

Kinetic Model of Carrier Recombination in Solid Dielectric

by

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Summary. In this paper the model of solid dielectric is presented, in which the space-charge is formed by free and trapped electrons, as well as by holes. Charge transport is described by means of the Gauss law, the continuity equation and the system of equations describing the contribution of electron localization and delocalization states in the generation-recombination processes.

It is assumed that initial values of carrier concentration are equal to the values of equilibrium concentration. Boundary values of free carriers concentration are established basing on mechanisms of carriers injection from metal into the dielectric. The influence of generation-recombination processes and of mechanisms of injection on the time-course of absorption current density are also determined, the latter being evaluated numerically.

1. Introduction. The objective of the theory of space charge in a solid dielectric is the creation of theoretical bases of identifying processes occurring during charge transport in the metal-dielectric-metal system. Till now [4-6] two conceptions of conductance identification in the system metal-dielectric-metal were considered:

— the resorption state conception

$$(1) \quad \int_0^L E(x, t) dx = 0; \quad E(x, 0) \neq 0; \quad 0 \leq x \leq L$$

— the absorption state conception

$$(2) \quad \int_0^L E(x, t) dx = U; \quad U = \text{const}; \quad U > 0$$

where E — electric field intensity, t — time, x — distance of point from the electrode, L — distance between electrodes, U — voltage applied to the electrodes.

Describing the bipolar conductivity of resorption state and of absorption state, one must simultaneously consider processes occurring inside the dielectric and those at the electrodes. The further studies are intended to relate the processes inside the dielectric and electrode processes with the time courses of resorption and absorption current densities.

In this work we consider absorption state with carriers of positive and negative charge. The basic equations in the description of bipolar conductivity are two Maxwell equations:

— the Gauss law

$$(3) \quad \frac{\partial}{\partial x}(\varepsilon E) = e_0 \{(p - p_0) - (n - n_0)\}$$

— the continuity equation

$$(4) \quad \frac{\partial}{\partial x}(\mu_p p E + \mu_n n E) + \frac{\partial p}{\partial t} - \frac{\partial n}{\partial t} = 0$$

where μ_n, μ_p — mobility of electrons and holes, $e_0 = 1.6 \cdot 10^{-11}$ C, ε — dielectric constant, n, p — nonequilibrium concentrations of electrons and holes, n_0, p_0 — equilibrium concentrations of electrons and holes. In order to give a full description of conductivity in this approach, one must take into consideration an additional equation describing the dependence between carrier concentrations, e.g. of the form [6]

$$(5) \quad F\left(\frac{\partial n}{\partial t}; \frac{\partial n}{\partial x}; \frac{\partial E}{\partial x}; E; n; p\right) = 0.$$

The form of function F depends on the generation-recombination processes in the dielectric. In [6] a model of dielectric was considered in which Eq. (5) described the "bimolecular recombination law"

$$(6) \quad \frac{\partial n}{\partial t} = \frac{\partial}{\partial x}(\mu_n n E) - \beta (np - n_0 p_0)$$

where β is the recombination coefficient.

It may be demonstrated that the coefficient of recombination may be related to material constants ε and μ , e.g. as follows [3]

$$(7) \quad \beta = \frac{e_0 \mu}{\varepsilon}; \quad \mu = \mu_n = \mu_p.$$

In this description the concise Eq. (6) does not describe in detail the

effect of defects in the dielectric's crystalline structure on the generative-recombination processes, and so the model (3), (4), (6) needs to be modified.

Due to defects in the crystalline structure, impurities, in the dielectric there appear the states of electron localization and delocalization. In addition, light and temperature are additional factors determining the change of free carrier concentration [1, 3]. Taking into consideration trapping states, we introduce in Eqs (3) and (4) concentrations of trapped carriers [3]

$$(8) \quad \frac{\partial}{\partial x}(\varepsilon E) = e_0 \{(p - p_0) - (n - n_0) - \sum_{i=1}^m (n_{ti} - n_{ti,0})\}$$

$$(9) \quad \frac{\partial}{\partial x}(\mu_p p E + \mu_n n E) + \frac{\partial p}{\partial t} - \frac{\partial n}{\partial t} - \sum_{i=1}^m \frac{\partial n_{ti}}{\partial t} = 0$$

where n_{ti} — nonequilibrium concentration of trapped electrons in the i -th group of trapping states, $n_{ti,0}$ — equilibrium concentration of trapped electrons in the i -th group of trapping states, m — number of trapping state groups. Equation (5) should be replaced by a suitable system of equations describing the participation of trapping states in generation-recombination processes of charge carriers. The equations thus formulated, will serve as a basis for the study of the effect of generation-recombination and electrode processes on the time courses of the density of absorption current $j_a(t)$.

