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The Idea of Surface Recombination in Analysis of Bipolar-Charge Transport in Metal-Dielectric-Metal Configuration with a Thick Dielectric

by

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Summary. A problem of the boundary-condition formulation in the analysis of space bipolar-charge transport in a planar capacitor at constant supply voltage was developed. Influence of surface charge on electric conductivity in the system was investigated. Absorption-current densities $j(t)$ and surface-charge densities $q_s(t)$ as functions of time on the interface surfaces between dielectric and metal have been obtained.

1. Introduction. The formulation of boundary conditions in solid dielectrics at a given voltage condition is one of the basic tasks of the *space charge theory.* In the concept of *space bipolar-charge* two boundary conditions describing a mechanism of carriers injection from electrodes to a dielectric have to be formulated [1, 2]. The problem of formulation of boundary conditions is closely connected with a model system, in which the electrical charge transport is considered. In order to describe fully the electrical conductivity in the planar capacitor one needs to give equations describing carrier transport into the dielectric and also equations describing two mechanisms of carrier injections from the metal to the dielectric [1, 2]. According to general premises of *solid state theory,* during the electrical charge transport, the surface charge can appear on the interface planes between dielectric and metal. The surface charge density q_s, the transport-current density $\boldsymbol{j}_{tr}$ and the electrical field intensity $\boldsymbol{E}$ fulfil two elementary boundary equations of electrodynamics:

— the variation of the normal component of the vector $\boldsymbol{j}_{tr}$

$$j_{n_1} - j_{n_2} = \pm\frac{dq_s}{dt}, \quad j_n = \boldsymbol{j}\cdot\boldsymbol{n}^0, \quad |\boldsymbol{n}^0| = 1 \tag{1}$$

— the variation of the normal component of electrical induction

$$\varepsilon_1 E_{n_1} - \varepsilon_2 E_{n_2} = \pm q_s, \quad E_n = \boldsymbol{E} \cdot \boldsymbol{n}^0, \quad |\boldsymbol{n}^0| = 1 \tag{2}$$

where $\boldsymbol{n}^0$ — unit vector normal to the interface surface of two conducting media, t — time, ε_1, ε_2 — high-frequency permittivity of conducting media.

Condition (2) exists in the case of instantaneous polarization. Condition (1) characterize generation-recombination processes on the interface surface between dielectric and metal.

The planar capacitor system is characterized by the absorption current density $j(t)$:

$$j(t) = \varepsilon \frac{\partial \boldsymbol{E}(x,t)}{\partial t} + j_{t_r}(x,t) \tag{3}$$

where x — the distance from the electrode, ε — the high frequency electrical permittivity of the dielectric.

The aim of this paper is a determination of the correlation between generation-recombination processes on the interface surfaces of the solid dielectric with electrodes and the time-dependent densities of absorption-currents $j(t)$ of the planar capacitor system.

2. Basic equations. In order to link the absorption-current $j(t)$ and the boundary values of surface charge q_s, a model of electrical conductivity in a dielectric is to be stated. It will be assumed in the sequel that space charge is composed of free negative-charge carriers and free positive-charge carriers with concentrations $n(x,t)$ and $p(x,t)$, respectively. The trap states in electrical conductivity are here neglected. Such an assumption consists some simplification of the considered problem but does not change a mathematical gist of description of bipolar charge transport as a whole issue of electrical conductivity analysis in the metal-dielectric-metal system. This assumption has been done in order to reduce redundant internal parameters of the dielectric and to expose the influence of contacts on time functions $j(t)$.

