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Development of Idea of Surface Recombination in Analysis of Bipolar-Charge Transport in Metal-Dielectric-Metal System with Thick Dielectric

by

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Summary. In this model system there is presented the electric conduction with three mobilities of carriers when the surface traps exist. The free electrons and holes as well as the trapped electrons form the space charge in the dielectric. The transient state is examined for the different effects of the injection of carriers. There are determined the functions $j(t)$ and $q_s(t)$ of current density and surface charge.

1. Introduction. The idea of a surface charge on an interface planes between solid dielectric and metal is one of the conceptions of the determination of the boundary values' concentration of free carriers of the positive and negative charge [1]. This idea exists in two basic boundary equations of electrodynamics: the change of the normal component of the vector's current density, the change of the normal component of the vector's electric induction. In this problem, there are distinguished the domain of the space-charge and the domain of the surface charge. Assuming existence of the surface charge in the planar capacitor system, the integral condition can be described by the formula:

$$\int_{0_-}^{0_+} \boldsymbol{E}\,dx + \int_{0_+}^{L_-} \boldsymbol{E}\,dx + \int_{L_-}^{L_+} \boldsymbol{E}\,dx = U = \text{const}; \quad U > 0 \tag{1a}$$

or in case of thick dielectric [1], when the contact voltage may be neglected, condition (1a) has the form:

$$\int_{0_+}^{L_-} \boldsymbol{E}(x,t)\,dx = U \tag{1b}$$

where E — electric field intensity, U — voltage applied to the electrodes, L — distance between electrodes, x — distance from the electrode, t — time, $x = 0_+$ and $x = L_+$ — a right-hand limit at $x = 0$ and $x = L$, respectively, $x = 0_-$ and $x = L_-$ — a left-hand limit at $x = 0$ and $x = L$, respectively. The planes $x = 0$ and $x = L$ are the interfaces between the dielectric and metal. In the concept of space bipolar-charge, the value of electric field intensity $E(0_-, t)$ characterizes the electron emission from the dielectric plane $x = 0$ to the electrode $x = 0_-$, whereas $E(L_+, t)$ characterizes the electron emission from the electrode $x = L_+$ to the dielectric plane $x = L$. The points $x = 0_+$ and $x = L_-$ are internal points of the dielectric. This two basic boundary equations have the form:

$$(2)\qquad \begin{aligned} -\frac{dq_s}{dt}_{|x=0} &= -f_0[E(0_-, t)] + j_{tr}(0_+, t) \\ -\frac{dq_s}{dt}_{|x=L} &= f_L[E(L_+, t)] - j_{tr}(L_-, t) \end{aligned}$$

and

$$(3)\qquad \begin{aligned} q_{s|x=0} &= \varepsilon_0[\varepsilon_r E(0_+, t) - E(0_-, t)] \\ q_{s|x=L} &= \varepsilon_0[E(L_+, t) - \varepsilon_r E(L_-, t)] \end{aligned}$$

where $\varepsilon_0 = 8.85 \cdot 10^{-12} \frac{\mathrm{F}}{\mathrm{m}}$, q_s — surface-charge density, f_0 and f_L — the functions of current emission density from a dielectric and metal surface, respectively, ε_r — high frequency permittivity, j_{tr} — current density of a transport. According to the mean-value theorem in the planar capacitor system, the $q_s(t)$ function is described by the formula:

$$(4)\qquad q_s(t) = x_s \cdot q_v(c, t); \quad 0 \leqslant x_s \leqslant L; \quad 0 \leqslant c \leqslant x_s,$$

where q_v — the value of space-charge density, and if $x_s = 0$, then $q_s(t) = 0$. In the present work, it was assumed that the space charge is formed by free and trapped electrons and free holes. Trapped electrons can displace from a trap to a trap at the mobility μ_t = constant. In consequence, the space-charge density q_v and the current density of a transport j_{tr} have the form:

$$(5)\qquad q_v(x, t) = e_0\{(p(x, t) - p_0) - (n(x, t) - n_0) - (n_t(x, t) - n_{t,0})\}; \qquad p_0 = n_0 + n_{t,0}$$