2. Assumption of dielectric model. The following levels were distinguished in the set of trapping levels:

— the trapping level closest to the electron conductance region, termed the "first level", with trapped electron concentration n_{t1} , and

— the trapping level nearest to the hole conductance region termed the "second level" with trapped electron concentration n_{t2} .

It was assumed in the present work that the transition of electrons from the first to the second level through the states between them may be replaced by the so called effective transition [2] by introducing the coefficients C_{12} and C_{21} into the equations. This assumption does not bring about a loss of generality of considerations and its purpose is to avoid an excess of equations and parameters. After reduction to two trapping levels $m = 2$, the equations of positive and negative charge carrier transport take the form

$$(10) \quad \frac{\varepsilon}{e_0} \frac{\partial E}{\partial x} = (p - p_0) - (n - n_0) - (n_{t1} - n_{t1,0}) - (n_{t2} - n_{t2,0})$$

$$(11) \quad \frac{\partial}{\partial x} (\mu_p p E + \mu_n n E) + \frac{\partial p}{\partial t} - \frac{\partial n}{\partial t} - \frac{\partial n_{t1}}{\partial t} - \frac{\partial n_{t2}}{\partial t} = 0$$

$$(12) \quad \frac{\partial n_{t1}}{\partial t} = C_n n (N_{t1} - n_{t1}) - v_1 n_{t1} - C_{12} n_{t1} (N_{t2} - n_{t2}) + C_{21} n_{t2} (N_{t1} - n_{t1})$$

$$(13) \quad \frac{\partial n_{t2}}{\partial t} = C_{12} n_{t1} (N_{t2} - n_{t2}) - C_{21} n_{t2} (N_{t1} - n_{t1}) - C_p p n_{t2} + v_2 (N_{t2} - n_{t2})$$

$$(14) \quad \frac{\partial n}{\partial t} = \frac{\partial}{\partial x} (\mu_n n E) - C_n n (N_{t1} - n_{t1}) + v_1 n_{t1}$$

where N_{t1}, N_{t2} — trap concentration in the first and second trapping level, respectively; $C_n, v_1, C_{12}, C_{21}, C_p, v_2$ — material coefficients. Equations (10)–(14) and the integral condition (2) describe the absorption transition state. The material constants in the equations usually depend on the electric field intensity. In this work we assume these coefficients to be independent of electric field intensity, which makes possible to reduce their number:

$$(15) \quad v_1 = C_n (N_{t1} - n_{t1,0}) \frac{n_0}{n_{t1,0}}$$

$$(16) \quad C_{21} = C_{12} \frac{(N_{t2} - n_{t2,0})}{(N_{t1} - n_{t1,0})} \frac{n_{t1,0}}{n_{t2,0}}$$

$$(17) \quad C_p = v_2 \frac{(N_{t2} - n_{t2,0})}{p_0 n_{t2,0}}$$

Relations (15)–(17) result from the equations (12)–(14) written for equilibrium conditions.

Determined next was the time course of the density of absorption current

$$(18) \quad j_a(t) = \frac{e_0}{L} \int_0^L (\mu_p p E + \mu_n n E) dx.$$

Equation (18) results from (10), (11) and the voltage condition (2).

The aim of this work is the study of the effect of generation-recombination and electrode processes on the time courses of the density of absorption current $j_a(t)$.