In a case of the planar capacitor system, with the constant voltage applied to the electrodes, values of carriers concentrations $n(x,t)$, $p(x,t)$ and electric field intensity $E(x,t)$ are related with Gauss, continuity and recombination equations in the form [1]:

$$\varepsilon \frac{\partial \boldsymbol{E}(x,t)}{\partial x} = e_0(p(x,t) - n(x,t)), \tag{4}$$

$$\frac{\partial}{\partial x}\{\mu_n \cdot n(x,t) \cdot \boldsymbol{E}(x,t) + \mu_p \cdot p(x,t) \cdot \boldsymbol{E}(x,t)\} + \frac{\partial p(x,t)}{\partial t} - \frac{\partial n(x,t)}{\partial t} = 0, \tag{5}$$

$$\frac{\partial n(x,t)}{\partial t} = \frac{\partial}{\partial x}\{\mu_n \cdot n(x,t) \cdot \boldsymbol{E}(x,t)\} - \beta(n(x,t) \cdot p(x,t) - n_0 p_0), \tag{6}$$

where $e_0 = 1{,}6 \cdot 10^{-19}$ C, μ_n, μ_p — mobilities of negative and positive charge carriers, respectively, β — a coefficient of bimolecular recombination, $n_0 = p_0$ — equilibrium concentrations of negative and positive charge carriers, respectively. Equations (4–6) describe the transport of bipolar charge carriers in the dielectric. The voltage condition of the planar capacitor system supplied by an ideal source of constant voltage is the complementary dependence to Eqs (4–6). In the sequel there is assumed that the distance between electrodes of the metal-dielectric-metal system is L, and that the interface surfaces are $x = 0$ and $x = L$. Assuming existence of the surface charges with $q_{s|x=0}$ and $q_{s|x=L}$ densities, the voltage condition has the form:

$$\int_{0_-}^{0_+} \boldsymbol{E}(x,t)dx + \int_{0_+}^{L_-} \boldsymbol{E}(x,t)dx + \int_{L_-}^{L_+} \boldsymbol{E}(x,t)dx = U = \text{const}, \quad U > 0, \tag{7}$$

where 0_- — a left-side limit at the point $x = 0$, L_+ — a right-side one in the point $x = L$. The integrals $\int_{0_-}^{0_+}$ and $\int_{L_-}^{L_+}$ — represent the value of metal-dielectric contact voltage.

Depending on the values of U and L the contact voltages may be neglected or not as compared to U. The basis of this estimation are Schottky' and tunnel effects when the assumed thickness of double layer is in the range 1 — 10 Å. Dielectrics, in which contact voltages may be neglected, are named the thick dielectrics [3]. In this paper the transient state of electrical conductivity in the thick dielectrics will be examined so

$$\int_0^L \boldsymbol{E}(x,t)dt = U = \text{const} \quad U > 0. \tag{8}$$

Hence, on the base of (4), (5) the function of absorption-current density $j(t)$ (3) can be presented in the equivalent form

$$j(t) = \frac{e_0}{L}\int_0^L [\mu_n \cdot n(x,t) + \mu_p \cdot p(x,t)]\boldsymbol{E}(x,t)dx \tag{9}$$

The purpose of this paper is to determine the function $j(t)$ when there exists the surface charge with densities $q_{s|x=0}$ and $q_{s|x=L}$ on interface planes of the dielectric and electrodes. According to condition (8) the case $E(x,t) > 0$ in the whole region of dielectric will be taken into consideration. Thus, from (4–6) it follows the conclusion that in order to determine the function $j(t)$ there are needed two boundary conditions [1], one for the electrode next to the plane $x = 0$ injecting positive-charge carriers and the second one for the electrode next to the plane $x = L$ injecting negative-charge carriers to the dielectric. A mechanism of carriers injection from metal or dielectric surface to vacuum is described by the current and electrical field densities functions at the emitting surface.

Let the electrical conductivity mechanism be an electron-hole type and let the limit values 0_- and L_+ is applied, thus boundary condition (1) for the surfaces $x = 0$ and $x = L$ gets the form

$$(10)\quad -\frac{dq_s}{dt}_{|x=0} = -f_0[E(0_-,t)]+[e_0\cdot\mu_n\cdot n(0_+,t)+e_0\cdot\mu_p\cdot p(0_+,t)]E(0_+,t),$$

$$(11)\quad -\frac{dq_s}{dt}_{|x=L} = -[e_0\cdot\mu_n\cdot n(L_-,t)+e_0\cdot\mu_p\cdot p(L_-,t)]E(L_-,t)+f_L[E(L_+,t)],$$

