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Development of a bipolar space charge–limited current problem for metal-insulator-metal system. Some numerical results

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A solid in which the trapped negative charge can become mobile or immobile is considered. The different contact processes for a bipolar space charge transport are taken into account. A problem of the current flow through a solid is solved by a numerical method. The integral problem basing on the theory of characteristics for numerical calculations is defined.

1. INTRODUCTION

The fundamental problem for electric conduction in the metal-insulator-metal system is to determine the internal and boundary conditions describing interactions between the positive and negative charge carriers in a solid. A mathematical problem of a space charge theory is to find the conditions for the existence of the solutions [1–7]. Generally, the boundary and internal problem of electric conduction corresponds to the electrode-bulk contact processes and to the given material structure [8–20]. In this paper, the boundary and internal problem of a bipolar space charge transport in a solid placed between the two electrodes will be continued and developed.

The purpose of this work is to determine the effect of the internal and boundary processes on the shape of the current characteristics. This problem will be solved by a numerical method.

2. TWO MATHEMATICAL MODELS

In general, under conditions of an external electric field, interactions between positive and negative charge carriers depend on a configuration of atoms in space. On this basis, we make the following assumptions:

(I) The system of atoms defining the bulk (insulator) is very chaotic (that is, we will assume that the given configuration of atoms is permanently perturbed),

(II) The concentration of atoms is possibly maximal and the splitting of the energy states (the Zeeman internal effect) occurs (this property corresponds to the different structural dislocations and to the Frenkl defects caused by impurities and pollutants),

(III) The Stark external (linear or non-linear) effect is sufficiently weak (this property is characterised by a dielectric constant),

(IV) As a model system, we consider the planar capacitor system,

(V) For the trapped electron we will consider two following cases:

(Va) The first case is when the additional kinetic energy is given by an external elecric field to the trapped electron in a small portion. Under these conditions, for the external electric field, the trapped electrons are immobile,

(Vaa) The second case is when (for example, the Pool internal effect, hopping conduction and others can occur) the trapped electron flow is observed.

In this paper, using (I)—(V) for a charging capacitor system, we will investigate electric conduction. For this problem, the basic equations are the Gauss equation, the continuity equation, the generation-recombination equations and the field integral. These equations describing the bipolar space charge transport in the planar capacitor sytem are written as follows [21]:

$$\frac{\varepsilon}{q}\frac{\partial E'(x',t')}{\partial x'}=p'(x',t')-\{n'(x',t')+n'_{t1}(x',t')+n'_{t2}(x',t')\}, \tag{1}$$

$$\begin{aligned}&\frac{\partial}{\partial x'}\{[\mu_p p'(x',t')+\mu_n n'(x',t')+\mu_{t1}n'_{t1}(x',t')+\mu_{t2}n'_{t2}(x',t')]E'(x',t')\}+\\&+\frac{\partial p'(x',t')}{\partial t'}-\frac{\partial n'(x',t')}{\partial t'}-\frac{\partial n'_{t1}(x',t')}{\partial t'}-\frac{\partial n'_{t2}(x',t')}{\partial t'}=0,\end{aligned} \tag{2}$$

$$\begin{aligned}\frac{\partial n'_{t1}(x',t')}{\partial t'}&=C_n n'(x',t')-v_{n1}n'_{t1}(x',t')-C_{12}n'_{t1}(x',t')+C_{21}n'_{t2}(x',t')+\\&+v_{p1}N_{t1}-C_{p1}p'(x',t')n'_{t1}(x',t')+\frac{\partial}{\partial x'}[\mu_{t1}n'_{t1}(x',t')E'(x',t')];\quad N_{t1}\gg n'_{t1},\end{aligned} \tag{3}$$

$$\begin{aligned}\frac{\partial n'_{t2}(x',t')}{\partial t'}&=C_{12}n'_{t1}(x',t')-C_{21}n'_{t2}(x',t')-v_{n2}n'_{t2}(x',t')+v_{p2}N_{t2}+\\&-C_{p2}p'(x',t')n'_{t2}(x',t')+\frac{\partial}{\partial x'}[\mu_{t2}n'_{t2}(x',t')E'(x',t')];\quad N_{t2}\gg n'_{t2},\end{aligned} \tag{4}$$

$$\begin{aligned}\frac{\partial n'(x',t')}{\partial t'}&=v_{n1}n'_{t1}(x',t')+v_{n2}n'_{t2}(x',t')-C_n n'(x',t')+\\&+\frac{\partial}{\partial x'}[\mu_n n'(x',t')E'(x',t')],\end{aligned} \tag{5}$$

$$V=\int_0^L E'(x',t')\mathrm{d}x'; \quad V=\text{constant}>0. \tag{6}$$

where: $q=1.6\times10^{-19}$ C, ε is the dielectric constant (electric permittivity), E' is the electric field intensity, x' is the distance from the electrode, t' is the time, p' and n' denote the free hole and electron concentrations, respectively, μ_p and μ_n are the hole and electron mobilities, respectively, μ_{t1} and μ_{t2} are the mobilities of trapped electrons in the first and second trapping level, respectively, n'_{t1} and n'_{t2} are the trapped electron concentrations in the first and second trapping level, respectively N_{t1} and N_{t2} are the concentrations of traps in the first and second trapping level, respectively, $v_{p1,2}$, C_{21}, $v_{n1,2}$, C_n, C_{12}, $C_{p1,2}$ are the generation-recombination parameters, L is the distance between the electrodes, and V is the applied voltage. Equations (3)–(5) are written when allowed electron transitions are independent of the external electric field and the bulk acts as an unlimited reservoir of trapped carriers. Thus, taking into account the equilibrium conditions (that is $E'\equiv0$), the generation-recombination parameters can be expressed by the equilibrium concentrations $p'_0=n'_0+n'_{t1,0}+n'_{t2,0}$ in the form

$$C_{12}n'_{t1,0}-C_{21}n'_{t2,0}-v_{n2}n'_{t2,0}=v_{p1}N_{t1}-C_{p1}p'_0n'_{t1,0}=C_{p2}p'_0n'_{t2,0}-v_{p2}N_{t2}; \tag{7}$$
$$v_{n1}n'_{t1,0}+v_{n2}n'_{t2,0}=C_nn'_0.$$

Under these conditions, we see that the number of internal parameters is reduced. From (1), (2) and (6) it follows that the total current density $J(t')$ has the form

$$J(t')=\frac{q}{L}\int_0^L[\mu_pp'(x',t')+\mu_nn'(x',t')+\mu_{t1}n'_{t1}(x',t')+\mu_{t2}n'_{t2}(x',t')]E'(x',t')\mathrm{d}x'. \tag{8}$$