3. Problem solution. The time course of the density of absorption current $j_a(t)$ was determined numerically. A low degree of trap filling in nonequilibrium conditions $N_{t1} \gg n_{t1}$ and $N_{t2} \gg n_{t2}$ and a low degree of trap filling in equilibrium conditions $N_{t1} \gg n_{t1,0}$ and $N_{t2} \gg n_{t2,0}$ was assumed in the numerical calculations. This assumption makes possible to simplify the r.h.s. of Eqs (12)–(14) and relations (15)–(17). A system of nondimensional variables: $E', u', t', p', n', n'_t, \tau'_n, \tau'_p, \tau'_1, \tau'_2, \tau'_{12}, \tau'_{21}, j'_a, r$ described by the formulas

$$(19) \quad \begin{aligned} E' &= \frac{LE}{U_0}; & u' &= \frac{U}{U_0}; & x' &= \frac{x}{L}; & p' &= \frac{L^2 e_0 p}{\varepsilon U_0}; & n' &= \frac{L^2 e_0 n}{\varepsilon U_0} \\ n'_t &= \frac{L^2 e_0 n_t}{\varepsilon U_0}; & t' &= \frac{\mu_n U_0 t}{L^2}; & \tau'_n &= \frac{\mu_n U_0}{L^2 C_n N_{t1}}; & \tau'_p &= \frac{e_0 \mu_n}{\varepsilon C_p} \\ \tau'_1 &= \frac{\mu_n U_0}{L^2 v_1}; & \tau'_2 &= \frac{\varepsilon \mu_n U_0^2}{L^4 e_0 v_2 N_{t2}}; & \tau'_{12} &= \frac{\mu_n U_0}{L^2 C_{12} N_{t2}} \\ \tau'_{21} &= \frac{\mu_n U_0}{L^2 C_{21} N_{t1}}; & j'_a &= \frac{L^3 j_a}{\varepsilon \mu_n U_0^2}; & r &= \frac{\mu_p}{\mu_n} \end{aligned}$$

(where U_0 is the reference voltage) was used in the numerical analysis. After omitting the prime symbol, the charge transport equations take the following form in the system of nondimensional variables

$$(20) \quad \frac{\partial E}{\partial x} = (p - p_0) - (n - n_0) - (n_{t1} - n_{t1,0}) - (n_{t2} - n_{t2,0})$$

$$(21) \quad \frac{\partial}{\partial x} (rpE + nE) + \frac{\partial p}{\partial t} - \frac{\partial n}{\partial t} - \frac{\partial n_{t1}}{\partial t} - \frac{\partial n_{t2}}{\partial t} = 0$$

$$(22) \quad \frac{\partial n_{t1}}{\partial t} = \frac{n}{\tau_n} - \frac{n_{t1}}{\tau_1} - \frac{n_{t1}}{\tau_{12}} + \frac{n_{t2}}{\tau_{21}}$$

$$(23) \quad \frac{\partial n_{t2}}{\partial t} = \frac{n_{t1}}{\tau_{12}} - \frac{n_{t2}}{\tau_{21}} - \frac{pn_{t2}}{\tau_p} + \frac{1}{\tau_2}$$

$$(24) \quad \frac{\partial n}{\partial t} = \frac{\partial}{\partial x} (nE) - \frac{n}{\tau_n} + \frac{n_{t1}}{\tau_1}$$

with the integral condition

$$(25) \quad \int_0^1 E dx = u: \quad u = \text{const}; \quad u > 0.$$

The equilibrium concentrations satisfy the condition of neutrality

$$(26) \quad p_0 = n_0 + n_{t1,0} + n_{t2,0}.$$

The time course of absorption current density $j_a(t)$ described by the integral (18) has the following integral form in the system of nondimensional variables

$$(27) \quad j_a(t) = \int_0^1 (rpE + nE) dx.$$

After taking into consideration transformations (19), the relations (15)–(17) describing the dependence between coefficients describing generation-recombination processes are reduced to the form

$$(28) \quad \tau_{21} = \tau_{12} \frac{n_{t2,0}}{n_{t1,0}}; \quad \tau_1 = \tau_n \frac{n_{t1,0}}{n_0}; \quad \tau_2 = \frac{\tau_p}{p_0 n_{t2,0}}.$$

After transformations we get the following quasi-linear partial differential equations:

$$(29) \quad \frac{\partial n}{\partial t} - E \frac{\partial n}{\partial x} - n(p - n - n_{t1} - n_{t2}) + \frac{n}{\tau_n} - \frac{n_{t1}}{\tau_1} = 0$$

$$(30) \quad \frac{\partial p}{\partial t} + rE \frac{\partial p}{\partial x} + rp(p - n - n_{t1} - n_{t2}) + \frac{pn_{t2}}{\tau_p} - \frac{1}{\tau_2} = 0.$$