where f_0 and f_L — functions describing mechanism of emission from a dielectric and metal surface to vacuum, respectively, $E(0_-,t)$ and $E(L_+,t)$ — electric field intensity at $x = 0$ and $x = L$, respectively, both seen from the side of the metal. Introduction of the values $E(0_-,t)$ and $E(L_+,t)$ is due to the granular character of interface surfaces and the possible surface deviations. In consequence, the surface charge densities $q_{s|x=0}$ and $q_{s|x=L}$ fulfilling condition (2) have the form

$$(12)\quad q_{s|x=0} = \varepsilon_0[\varepsilon_r E(0_+,t) - E(0_-,t)]$$

$$(13)\quad q_{s|x=L} = \varepsilon_0[E(L_+,t) - \varepsilon_r E(L_-,t)]$$

where ε_r — high frequency relative permittivity of dielectric, ε_0 — permittivity of vacuum.

The boundary values $p(0_+,t)$ and $n(L_-,t)$ defined by Eqs (10) and (11) are necessary for complete description of electrical conductivity. For this purpose, one needs to define the positive surface charge $^+q_{s|x=0}$ and the negative one $^-q_{s|x=0}$. The mean-value theorem can be used to the system of the planar capacitor

$$(14)\quad \int_S ds \int_0^{x_s} q_v\, dx = \int_S x_s \cdot \tilde{q}_v\, ds, \quad \tilde{q}_v = q_v(c,t), \quad 0 \leqslant c \leqslant x_s,$$

where q_v — the value of space charge density, to obtain dependencies linking the values $^+q_{s|x=0}$ and $^-q_{s|x=L}$ with the boundary values $p(0_+,t)$ and $n(L_-,t)$

$$(15)\quad ^+q_{s|x=0} = e_0 \cdot x_s \cdot p(0_+,t), \qquad 0 \leqslant x_s \leqslant L,$$

$$(16)\quad ^-q_{s|x=L} = -e_0 \cdot x_s \cdot n(L_-,t), \quad 0 \leqslant x_s \leqslant L.$$

In the electron-hole description of electrical conductivity, a generation-recombination process of electron-hole pair proceeds together with the process carriers injection into the dielectric on the contact surface between the dielectric and metal. If the law of bimolecular surface recombination is taken into account dependencies (10) and (11) for $^+q_{s|x=0}$ and $^-q_{s|x=L}$ described

by Eqs (15), (16) have the form

$$(17)\quad x_s\frac{dp(0_+,t)}{dt} = -\beta_0(n(0_+,t)\cdot p(0_+,t) - n_0\cdot p_0) - \mu_p\cdot p(0_+,t)\cdot E(0_+,t) + \frac{f_0(E(0_-,t))}{e_0}$$

$$(18)\quad x_s\frac{dn(L_-,t)}{dt} = -\beta_L(n(L_-,t)\cdot p(L_-,t) - n_0\cdot p_0) - \mu_n\cdot n(L_-,t)\cdot E(L_-,t) + \frac{f_L(E(L_+,t))}{e_0}$$

where β_0, β_L — surface recombination coefficients. Thus, Eqs. (4)–(6), (8), (10)–(13), (16), (17) describe completely the electrical conductivity in the planar capacitor system and allow to calculate the function $j(t)$ described by Eq. (9). Further, the function $j(t)$ with given boundary conditions (17), (18), (10)–(13) is determined.

3. Solution of the problem. The function $j(t)$ has been found numerically utilizing the method of characteristics [1, 2, 3] in the set of normalized variables: u', E', x', n', p', t', j', τ_R, τ_1, τ_2, r, q'_s determined by the equations:

$$(19)\quad \begin{array}{llll} u' = \dfrac{U}{U_0}, & E' = \dfrac{L\cdot E}{U_0}, & x' = \dfrac{X}{L}, & n' = \dfrac{e_0 L^2 n}{\varepsilon\cdot U_0}, \\ p' = \dfrac{e_0 L^2 p}{\varepsilon\cdot U_0}, & t' = \dfrac{\mu_n U_0 t}{L^2}, & j' = \dfrac{L^3 j}{\varepsilon\cdot U_0^2\mu_n}, & \tau_R = \dfrac{e_0\mu_n}{\varepsilon\cdot\beta}, \\ \tau_1 = \dfrac{e_0\mu_n L}{\varepsilon\cdot\beta_0}, & \tau_2 = \dfrac{e_0\mu_n L}{\varepsilon\cdot\beta_L}, & r = \dfrac{\mu_p}{\mu_n}, & q'_s = \dfrac{L\cdot q_s}{\varepsilon\cdot U_0}, \end{array}$$

where U_0 — the reference voltage.

In further dependences the apostrophe is omitted, and the results are

the absorption current density

$$(20)\quad j(t) = \int_0^1 (n + rp)\cdot E\, dx$$

— the characteristics equations

$$(21)\quad dx_n/dt = -E \quad\text{and}\quad dn/dt = n(p-n) - (np - n_0p_0)/\tau_R$$

$$(22)\quad dx_p/dt = rE \quad\text{and}\quad dp/dt = -rp(p-n) - (np - n_0p_0)/\tau_R$$

— the electric field density distribution

$$(23)\quad E(x,t) = E(0_+,t) + \int_0^x (p-n)dx, \quad E(0_+,t) = u - \int_0^1 (1-x)\cdot(p-n)dx,$$

— the boundary equations

$$\varepsilon_r E(0_+,t) - E(0_-,t) = \varepsilon_r \cdot q_{s|x=0} \tag{24}$$
$$E(1_+,t) - \varepsilon_r E(1_-,t) = \varepsilon_r \cdot q_{s|x=1}$$

$$\frac{dq_s}{dt}_{|x=0} = f_0[E(0_-,t)] - [n(0_+,t) + rp(0_+,t)] \cdot E(0_+,t) \tag{25}$$

$$\frac{dq_s}{dt}_{|x=1} = [n(1_-,t) + rp(1_-,t)] \cdot E(1_-,t) - f_1[E(1_+,t)] \tag{26}$$

$$\frac{dp(0_+,t)}{dt} = \frac{1}{x_s}\Big\{-\frac{1}{\tau_1}(n(0_+,t)\cdot p(0_+,t) - n_0p_0) - rp(0_+,t)\cdot E(0_+,t) + f_0[E(0_-,t)]\Big\} \tag{27}$$

$$\frac{dn(1_-,t)}{dt} = \frac{1}{x_s}\Big\{-\frac{1}{\tau_2}(n(1_-,t)\cdot p(1_-,t) - n_0p_0) - n(1_-,t)\cdot E(1_-,t) + f_1[E(1_+,t)]\Big\}. \tag{28}$$

Dependences (21)–(28) form a basis of the algorithm to calculate the values of function $j(t)$ (20). Because integral condition (8) is fulfilled, the case of carriers transport, where $E(x,t) > 0$, is considered in numerical calculations. Moreover, the initial values have been applied

$$p(x,0) = n(x,0) = n_0 = p_0 = 1 \tag{29}$$
$$q_s(t=0)_{|x=0} = q_s(t=0)_{|x=1} = 0.$$

The Fauler–Nordheim and Schottky type functions were chosen as the boundary functions f_0 and f_1. The calculations were done for constant values $u = 5$, $\varepsilon_r = 2$, $x_s = 1$. Some results of numerical calculations of absorption-current density $j(t)$ as function of time and the entire surface-charge densities $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$ are given below in the set of dimensionless variables.

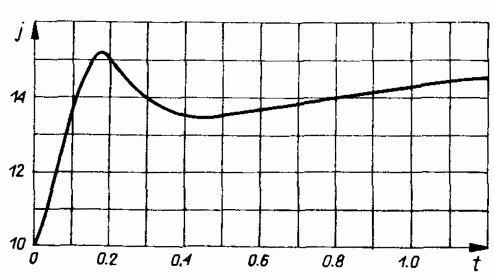

Fig. 1. Time-varying wave form of absorption current density $j(t)$
$f_0 \equiv 0$; $f_1 = a_1 E^2(1_+,t)\exp(-b_1/E(1_+,t))$; $r = 1$; $a_1 = b_1 = 1$; $\tau_R = 1$; $\tau_1 = \tau_2 = 0.5$

4. Conclusions. It results from the numerous numerical calculations of the presented model of electrical conductivity that surface processes contribute to the electrical conductivity of relaxation type in the metal-dielectric-metal set.