According to the purpose of this work, the effect of the internal parameters and the mechanisms of carrier injection on the shape of $J(t')$ curve will be investigated. This problem will be solved by the use of the normalised variables in the form:

$$E=\frac{E'L}{V_0};\ u=\frac{V}{V_0};\ x=\frac{x'}{L};\ p=\frac{p'qL^2}{\varepsilon V_0};\ n=\frac{n'qL^2}{\varepsilon V_0};\ n_{t1,2}=\frac{n'_{t1,2}qL^2}{\varepsilon V_0}; \tag{9}$$

$$t=\frac{\mu_nV_0t'}{L^2};\ \tau_n=\frac{\mu_nV_0}{L^2C_n};\ \tau_p=\frac{q\mu_n}{\varepsilon C_{p2}};\ \tau'_p=\frac{q\mu_n}{\varepsilon C_{p1}};\ \tau_1=\frac{\mu_nV_0}{L^2v_{n1}};\ \tau'_1=\frac{\mu_nV_0}{L^2v_{n2}};$$

$$\tau_2=\frac{\varepsilon\mu_nV_0^2}{qL^4v_{p2}N_{t2}};\ \tau'_2=\frac{\varepsilon\mu_nV_0^2}{qL^4v_{p1}N_{t1}};\ \tau_{12}=\frac{\mu_nV_0}{L^2C_{12}};\ \tau_{21}=\frac{\mu_nV_0}{L^2C_{21}};\ j=\frac{L^3J}{\varepsilon\mu_nV_0^2};\ r=\frac{\mu_p}{\mu_n},$$

where V_0 denotes a reference voltage. On the basis (1)–(7), we will consider two special cases of a bipolar space charge transport between two electrodes.

2.1. Current flow with $\mu_{t1}=\mu_{t2}=0$.

In this section we will consider the current flow through a solid when the trapped electrons are immobile as well as $\tau'_1=\tau'_2=\tau'_p=\infty$ (a case of an insulator). For this problem, from (1)–(6) and (9) it follows that the bipolar space charge transport can be described by the following equation system:

$$\frac{\partial n_{t1}}{\partial t}=\frac{n}{\tau_n}-\frac{n_{t1}}{\tau_1}-\frac{n_{t1}}{\tau_{12}}+\frac{n_{t2}}{\tau_{21}}, \tag{10}$$

$$\frac{\partial n_{t2}}{\partial t}=\frac{n_{t1}}{\tau_{12}}-\frac{n_{t2}}{\tau_{21}}-\frac{pn_{t2}}{\tau_p}+\frac{1}{\tau_2}, \tag{11}$$

$$\begin{cases}\dfrac{dx_n}{dt}=-E(x_n(t),t),\\ \dfrac{dn}{dt}=n(p-n-n_{t1}-n_{t2})-\dfrac{n}{\tau_n}+\dfrac{n_{t1}}{\tau_1},\end{cases} \tag{12}$$

$$\begin{cases}\dfrac{dx_p}{dt}=rE(x_p(t),t),\\ \dfrac{dp}{dt}=-rp(p-n-n_{t1}-n_{t2})-\dfrac{pn_{t2}}{\tau_p}+\dfrac{1}{\tau_2},\end{cases} \tag{13}$$

$$\int_0^1 E(x,t)dx=u=\mathrm{const}>0, \tag{14}$$

where $x_n=x_n(t)$ and $x_p=x_p(t)$ are the characteristics of free electrons and holes, respectively.
With the voltage condition (14), the Gauss equation is of the integral form

$$\begin{cases}E(0,t)=u-\int_0^1(1-x)(p-n-n_{t1}-n_{t2})dx\\ E(x,t)=E(0,t)+\int_0^x(p-n-n_{t1}-n_{t2})dx, \quad 0\leqslant x\leqslant 1.\end{cases} \tag{15}$$

Now, instead of (8), we have

$$j(t)=\int_0^1[rp(x,t)+n(x,t)]E(x,t)dx. \tag{16}$$

The relations (7) between the internal parameters and the equilibrium concentrations take the form

$$\tau_{21}=\tau_{12}\frac{n_{t2,0}}{n_{t1,0}}; \quad \tau_1=\tau_n\frac{n_{t1,0}}{n_0}; \quad \tau_2=\frac{\tau_p}{p_0 n_{t2,0}}. \tag{17}$$

Referring to (14), there will be considered such conduction conditions in which the electric field intensity is always positive $E(x,t)>0$. Hence, it follows that $\frac{\mathrm{d}x_p}{\mathrm{d}t}>0$ at the electrode $x=0$ and $\frac{\mathrm{d}x_n}{\mathrm{d}t}<0$ at the electrode $x=1$. Thus, in order to find $j(t)$ curve expressed by (16) we have to define the boundary and initial conditions. In this paper we assume that the initial conditions for our problem are determined by the equilibrium conditions, that is

$$p(x,0)=p_0=2; \quad n(x,0)=n_0=1; \quad n_{t1}(x,0)=n_{t1,0}=0.5; \quad n_{t2}(x,0)=n_{t2,0}=0.5. \tag{18}$$

Also, we will assume that the boundary values $p(0,t)$ and $n(1,t)$ are determined by the mechanisms of carrier injection from the electrodes into the bulk. To this end, referring to the field theory, the convection current density

$$j_c(x,t)=[rp(x,t)+n(x,t)]E(x,t) \tag{19}$$

and the emission current density $j_0=f(E_0)$ must satisfy the following boundary condition

$$\begin{cases} j_0=f(E_0) \\ j_c(x_0,t)-j_0(x_0,t)=\pm\left.\frac{\mathrm{d}q_s}{\mathrm{d}t}\right|_{x=x_0} \end{cases}, \tag{20}$$

where $f(E_0)$ is a function describing the mechanism of carrier injection from the electrode into the bulk, E_0 denotes $E(0,t)$ or $E(1,t)$, q_s is the surface charge density, and x_0 denotes the electrode $x=0$ or $x=1$. Thus, taking into account (20), the boundary values $p(0,t)$ and $n(1,t)$ corresponding to the quasi-stationary boundary processes are determined by

$$\begin{cases} [rp(0,t)+n(0,t)]E(0,t)=f_0[E(0,t)] \\ [rp(1,t)+n(1,t)]E(1,t)=f_1[E(1,t)] \end{cases}, \tag{21}$$

where f_0 and f_1 are the boundary functions describing the mechanisms of carrier injection from the electrode $x=0$ and $x=1$ into the bulk. Also, for numerical calculations, the stationary and quasi-stationary electrode processes characterised by

$$\begin{cases} p(0,t)=\mathrm{const} \\ [rp(1,t)+n(1,t)]E(1,t)=f_1[E(1,t)] \end{cases} \tag{21a}$$

are considered. For the equations (10) – (13), (15) – (18), (21) and (21a), a numerical algorithm has been made. As the boundary functions, the Schottky and Fowler-Nordheim functions have been used. Some numerical results are presented in Fig. 1 – 7. In the next part of this paper, we shall develop the importance of the voltage condition (6).

