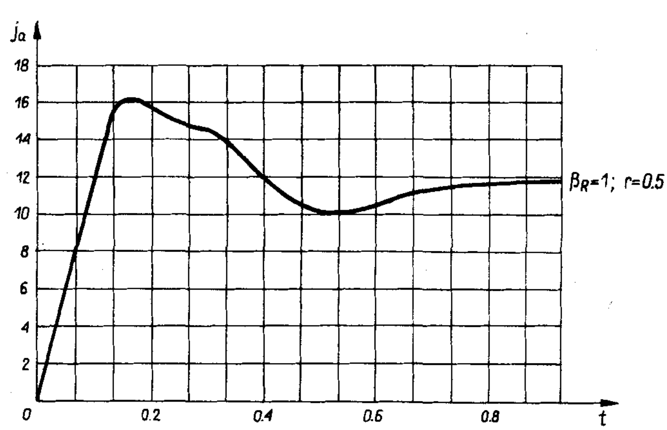
Eqs (21)–(24) and (28)–(30) were solved numerically. The density of the absorption current was determined from Eq. (18). In this work we also considered the electrode-dielectric contact for which the boundary values $p(0, t)$ and $n(1, t)$ are constant, without precluding, however, other ways



$j_{(0,t)} = a_1 E^2_{(0,t)} \exp(-b_1/E_{(0,t)})$; $j_{(1,t)} = a_1 E^2_{(1,t)} \exp(-b_1/E_{(1,t)})$

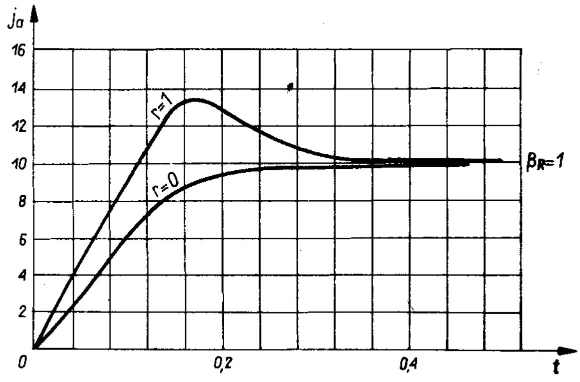


$j_{(0,t)} = a_1 E^2_{(0,t)} \exp(-b_1/E_{(0,t)})$; $j_{(1,t)} = a_1 E^2_{(1,t)} \exp(-b_1/E_{(1,t)})$

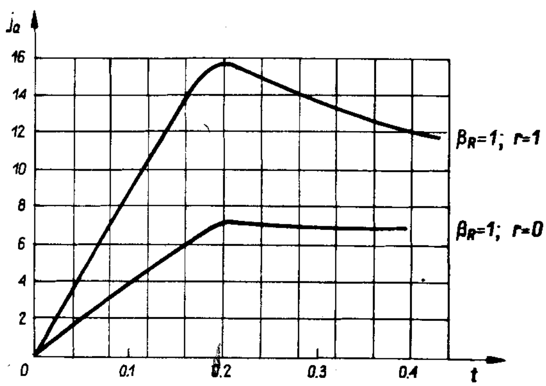


$j_{(0,t)} = a \exp(b\sqrt{E_{(0,1)}})$; $j_{(1,t)} = a_1 E^2_{(1,t)} \exp(-b_1/E_{(1,t)})$

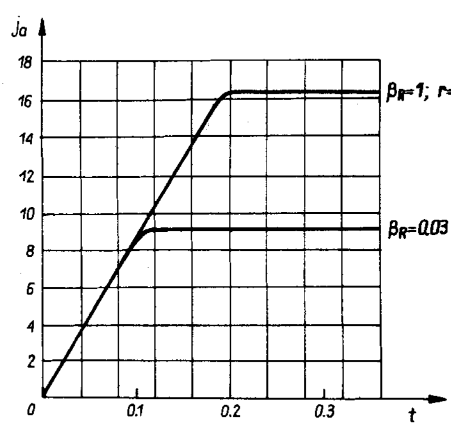
Figs. 2–4. Time course of absorption current density



$p_{(0,t)} = const$; $j_{(1,t)} = const$



$p_{(0,t)} = const$; $j_{(1,t)} = a_1 E^2_{(1,t)} \exp(-b_1/E_{(1,t)})$



$p_{(0,t)} = const$; $n_{(1,t)} = const$

Figs. 5–7. Time course of absorption current density of determining the boundary conditions. The results of numerical calculations are shown in the Figures 2–7.

4. Conclusions. As it was mentioned in the Introduction, we intended to determine the time course of absorption current density $j_a(t)$ at given mechanisms of charge injection from the electrodes into the dielectric and for given function F describing carrier recombination. We considered a case of charge flow in which the distribution of electric field intensity $E(x, t)$ is always positive. Under such conditions it was found that the injection mechanism has an effect on the shape of the curve of $j_a(t)$ at given parameters μ_n, μ_p, β. When the density of transport current at the electrodes $j(0, t)$ and $j(L, t)$ is a function of electric field intensity — $E(0, t)$ and $E(L, t)$, respectively — there appear extrema (maximum followed by a minimum) on the $j_a(t)$ curve, or only a maximum $(p(0, t) = \text{const})$. Moreover, the curve of $j_a(t)$ at first grows from zero to maximum value and after a time attains a steady value. In the case of constant concentration values $p(0, t) = \text{const}$ and $n(L, t) = \text{const}$ on the boundaries, the time course of absorption current density $j_a(t)$ grows initially to finally attain a steady value.

An increase of recombination coefficient β or a change of parameter $r = \frac{\mu_p}{\mu_n}$ from $r = 1$ to $r < 1$ improves the stability of the $j_a(t)$ curve $\left(\frac{dj_a}{dt} \approx 0 \text{ and } j_a \neq 0\right)$ and reduces the value of $j_a(t)$.

In contrast to the dielectric with conductance in which at time $t = 0$ there occurs a jump of absorption current value, the ideal dielectric with carrier recombination exhibits a time course of absorption current that is relaxational in nature.

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Б. Свистач, **Нестационарные инжекционные токи в твердом диэлектрике с рекомбинацией носителей зарядов. Част I. Идеальный диэлектрик без ловушек**

В настоящей статье рассматривается модель диэлектрика с инжектированными электронами и дырками. Перенос заряда описывается системой уравнений: уравнение Гаусса, закон сохранения заряда, уравнение, описывающее рекомбинацию носителей. Граничные условия определяются по механизму инжектирования носителей заряда с электродов в диэлектрик. Исследуется влияние механизмов инжекции, подвижности носителей и коэффициента рекомбинации на переходные характеристики плотности тока абсорбции. Задача решена на вычислительной машине ВМ.