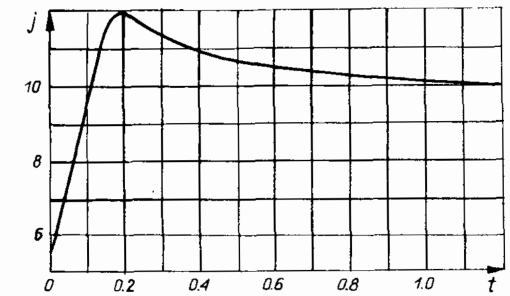

Fig. 2. Time-varying wave form of absorption current density $j(t)$
$f_0 \equiv 0$; $f_1 = a_1 E^2(1_+,t)\exp(-b_1/E(1_+,t))$; $r = 0.1$; $a_1 = b_1 = 1$; $\tau_R = 1$; $\tau_1 = \tau_2 = 0.5$

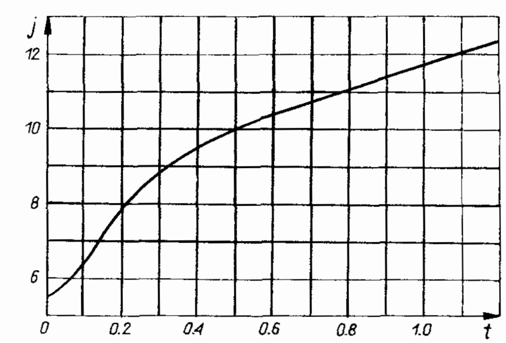

Fig. 3. Time-varying wave form of absorption current density $j(t)$
$f_0 = a_0 E^2(0_-,t)$; $f_1 = a_1 \exp(b_1\sqrt{E(1_+,t)})$; $r = 0.1$; $a_0 = 1$; $a_1 = 5$; $b_1 = 0.2$; $\tau_R = \tau_1 = \tau_2 = 10000$

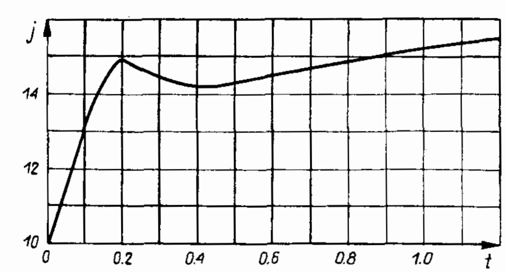

Fig. 4. Time-varying wave form of absorption current density $j(t)$
$f_0 = a_0 E^2(0_-,t)$; $f_1 = a_1 \exp(b_1\sqrt{E(1_+,t)})$; $r = 1$; $a_0 = 0.5$; $a_1 = 1$; $b_1 = 0.2$; $\tau_R = 1$; $\tau_1 = \tau_2 = 0.5$

The surface processes on the metal-dielectric contacts can affect the wave forms $j(t)$ plotted in Fig. 1 to Fig. 5. The wave form $j(t)$ in Fig. 2 is typical function of time obtained in [1, 2].

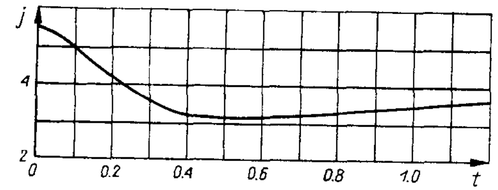

Fig. 5. Time-varying wave form of absorption current density $j(t)$

$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 \exp(b_1\sqrt{E(1_+, t)})$; $r = 0.1$; $a_0 = 0.2$; $a_1 = 1$; $b_1 = 0.2$; $\tau_1 = \tau_2 = \tau_R = 10000$