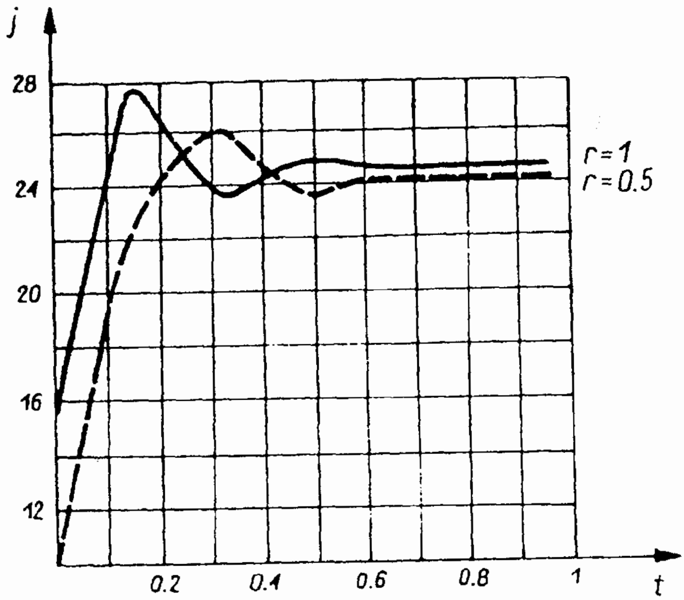

Fig. 1. The time-current characteristics in the normalised variable system:
$f_0 = a_0 E^2(0,t)$; $f_1 = a_1 E^2(1,t)$; $a_0 = a_1 = 1$; $\tau_n = \tau_p = \tau_{12} = 1$

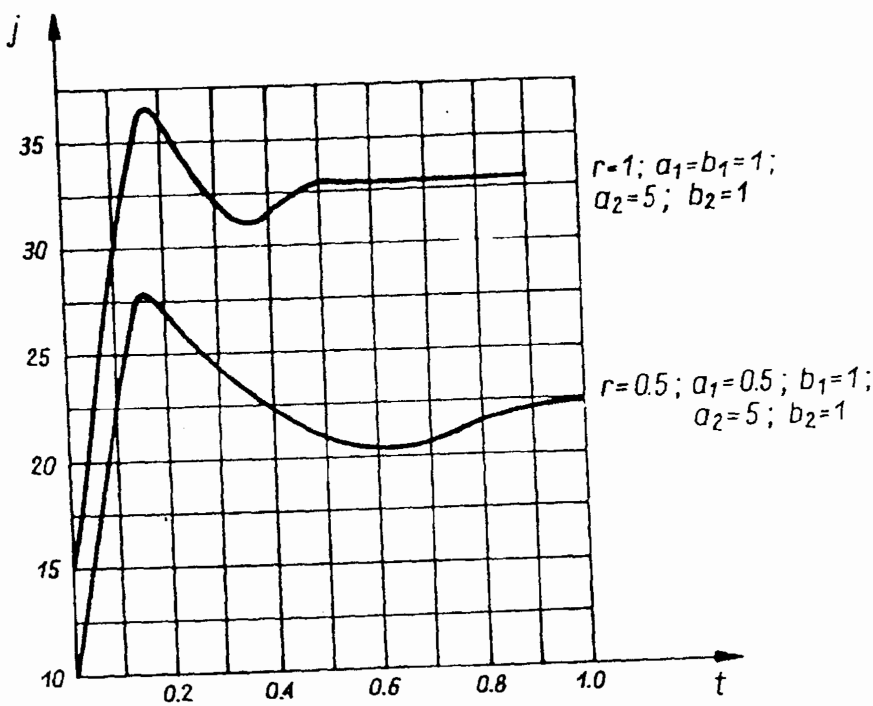

Fig. 2. The time-current characteristics in the normalised variable system:
$f_0 = a_1 E^2(0,t)\exp(-b_1/E(0,t))$; $f_1 = a_2\exp(b_2\sqrt{E(1,t)})$; $\tau_n = \tau_p = \tau_{12} = 1$

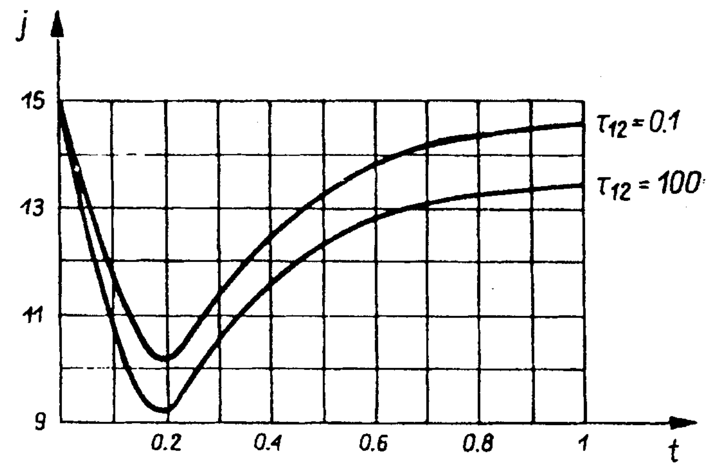

Fig. 3. The time-current characteristics in the normalised variable system: $p(0,t)\equiv 0$; $f_1 = a\exp(b_1\sqrt{E(1,t)})$; $a=11$; $b=0.2$; $r=1$; $\tau_n=0.2$; $\tau_p=0.1$

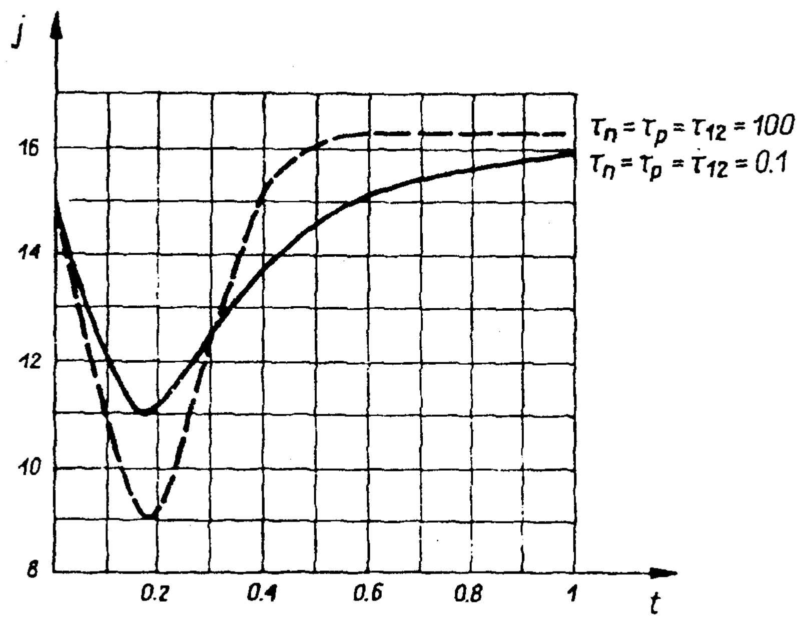

Fig. 4. The time-current characteristics in the normalised variable system: $p(0,t)\equiv 0$; $f_1 = a\exp(b\sqrt{E(1,t)})$; $a=12$; $b=0.2$; $r=1$