Hence we write the characteristics equations

$$(31) \quad \frac{dx_n}{dt} = -E \quad \text{and} \quad \frac{dn}{dt} = n(p - n - n_{t1} - n_{t2}) - \frac{n}{\tau_n} + \frac{n_{t1}}{\tau_1}$$

$$(32) \quad \frac{dx_p}{dt} = rE \quad \text{and} \quad \frac{dp}{dt} = -rp(p - n - n_{t1} - n_{t2}) - \frac{pn_{t2}}{\tau_p} + \frac{1}{\tau_2}.$$

Basing on the integral condition (25) we considered such conditions of charge flow in which the electric field intensity is always positive $E(x, t) > 0$. It results from this that the gradients of characteristics (31) and (32) in the dielectric and next to the electrodes are always positive for holes $dx_p/dt > 0$ and negative for electrons $dx_n/dt < 0$. Thus, in order to determine the time course of absorption current density $j_a(t)$ we need to know the boundary and initial conditions. The following initial conditions are assumed here:

$$(33) \quad p(x, 0) = p_0; \quad n(x, 0) = n_0; \quad n_{t1}(x, 0) = n_{t1,0}; \quad n_{t2}(x, 0) = n_{t2,0}$$

The boundary values $n(1, t)$ and $p(0, t)$ were determined on the basis of the mechanism of carrier injection from the metal into the dielectric. To this end the density of current of transport $j(x, t)$ of carriers in the dielectric

$$(34) \quad j(x, t) = [rp(x, t) + n(x, t)] E(x, t)$$

was bound with the density of the current j_0 of the injected carriers

$$(35) \quad j_0 = f(E_0)$$

with the boundary equation

$$(36) \quad j(x_0, t) - j_0(x_0, t) = \pm \frac{dq_s}{dt} \Big|_{x=x_0}$$

where x_0 — value $x = 0$ or $x = 1$, E_0 — value of $E(0, t)$ or $E(1, t)$, $f(E_0)$ — function describing the mechanism of electron emission from the metal or dielectric surface into vacuum, q_s — surface density of charge at the dielectric surface next to the electrode.

The boundary equation (36) describes the dependence between transport current density in the dielectric at the surface of contact with the electrode and the density of the injected carrier current density. The surface density of charge q_s results from the deviation of the contact surfaces between the metal and the dielectric and from the existence of surface trapping states.

In the numerical calculations we assume zero value of the derivative of surface charge $dq_s/dt = 0$. Hence, on the basis of (34)–(36) we determined the boundary values of $p(0, t)$ and $n(1, t)$

$$(37) \quad \begin{aligned} [rp(0, t) + n(0, t)] E(0, t) &= f_0[E(0, t)] \\ [rp(1, t) + n(1, t)] E(1, t) &= f_1[E(1, t)] \end{aligned}$$

where f_0 and f_1 are functions describing the mechanism of carrier injection from the electrode to the dielectric. In numerical calculations there were given functions f_0 and f_1 describing the tunnel effect and the Schottky effect. Also considered were contacts described by the equations

$$(38) \quad \begin{aligned} p(0, t) &= \text{const} \\ j(1, t) &= f_1[E(1, t)]. \end{aligned}$$

Boundary values of electric field intensity $E(0, t)$ and $E(1, t)$ were determined on the basis of Eq. (20) and the integral condition (25)

$$(39) \quad \begin{aligned} E(0, t) &= \int_0^1 (1-x)(p-n-n_{t1}-n_{t2}) dx \\ E(1, t) &= E(0, t) + \int_0^1 (p-n-n_{t1}-n_{t2}) dx. \end{aligned}$$

The aim of numerical calculations is the determination of the time course of absorption current density $j_a(t)$ described by the integral formula (27). Equations (31), (32), (22), (23), (23), (28) and (37)–(39) were used in the algorithm that was worked out. The results of numerical calculations are shown in the figures.