$$(6)\qquad j_{tr}(x, t) = e_0 E(x, t)\{\mu_p p(x, t) + \mu_n n(x, t) + \mu_t n_t(x, t)\}; \qquad \mu_p > 0; \quad \mu_n > 0; \quad \mu_t > 0$$

where $e_0 = 1.6 \cdot 10^{-19}$ C, μ_n, μ_p — mobility of electron and hole, respectively, n, p — concentrations of free electrons and holes, respectively, n_t — concentrations of trapped electrons, n_0, p_0, $n_{t,0}$ — equilibrium concentrations. Equation (5) and (6) can describe one trapping level or more discrete trapping levels with the same parameter μ_t on condition that a distance between energy levels of trapped electrons is small.

The aim of the paper is an investigation of the electric conduction with three mobilities of carriers and the surface recombination in the planar capacitor system with constant voltage between the electrodes.

2. Problem solution. In this work, it will be considered the transient state of the transport of positive and negative charges with the integral condition (1b). The transient state is characterized by the function of current density $j(t)$ [1]

$$(7)\qquad j(t) = \frac{1}{L}\int_{0_+}^{L_-} j_{tr}(x, t)\, dx$$

and by the functions of surface charge $q_s(t)_{|x=0}$ and $q_s(t)_{|x=L}$. In this case of the electric conduction, the transport of the carriers is described by the equations:

$$(8)\qquad \varepsilon\frac{\partial E(x, t)}{\partial x} = q_v(x, t); \qquad \varepsilon = \varepsilon_0\varepsilon_r$$

$$(9)\qquad \frac{1}{e_0}\frac{\partial}{\partial x}\{j_{tr}(x, t)\} + \frac{\partial p(x, t)}{\partial t} - \frac{\partial n(x, t)}{\partial t} - \frac{\partial n_t(x, t)}{\partial t} = 0$$

$$(10)\qquad \frac{\partial n_t(x, t)}{\partial t} = C_n N_t n(x, t) + \nu_p N_t - \nu_n n_t(x, t) - C_p p(x, t) n_t(x, t) + \frac{\partial}{\partial x}\{\mu_t n_t(x, t) E(x, t)\}$$

$$(11)\qquad \frac{\partial n(x, t)}{\partial t} = \nu_n n_t(x, t) - C_n N_t n(x, t) + \frac{\partial}{\partial x}\{\mu_n n(x, t) E(x, t)\},$$

where equations (8) and (9) are the Gauss' and the continuity equations, respectively. Recombination equations (10) and (11) are used for the concentration of the traps N_t when $N_t \gg n_t$, and the material coefficients C_n, C_p, ν_n are independent of electric field intensity. If $E \equiv 0$, then the recombination equations make the forms:

$$(12)\qquad \nu_n = \frac{C_n N_t n_0}{n_{t,0}}; \quad \nu_p = \frac{C_p p_0 n_{t,0}}{N_t};$$

In the paper, we assume the relation $E(x, t) > 0$ (it is possible). According to the transport equation, there are determined the boundary values: $p(0_+, t)$, $n(L_-, t)$ and $n_t(L_-, t)$ at $x = 0_+$ and $x = L_-$. Assuming that the generation-recombination processes exist on the contact surfaces $x = 0$ and $x = L$, the boundary values fulfil the equation [1]:

$$\text{(13)}\quad \frac{dp(0_+,t)}{dt} = \frac{1}{x_s}\{\nu'_{ps}N'_{ts} + f_0/\epsilon_0 - \mu_p p(0_+,t)E(0_+,t) - C_{ps}p(0_+,t)n_t(0_+,t)\}$$

$$\text{(14)}\quad \frac{dn(L_-,t)}{dt} = \frac{1}{x_s}\{f_L/\epsilon_0 + \nu_{ns}n_t(L_-,t) - C_{ns}N_{ts}n(L_-,t) - \mu_n n(L_-,t)E(L_-,t)\}$$