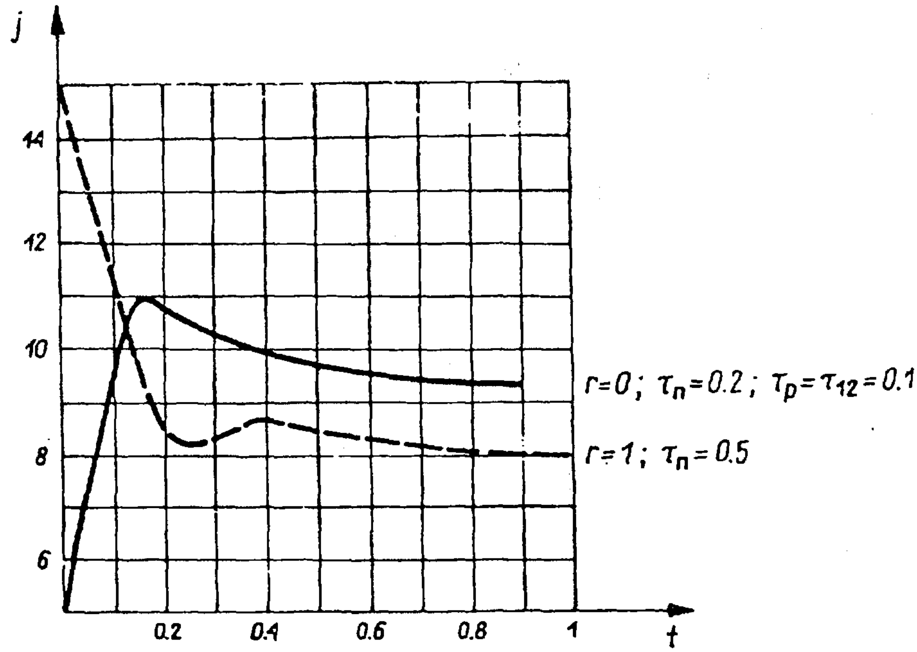

Fig. 5. The time-current characteristics in the normalised variable system: $p(0,t)\equiv 0$; $f_1=a\,E^2(1,t)\exp(-b/E(1,t))$; $a=b=1$

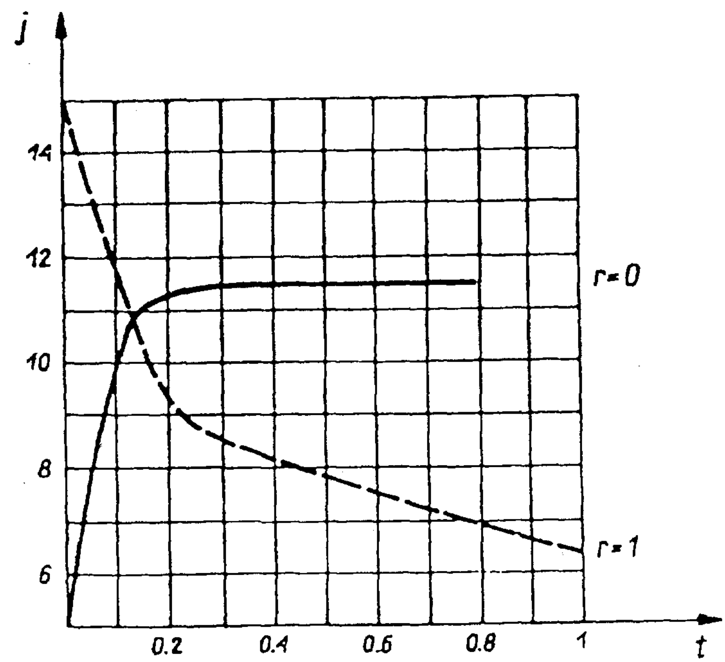

Fig. 6. The time-current characteristics in the normalised variable system: $p(0,t)\equiv 0$; $f_1=a\,E^2(1,t)\exp(-b/E(1,t))$; $a=b=1$; $\tau_n=0.2$; $\tau_p=0.1$; $\tau_{12}=100$

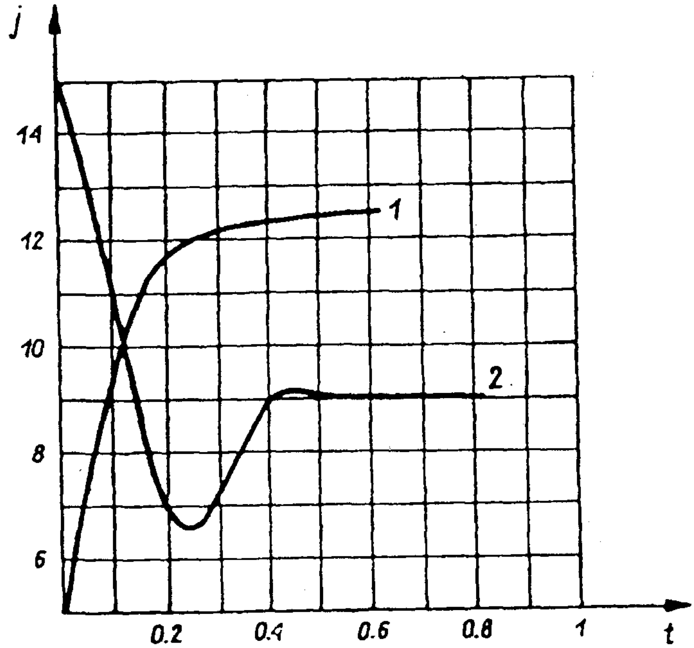

Fig. 7. The time-current characteristics in the normalised variable system:
1 — $p(0,t)\equiv 0$; $f_1 = a\exp(b\sqrt{E(1,t)})$; $a=10$; $b=0.2$; $r=0$; $\tau_n=0.2$; $\tau_p=\tau_{12}=0.1$;
2 — $p(0,t)\equiv 0$; $f_1=aE^2(1,t)\exp(-b/E(1,t))$; $a=b=1$; $r=1$; $\tau_n=\tau_p=\tau_{12}=100$

2.2. The electric conduction under conditions of the mobile trapped electrons and $C_{p1}=C_{p2}=C_p$.

Now, we shall consider a bipolar space charge transport when the electrode processes are not stationary, that is, the planar capacitor system will be characterised by the surface charge density $q_s'(t')$ at the electrodes $x=0$ and $x=1$. In this case, the field integral (6) must be written as

$$V = V_{c1} + \int_{0_+}^{L_-} E'(x',t')\mathrm{d}x' + V_{c2}, \tag{22}$$

where V_{c1} and V_{c2} denote the contact voltages at the electrodes $x'=0$ and $x'=L$, respectively, 0_+ and L_- are the right and left hand side limits at the point $x'=0$ and $x'=L$, respectively.