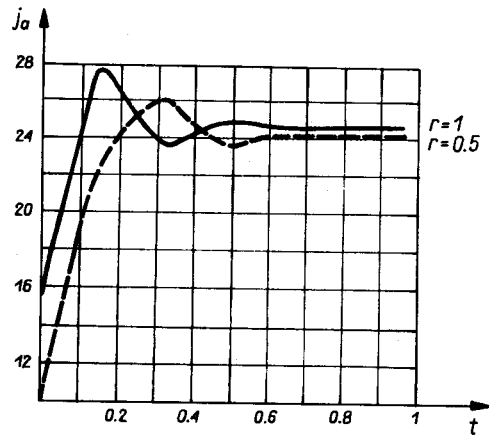


Fig. 1. Time courses of absorption current density in the system of nondimensional variables

$$j(0, t) = aE^2(0, t); j(1, t) = a_1 E^2(1, t); a = a_1 = 1; \tau_n = \tau_p = \tau_{12} = 1$$

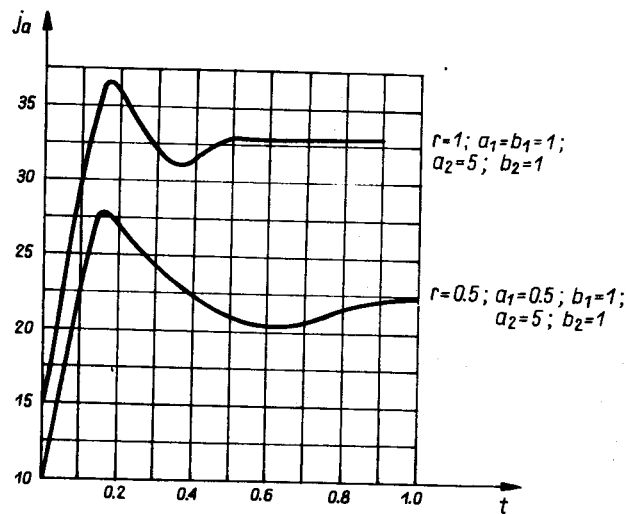


Fig. 2. Time courses of absorption current density in the system of nondimensional variables

$$j(0, t) = a_1 E^2(0, t) \exp(-b_1/E(0, t)); j(1, t) = a_2 \exp(b_2 \sqrt{E(1, t)})$$

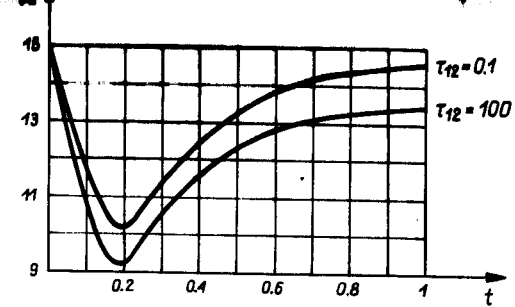


Fig. 3. Time courses of absorption current density in the system of nondimensional variables

$$p(0, t) = 0; j(1, t) = a \exp(b \sqrt{E(1, t)}); a = 11; b = 0.2; r = 1; \tau_n = 0.2; \tau_p = 0.1$$

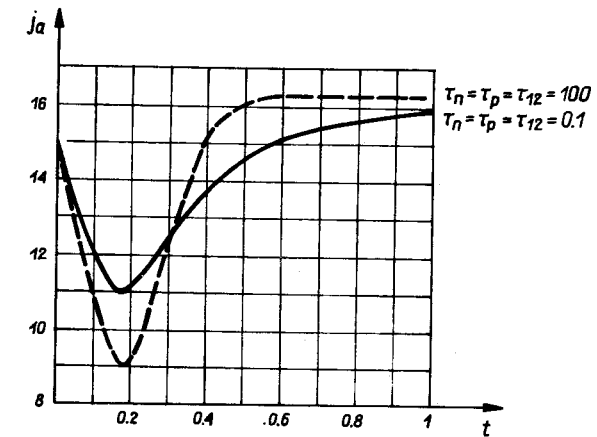


Fig. 4. Time courses of absorption current density in the system of nondimensional variables