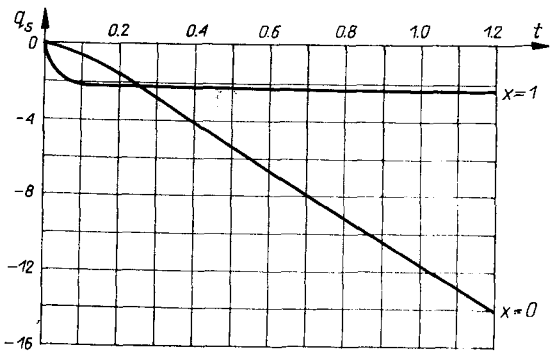

Fig. 6. Time-varying wave form of surface charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$

$f_0 \equiv 0$; $f_1 = a_1 E^2(1_+, t)\exp(-b_1/E(1_+, t))$; $r = 0.1$; $a_1 = b_1 = 1$; $\tau_R = 1$; $\tau_1 = \tau_2 = 0.5$

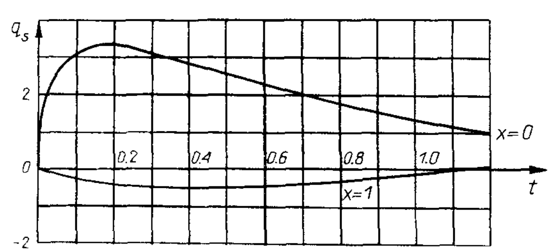

Fig. 7. Time-varying wave form of surface charge density $q_s(t)_{x=0}$ and $q_s(t)_{|x=1}$

$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 \exp(b_1\sqrt{E(1_+, t)})$; $r = 0.1$; $a_0 = 1$; $a_1 = 5$; $b_1 = 0.2$; $\tau_1 = \tau_2 = \tau_R = 10000$

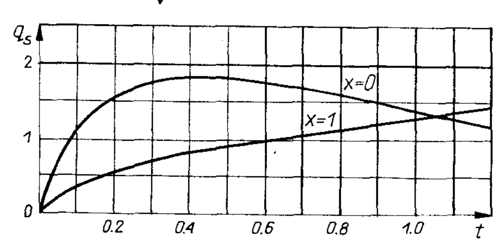

Fig. 8. Time-varying wave form of surface charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$

$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 \exp(b_1\sqrt{E(1_+, t)})$; $r = 0.1$; $a_0 = 0.2$; $a_1 = 1$; $b_1 = 0.2$; $\tau_1 = \tau_2 = \tau_R = 10000$

Depending on the values of boundary functions which describe the mech-

anism of carriers injection, an influence of internal and boundary parameters on the shapes of $j(t)$, $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$ wave forms is observed. A maximum appearing in the plot $j(t)$ is characteristic for a tunnel effect while a minimum is characteristic for generation-recombination processes. The wave form $j(t)$ corresponding to the plot $q_s(t)$ from Fig. 9 is similar to that in Fig. 5.

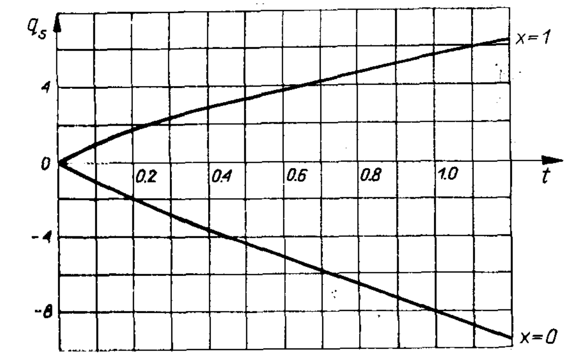

Fig. 9. Time-varying wave form of surface charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$

$f_0 \equiv 0$, $f_1 = a_1 \exp(b_1\sqrt{E(1_+, t)})$; $r = 1$; $a_1 = 1$; $b_1 = 0.2$; $\tau_R = 1$; $\tau_1 = \tau_2 = 0.5$

The ideas of formulation of boundary conditions presented in this work will be the basis of further analysis of the electrical conductivity of the metal-dielectric-metal system.

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