Additionally, we assume that the contact voltages are negligible (this is acceptable when the thickness of the double layer is $\leqslant 10^{-9}$ m and $E' \leqslant 10^9$ V/m). In the case when $V \gg |V_{c1}+V_{c2}|$, (22) becomes

$$V = \int_{0_+}^{L_-} E'(x',t')\mathrm{d}x'. \tag{22a}$$

The boundary conditions describing the behaviour of the normal components of the convection current $J_c(x',t')$ and electric field $E'(x',t')$ take the form

$$\begin{cases} -\left.\dfrac{dq_s'}{dt'}\right|_{x'=0} = -f_0[E'(0_-,t')] + J_c(0_+,t') \\ -\left.\dfrac{dq_s'}{dt'}\right|_{x'=L} = f_L[E'(L_+,t')] - J_c(L_-,t') \end{cases} \tag{23}$$

and

$$\begin{cases} q_s' \mid_{x'=0} = \varepsilon_o[\varepsilon_r E'(0_+,t') - E'(0_-,t')] \\ q_s' \mid_{x'=L} = \varepsilon_o[E'(L_+,t') - \varepsilon_r E'(L_-,t')], \end{cases} \tag{24}$$

where $\varepsilon_o = 8.85 \times 10^{-12}$ F/m and ε_r is the relative dielectric constant of the bulk, f_0 and f_L are the boundary functions describing the mechanisms of carrier injection from the electrodes into the bulk.

Now, we must define the interface surface between the electrode and the bulk. Thus, using the mean-value theorem for the planar capacitor system, we have

$$\int_S ds \int_0^{x_s'} q_v(x',t')dx' = \int_S x_s' q_v(c,t')ds; \quad 0 \leqslant c \leqslant x_s',$$

where S denotes an integration surface and q_v is the space charge density. On this basis, the free surface charge densities are defined by

$$\begin{cases} {}^+q_s' \mid_{x'=0} = q x_s' p'(0_+,t'); \quad 0 \leqslant x_s' \leqslant L \\ {}^-q_s' \mid_{x'=L} = -q x_s' n'(L_-,t'); \quad 0 \leqslant x_s' \leqslant L, \end{cases} \tag{25}$$

where x_s' is a distance parameter defining the contact surface. With the boundary conditions (23)–(25), we will examine electric conduction in the case when $\mu_{t1} = \mu_{t2} = \mu_t$. With the voltage condition (22a), the total current density is of the form:

$$J(t') = \frac{q}{L} \int_{0_+}^{L_-} [\mu_p p'(x',t') + \mu_n n'(x',t') + \mu_t n_t'(x',t')]E'(x',t')dx'; \quad n_t' = n_{t1}' + n_{t2}'. \tag{26}$$

In order to find a function $J(t')$, we must define the boundary conditions describing the mechanisms of carrier injection from the electrodes $x'=0$ and $x'=L$ into the bulk. According to (23)–(25), we shall assume that the surface energy states exist on the interface $x'=0$ and $x'=L$, and the generation-recombination processes occur on these contact surfaces. As the basic equations describing the electrode processes, we shall take into account the following equations:

$$\frac{dp'(0_+,t')}{dt'} = \frac{1}{x_s'}\{v_{ps}' N_{ts}' + f_0/q - \mu_p p'(0_+,t')E'(0_+,t') + \\ - C_{ps} p'(0_+,t') n_t'(0_+,t')\} \tag{27}$$

$$\frac{\mathrm{d}n'(L_-,t')}{\mathrm{d}t'}=\frac{1}{x'_s}\{f_L/q+v_{ns}n'_t(L_-,t')-C_{ns}n'(L_-,t')+ \\ -\mu_n n'(L_-,t')E'(L_-,t')\} \tag{28}$$

$$\frac{\mathrm{d}n'_t(L_-,t')}{\mathrm{d}t'}=\frac{1}{x'_s}\{v_{ps}N_{ts}+C_{ns}n'(L_-,t')-v_{ns}n'_t(L_-,t')+ \\ -C'_{ps}p'(L_-,t')n'_t(L_-,t')-\mu_t n'_t(L_-,t')E'(L_-,t')\}, \tag{29}$$

where $f_0=f_0[E'(0_-,t')]$ and $f_L=f_L[E'(L_+,t')]$ are the emission current densities, v_{ps}, v'_{ps}, v_{ns}, N_{ts}, N'_{ts}, C_{ns}, C_{ps}, C'_{ps} are the surface parameters satisfying the following relations:

$$v_{ps}=\frac{C_{ps}p'_0n'_{t,0}}{N_{ts}};\quad v_{ns}=\frac{C_{ns}n'_0}{n'_{t,0}};\quad n'_{t,0}=n'_{t1,0}+n'_{t2,0}. \tag{30}$$

Thus, equations (1)–(5), (23)–(29) and (22a) describe a bipolar space charge transport through a solid between the two electrodes. On this basis the total current density $J(t')$ and the surface charge densities $q'_s(t')\mid_{x'=0}$ and $q'_s(t')\mid_{x'=L}$ will be found by a numerical method. To this end, we shall make use of the following dimensionless variable system:

$$E=\frac{E'L}{V_0};\ u=\frac{V}{V_0};\ x=\frac{x'}{L};\ p=\frac{p'qL^2}{\varepsilon V_0};\ n=\frac{n'qL^2}{\varepsilon V_0};\ n_t=\frac{n'_tqL^2}{\varepsilon V_0};\ j=\frac{L^3J}{\varepsilon\mu V_0^2};$$
$$\tau_{1s}=\frac{\mu V_0}{Lv_{ns}};\ \tau_{ns}=\frac{\mu V_0}{LC_{ns}};\ \tau_{ps}=\frac{q\mu L}{\varepsilon C_{ps}};\ \tau_{2s}=\frac{\varepsilon\mu V_0^2}{qL^3v'_{ps}N'_{ts}};\ q_s=\frac{Lq'_s}{\varepsilon V_0};\ \tau_1=\frac{\mu V_0}{L^2v_n}; \tag{31}$$
$$t=\frac{\mu V_0t'}{L^2};\quad \tau_2=\frac{\varepsilon\mu V_0^2}{qL^4(v_{p1}N_{t1}+v_{p2}N_{t2})};\ \tau_p=\frac{q\mu}{\varepsilon C_p};\ r_1=\frac{\mu_p}{\mu};\ r_2=\frac{\mu_t}{\mu};\ r_3=\frac{\mu_n}{\mu},$$