$$p(0, t) = 0; j(1, t) = a \exp(b \sqrt{E(1, t)}); a = 12; b = 0.2; r = 1$$

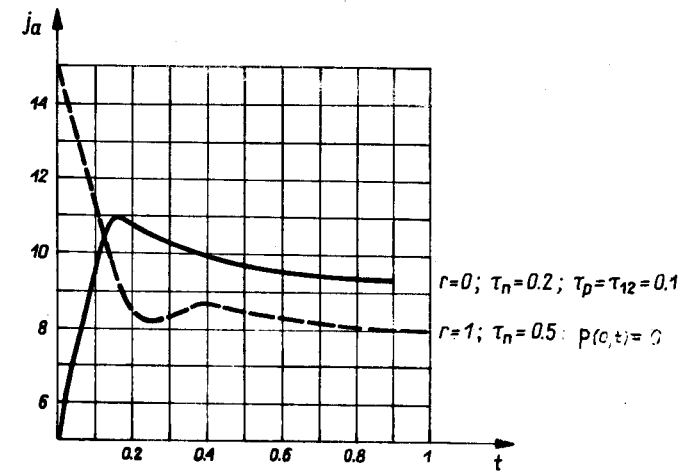


Fig. 5. Time courses of absorption current density in the system of nondimensional variables

$$j(1, t) = aE^2(1, t) \exp(-b/E(1, t)); a = b = 1$$

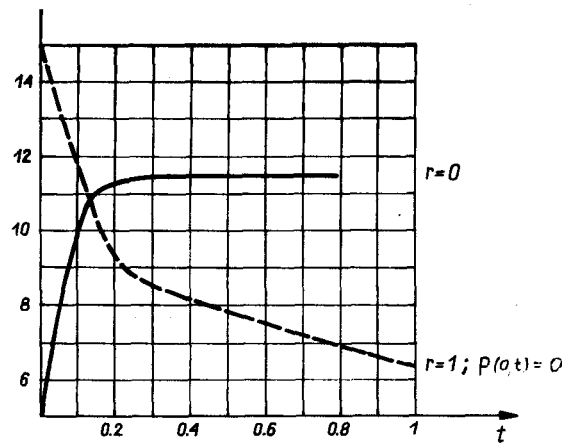


Fig. 6. Time courses of absorption current density in the system of nondimensional variables

$$j(1, t) = aE^2(1, t) \exp(-b/E(1, t)); a = b = 1; \tau_n = 0.2; \tau_p = 0.1; \tau_{12} = 100$$

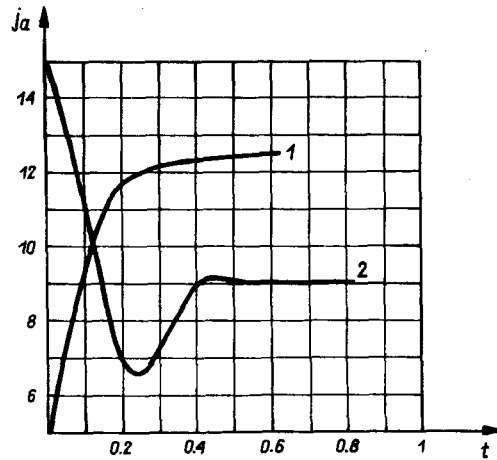


Fig. 7. Time courses of absorption current density in the system of nondimensional variables

$$1 - p(0, t) = 0; j(1, t) = a \exp(b\sqrt{E(1, t)}); a = 10, b = 0.2; r = 0; \tau_n = 0.2; \tau_p = \tau_{12} = 0.1$$

$$2 - p(0, t) = 0; j(1, t) = aE^2(1, t) \exp(-b/E(1, t)); a = b = 1; \tau_n = \tau_p = \tau_{12} = 100; r = 1$$

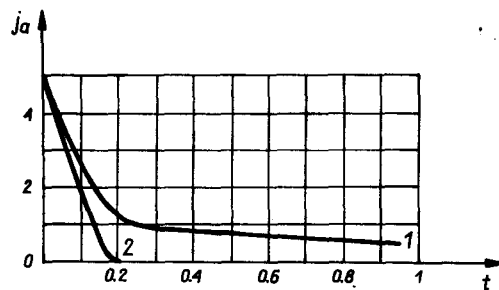


Fig. 8. Time courses of absorption current density in the system of nondimensional variables

$$1 - p(0, t) = 0; n(1, t) = 0; \tau_n = 0.2; \tau_p = \tau_{12} = 0.1; r = 0$$

$$2 - p(0, t) = 0; n(1, t) = 0; \tau_n = \tau_p = \tau_{12} = 100; r = 0$$

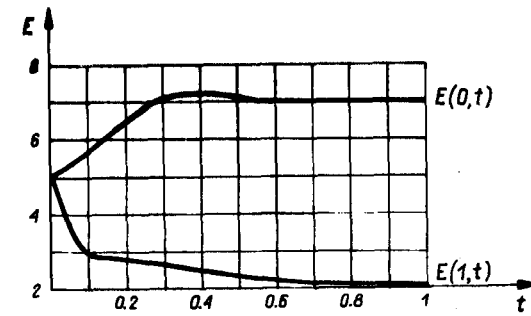


Fig. 9. Exemplary time courses of electric field intensity at the electrodes in the system of nondimensional variables

$$j(0, t) = aE^2(0, t) \exp(-b/E(0, t)); j(1, t) = a_1 \exp(b_1 \sqrt{E(1, t)}); a = 0.5; b = 1; a_1 = 5; b_1 = 1; r = 0.5; \tau_n = \tau_p = \tau_{12} = 1$$

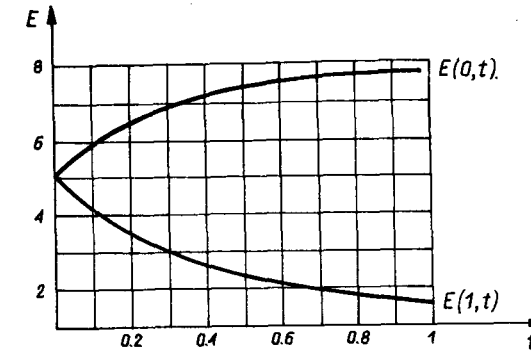


Fig. 10. Exemplary time courses of electric field intensity at the electrodes in the system of nondimensional variables

$$p(0, t) = 0; j(1, t) = a \exp(b\sqrt{E(1, t)}); a = 12; b = 0.2; r = 1; \tau_n = \tau_p = \tau_{12} = 0.1$$

4. Conclusions. In the presented model of a dielectric with conductance $p_0 \neq 0$ and $n_0 \neq 0$ there is a jump of absorption current density at time $t=0$ from zero value to the initial value $j_a(0)$. Calculations indicate that the shape of the $j_a(t)$ curve depends on the mechanisms of carrier injection and on carrier mobility. At the given injection mechanisms, the generation-recombination processes extend relaxation time and change the value of absorption current density $j_a(t)$.

When contacts are described by

a) dependences of transport current density and field intensity at the electrodes

$$j(0, t) = f_0 [E(0, t)] \quad \text{and} \quad j(L, t) = f_L [E(L, t)]$$

the $j_a(t)$ curve attains first a maximum and then a minimum, following which, after a certain time, it assumes a constant value;

b) when one of the electrodes does not inject holes $p(0, t) = 0$ or $p(0, t) < p_0$, and the other injects electrons according to the dependence $j(L, t) = f_L [E(L, t)]$ and when the carrier mobilities are equal $\mu_n = \mu_p$, then the $j_a(t)$ curve may be decreasing or may have a minimum; on the other hand, when the positive charge carriers are immobile $\mu_p = 0$, the $j_a(t)$ curve may be increasing or may have a maximum;

c) when both the electrodes do not inject carriers $p(0, t) = 0$ and $n(L, t) = 0$, the absorption current vanishes after some time, with the disappearance time extending with the increase of carrier generation process rate.

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Б. Свистач. Модель кинетики рекомбинации носителей заряда в твердом диэлектрике

В статье представляется модель твердого диэлектрика, в котором находится объемный заряд из свободных дырок, свободных и захваченных электронов. Транспорт заряда описывается системой уравнений: уравнением Гаусса, законом сохранения заряда и уравнениями, описывающими участие состояний локализации и делокализации электронов в процессах генерации-рекомбинации. Предполагается, что начальные величины концен-

траций имеют вид равновесных величин концентрации. Граничные величины концентраций носителей устанавливаются по механизмам инжектирования заряда из металла в диэлектрик. В данной статье исследуется влияние процессов генерации-рекомбинации и механизмов инжекции на переходные токи абсорбции. Переходные токи абсорбции определяются по вычислительному методу.