where

$$v_n=\frac{v_{n1}n'_{t1,0}+v_{n2}n'_{t2,0}}{n'_{t1,0}+n'_{t2,0}}. \tag{31a}$$

Here μ is a reference mobility parameter and v_n denotes the so-called effective frequency (this denotes that $v_{n1}n'_{t1}+v_{n2}n'_{t2}$ is replaced by $v_nn'_t$ in (5)). Moreover, using the effective frequency, the number of the boundary conditions is reduced. Thus, for a numerical algorithm, the equations describing electric conduction in the planar capacitor system are written as follows:

$$\begin{cases}\dfrac{\mathrm{d}x_p}{\mathrm{d}t}=r_1E(x_p(t),t)\\[2mm] \dfrac{\mathrm{d}p}{\mathrm{d}t}=-r_1p(p-n-n_t)-\dfrac{pn_t}{\tau_p}+\dfrac{1}{\tau_2}\end{cases} \tag{32}$$

$$\begin{cases} \dfrac{\mathrm{d}x_t}{\mathrm{d}t} = -r_2 E(x_t(t),t) \\ \dfrac{\mathrm{d}n_t}{\mathrm{d}t} = r_2 n_t(p-n-n_t) + \dfrac{n}{\tau_n} + \dfrac{1}{\tau_2} - \dfrac{n_t}{\tau_1} - \dfrac{pn_t}{\tau_p} \end{cases} \tag{33}$$

$$\begin{cases} \dfrac{\mathrm{d}x_n}{\mathrm{d}t} = -r_3 E(x_n(t),t) \\ \dfrac{\mathrm{d}n}{\mathrm{d}t} = r_3 n(p-n-n_t) + \dfrac{n_t}{\tau_1} - \dfrac{n}{\tau_n} \end{cases} \tag{34}$$

$$E(0_+,t) = u - \int_{0_+}^{1_-} (1-x)(p-n-n_t)\mathrm{d}x \tag{35}$$

$$E(x,t) = E(0_+,t) + \int_{0_+}^{x} (p-n-n_t)\mathrm{d}x; \quad 0_+ \leqslant x \leqslant 1_- \tag{36}$$

with the boundary conditions described by

$$\begin{cases} \varepsilon_r E(0_+,t) - E(0_-,t) = \varepsilon_r q_s \mid_{x=0} \\ E(1_+,t) - \varepsilon_r E(1_-,t) = \varepsilon_r q_s \mid_{x=1} \end{cases} \tag{37}$$

$$\begin{cases} \left.\dfrac{\mathrm{d}q_s}{\mathrm{d}t}\right|_{x=0} = f_0[E(0_-,t)] - [r_1 p(0_+,t) + r_2 n_t(0_+,t) + r_3 n(0_+,t)]E(0_+,t) \\ \left.\dfrac{\mathrm{d}q_s}{\mathrm{d}t}\right|_{x=1} = [r_1 p(1_-,t) + r_2 n_t(1_-,t) + r_3 n(1_-,t)]E(1_-,t) - f_1[E(1_+,t)] \end{cases} \tag{38}$$

$$\frac{\mathrm{d}p(0_+,t)}{\mathrm{d}t} = \frac{1}{x_s}\left\{\frac{1}{\tau_{2s}} + f_0[E(0_-,t)] - r_1 p(0_+,t)E(0_+,t) - \frac{p(0_+,t)n_t(0_+,t)}{\tau_{ps}}\right\} \tag{39}$$

$$\frac{\mathrm{d}n(1_-,t)}{\mathrm{d}t} = \frac{1}{x_s}\left\{f_1[E(1_+,t)] + \frac{n_t(1_-,t)}{\tau_{1s}} - \frac{n(1_-,t)}{\tau_{ns}} - r_3 n(1_-,t)E(1_-,t)\right\} \tag{40}$$

$$\frac{\mathrm{d}n_t(1_-,t)}{\mathrm{d}t} = \frac{1}{x_s}\left\{\frac{1}{\tau_{2s}} + \frac{n(1_-,t)}{\tau_{ns}} - \frac{n_t(1_-,t)}{\tau_{1s}} - r_2 n_t(1_-,t)E(1_-,t) - \frac{p(1_-,t)n_t(1_-,t)}{\tau_{ps}}\right\} \tag{41}$$

where f_0 and f_1 denote the normalised functions defining the emission current densities at the electrodes $x=0$ and $x=1$, respectively, $x_n = x_n(t)$ and $x_p = x_p(t)$ are the characteristics of free negative and positive charge carriers, respectively, and $x_t = x_t(t)$ is the characteristic of trapped mobile carriers.

For the boundary and internal parameters, we have the following relations:

$$\tau_1 = \tau_n \frac{n_{t,0}}{n_0}; \quad \tau_2 = \frac{\tau_p}{p_0 n_{t,0}}; \quad \tau_{1s} = \tau_{ns}\frac{n_{t,0}}{n_0}; \quad \tau_{2s} = \frac{\tau_{ps}}{p_0 n_{t,0}}. \tag{42}$$

According to (39)–(41), on the interfaces $x=0$ and $x=1$, the same values of τ_{2s} and τ_{ps} are taken into consideration, respectively. With this assumption, the number of the boundary parameters is reduced. As the initial values for (32)–(41), the equilibrium values are considered:

$$p(x,0)=p_0=2; \quad n(x,0)=n_0=1; \quad n_t(x,0)=n_{t,0}=1; \tag{43}$$

$$q_s(t=0)\mid_{x=0}=0; \quad q_s(t=0)\mid_{x=1}=0.$$

Thus, for the above space charge problem, the boundary functions $q_s(t)\mid_{x=0}$ and $q_s(t)\mid_{x=1}$ and the total current density $j(t)$

$$j(t)=\int_{0_+}^{1_-}[r_1p(x,t)+r_2n_t(x,t)+r_3n(x,t)]E(x,t)]\mathrm{d}x \tag{44}$$

are defined. Some numerical results are illustrated in Fig. 8–15.

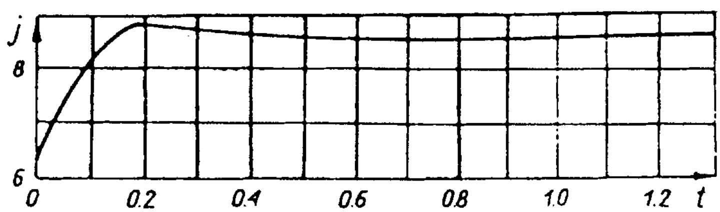

Fig. 8. The time-current characteristic in the normalised variable system: $f_0=a_0E^2(0_-,t)$; $f_1=a_1E^2(1_+,t)$; $a_0=0.2$; $a_1=0.5$; $r_1=r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=\tau_2=\tau_{2s}=0.1$

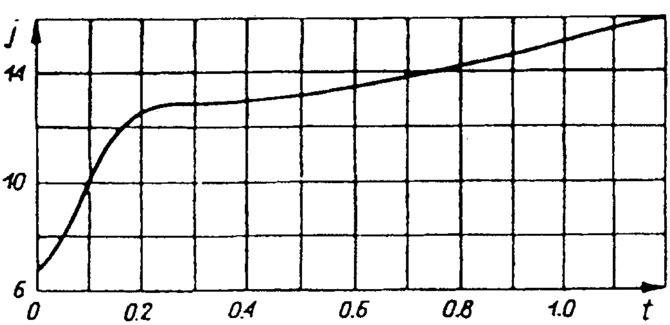

Fig. 9. The time-current characteristic in the normalised variable system: $f_0=a_0E^2(0_-,t)$; $f_1=a_1E^2(1_+,t)$; $a_0=0.2$; $a_1=0.5$; $r_1=r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=\tau_2=\tau_{2s}=1$

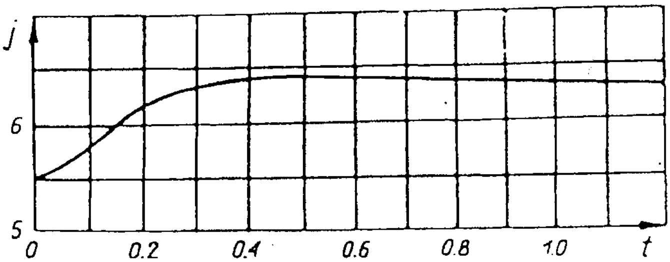

Fig. 10. The time-current characteristic in the normalised variable system:
$f_0=a_0E^2(0_-,t)\exp(-b_0/E(0_-,t))$; $f_1=a_1E^2(1_+,t)\exp(-b_1/E(1_+,t))$; $a_0=0.5$; $b_0=0.5$; $a_1=0.1$; $b_1=1$; $r_1=0$; $r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=0.1$; $\tau_2=\tau_{2s}=1$

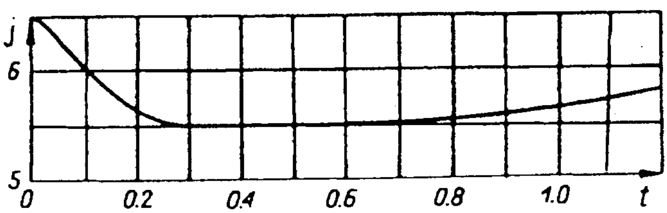

Fig. 11. The time-current characteristic in the normalised variable system:
$f_0=a_0E^2(0_-,t)\exp(-b_0/E(0_-,t))$; $f_1=a_1\exp(b_1\sqrt{E(1_+,t)})$; $a_0=0.2$; $b_0=1$; $a_1=1$; $b_1=0.1$; $r_1=r_3=0.1$; $r_2=1$; $\tau_n=\tau_2=10$; $\tau_n=\tau_{2s}=0.1$

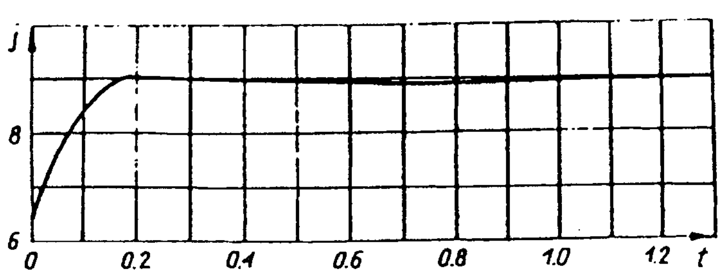

Fig. 12. The time-current characteristic in the normalised variable system:
$f_0\equiv 0$; $f_1=a_1E^2(1_+,t)\exp(-b_1/E(1_+,t))$; $a_1=0.5$; $b_1=1$; $r_1=r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=\tau_2=\tau_{2s}=0.1$

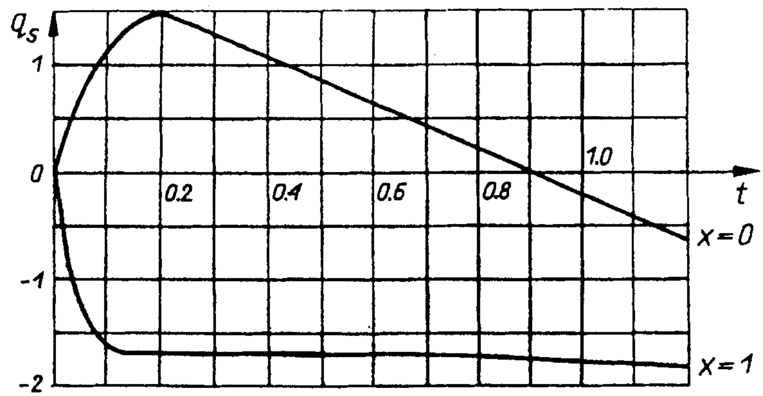

Fig. 13. The time – surface charge density characteristics at the electrodes $x=0$ and $x=1$ in the normalised variable system:
$f_0=a_0E^2(0_-,t)$; $f_1=a_1E^2(1_+,t)$; $a_0=0.2$; $a_1=0.5$; $r_1=r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=\tau_2=\tau_{2s}=1$

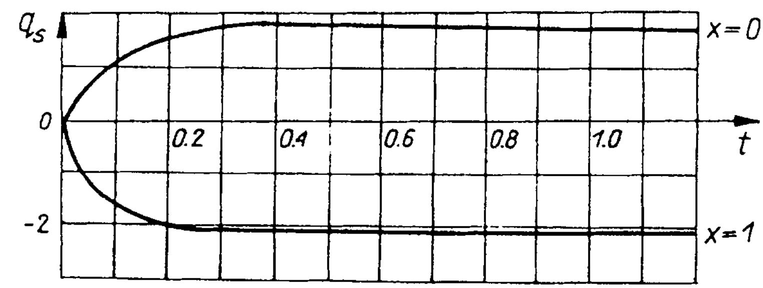

Fig. 14. The time – surface charge density characteristics at the electrodes $x=0$ and $x=1$ in the normalised variable system:
$f_0=a_0E^2(0_-,t)$; $f_1=a_1E^2(1_+,t)$; $a_0=0.2$; $a_1=0.5$; $r_1=r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=\tau_2=\tau_{2s}=0.1$

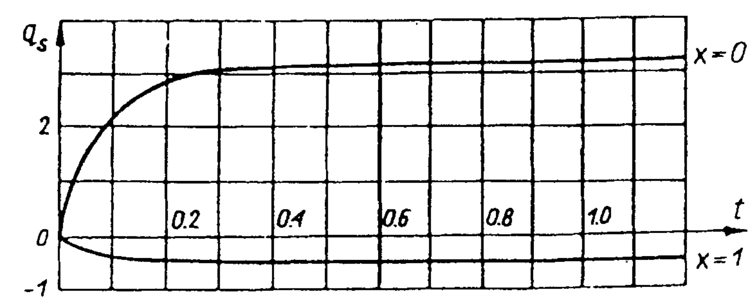

Fig. 15. The time surface charge density characteristics at the electrodes $x=0$ and $x=1$ in the normalised variable system:
$f_0=a_0E^2(0_-,t)\exp(-b_0/E(0_-,t))$; $f_1=a_1E^2(1_+,t)\exp(-b_1/E(1_+,t))$; $a_0=0.5$; $b_0=0.5$; $a_1=0.1$; $b_1=1$; $r_1=0$; $r_2=0.1$; $r_3=1$; $\tau_n=\tau_{ns}=0.1$; $\tau_2=\tau_{2s}=1$

3. DISCUSSION

In this work we have assumed that interactions between carriers are stimulated by an external electric field and by phonons and photons. Under conditions of an external electric field, in a capacitor system, we have distinguished two fundamental kinds of interactions in a solid. As a special case of blocking contacts $x'=0$ (or $x'=L$), we have considered the following boundary functions: $p'(0,t')\equiv 0$ (or $n'(L,t')\equiv 0$), (Fig. 3−7), and $f_0\equiv 0$, (Fig. 12). The condition $p'(0,t')\equiv 0$ denotes that all the empty energy states in the valence level can be filled by the free and trapped electrons in the bulk at the interface $x'=0$. This property can occur when the ionisation of atoms at this boundary is sufficiently weak and the electron-hole recombination processes are very quick (this is possible when the atomic numbers are sufficiently great). Analogously, at the contact $x'=L$, when the atomic numbers are sufficiently great and the number of unfilled energy states is also sufficiently great, we can have $n'(L,t')\equiv 0$. In the case when the concentrations of the trapped and valence electrons are much less than the concentration of the unfilled energy states in the valence level at the contact $x'=0$, a work function for the valence electrons in the bulk becomes very great because of the Coulomb force between the valence electrons and the positive nuclei of atoms in the bulk at the anode-bulk contact. In this situation, electron emission from the bulk into the anode does not occur or this emission is very weak. This property of the anode-bulk interface is characterised by $f_0\equiv 0$. In general, for the boundary conditions (21) and (21a), we assume that the contact processes are very quick or sufficiently quick. The inverse case occurs for (27)−(29). Here, these equations describe the mechanisms of the generation-recombination current emissions at the anode and cathode, respectively. Thus, we assume that the concentrations of injected carriers are stimulated by the electric-magnetic force interactions between atoms on the metal-bulk interfaces. These interactions correspond to the different electron-chemical and thermal processes. In particular, these boundary properties can be caused by impurities and pollutants. A distance parameter x_s' defining a metal-bulk contact surface denotes that a capacitance between the metal and the bulk at the contact exists. In this paper, we assumed that the contact voltage corresponding to a contact capacitance is much less than the applied voltage V. With this assumption, some $j(t)$ and $q_s(t)$ curves (Fig. 8−15) are found by a numerical method. These curves are obtained when the relative dielectric constant and the normalised distance parameter are $\varepsilon_r=2$ and $x_s=1$. From (39)−(41) it follows that the rate of change of the carrier concentrations at the electrodes is stimulated by the boundary parameters. Since those boundary parameters can be expressed by x_s, thus for numerical calculations we can assume that $x_s=1$. In general, for our numerical calculations, all the values of the internal and boundary parameters are of such the quantities for which all the derivatives are sufficiently small. Under these conditions, the numerical errors are suitably small. The same situation occurs when the relative dielectric constant is great (for example, in the case of the TiO_2 structure we have $\varepsilon_r=114$). It should be noted that the time constants characterising the generation-recombination processes depend on a material structure. For our numerical calculations, an initial configuration of atoms is characterised by the equilibrium concentrations (18) or (43) (other values can also be taken into account). In general, under conditions of an external electric field, from our numerical considerations it follows that the electric-magnetic force interactions between atoms in a solid and between atoms at the metal-bulk interfaces have an influence on the total energy of an electron. In particular, the electric-magnetic force interactions between atoms of the bulk and of the metal at the electrode contacts exist for which the electrons can be localised on the contact surfaces in the bulk. According to an experiment, we ascertain that the $j(t)$ curves presented in this paper are typical for materials basing on the structures such as polyethylene, Teflon, anthracene (a case of amorphous structure), CdS, SiC (a case of different hexagonal structures), Al_2O_3, TiO_2, polypropylene and others.

4. CONCLUSIONS

(1) Curve $j(t)$ can be monotone (Fig. 6, 7, 9) or can have an extreme (Fig. 1 – 5, 7, 8, 10, 11).

(2) When the boundary processes are very quick and the anode-bulk contact is perfectly blocking, then a function $j(t)$ is decreasing (Fig. 6), or it has a minimum (Fig. 3 – 5, 7).

(3) When the electrodes processes are very quick and allowed electron transition in the bulk are sufficiently slow, then the curve $j(t)$ can have a maximum (Fig. 1, 2).

(4) When the anode-bulk contact is perfectly blocking and the holes are immobile and the generation-recombination processes in the bulk are sufficiently quick, then the curve $j(t)$ can also have a maximum (Fig. 5).

(5) When the electrodes processes are sufficiently slow, then the total surface charge at the anode-bulk interface in the bulk is usually positive while this charge at the cathode-bulk interface in the bulk is usually negative (Fig. 14, 15).

(6) After a time, the surface charge on the contact surface at the anode can become negative when all the generation-recombination processes in a capacitor system are sufficiently slow (Fig. 13).

(7) In the case of (6), the curve $j(t)$ is permanently increasing. Under these conditions, the breakdown phenomenon can be observed. In the inverse case of (6), after a time the curve $j(t)$ is stabilised (Fig. 8, 12).

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ROZWINIĘCIE TEORII PRĄDÓW OGRANICZONYCH BIPOLARNYM ŁADUNKIEM PRZESTRZENNYM W UKŁADZIE METAL–DIELEKTRYK–METAL. PRZYKŁADOWE WYNIKI NUMERYCZNE

W niniejszym opracowaniu rozważa się dielektryk, w którym może istnieć ruchomy lub nieruchomy spułapkowany ujemny ładunek przestrzenny. W zagadnieniu podwójnego wstrzykiwania uwzględnia się różne procesy elektrodowe. Problem ten rozwiązuje się metodą numeryczną. Algorytm obliczeń numerycznych oparty jest na teorii charakterystyk.

ДАЛЬНЕЙШИЙ АНАЛИЗ ЗАДАЧИ ТОКА ДВОЙНОЙ ИНЖЕКЦИИ СООТНОШЕНИЯ МЕТАЛЛ-ИЗОЛЯТОР-МЕТАЛЛ. НЕКОТОРЫЕ ВЫЧИСЛИТЕЛЬНЫЕ РЕЗУЛЬТАТЫ

Рассматривается изолятор, в котором захваченные электроны являются подвижными или неподвижными. Граничные условия двойной инжекции образуют контактные процессы. Проблема переноса тока решается по вычислительному методу. Вычислительные решения получаются по теории характеристик.