$$\text{(15)}\quad \frac{dn_t(L_-,t)}{dt} = \frac{1}{x_s}\{\nu_{ps}N_{ts} + C_{ns}N_{ts}n(L_-,t) - \nu_{ns}n_t(L_-,t) - C'_{ps}p(L_-,t)n_t(L_-,t) + \mu_t n_t(L_-,t)E(L_-,t)\},$$

where ν_{ps}, ν'_{ps}, N_{ts}, N'_{ts}, C_{ns}, ν_{ns}, C_{ps}, C'_{ps} — the surface coefficients which fulfil the relations:

$$\text{(16)}\quad \nu_{ps} = \frac{C_{ps}p_0 n_{t,0}}{N_{ts}}; \quad \nu_{ns} = \frac{C_{ns}N_{ts}n_0}{n_{t,0}}.$$

Relations (13)–(15) follow also from Eq. (4). Thus, equations of carrier transport (5), (6), (8)–(11) with boundary functions (13)–(15) and with a initial state of the charged dielectric describe the transient state of the electric conduction. The functions: $j(t)$, $q_s(t)_{|x=0}$, $q_s(t)_{|x=L}$ will be determined numerically in the system of nondimensional variables: E', u', t', p', n', n'_t, τ'_p, τ'_1, τ'_2, τ'_{ns}, τ'_{ps}, τ'_n, τ'_{1s}, τ'_{2s}, r_1, r_2, r_3, x', j', q'_s which are defined by the formulas:

$$\text{(17)}\quad \begin{aligned}
&E' = \frac{LE}{U_0}; && u' = \frac{U}{U_0}; && x' = \frac{x}{L}; && p' = \frac{L^2\epsilon_0 p}{\varepsilon U_0};\\
&n' = \frac{L^2\epsilon_0 n}{\varepsilon U_0}; && n'_t = \frac{L^2\epsilon_0 n_t}{\varepsilon U_0}; && t' = \frac{\mu U_0 t}{L^2}; && \tau'_n = \frac{\mu U_0}{L^2 C_n N_t};\\
&\tau'_p = \frac{\epsilon_0\mu}{\varepsilon C_p}; && \tau'_1 = \frac{\mu U_0}{L^2\nu_n}; && \tau'_2 = \frac{\mu U_0^2}{L^4\epsilon_0\nu_p N_t}; && \tau'_{1s} = \frac{\mu U_0}{L\nu_{ns}};\\
&\tau'_{ns} = \frac{\mu U_0}{LC_{ns}N_{ts}}; && \tau'_{ps} = \frac{\epsilon_0\mu L}{\varepsilon C_{ps}}; && \tau'_{2s} = \frac{\mu U^2}{L^3\epsilon_0\nu'_{ps}N'_{ts}}; && j' = \frac{L^3 j}{\varepsilon\mu U_0^2};\\
&r_1 = \frac{\mu_p}{\mu}; && r_2 = \frac{\mu_t}{\mu}; && r_3 = \frac{\mu_n}{\mu}; && q'_s = \frac{Lq_s}{\varepsilon U_0},
\end{aligned}$$

where U_0, μ — the reference voltage and mobility, respectively. After omission the apostrophe, the equations of the electric charge transport take the following forms in the system of nondimensional variables:

— the equations of characteristics [2]

$$\text{(18)}\quad \frac{dx_n}{dt} = -r_3E \quad\text{and}\quad \frac{dn}{dt} = r_3 n(p-n-n_t) + \frac{n_t}{\tau_1} - \frac{n}{\tau_n}$$

$$\text{(19)}\quad \frac{dx_p}{dt} = r_1E \quad\text{and}\quad \frac{dp}{dt} = \frac{1}{\tau_2} - r_1 p(p-n-n_t) - \frac{pn_t}{\tau_p}$$

$$\text{(20)}\quad \frac{dx_t}{dt} = -r_2E \quad\text{and}\quad \frac{dn_t}{dt} = r_2 n_t(p-n-n_t) + \frac{n}{\tau_n} + \frac{1}{\tau_2} - \frac{n_t}{\tau_1} - \frac{pn_t}{\tau_p}$$

— the distribution of electric field intensity

$$\text{(21)}\quad \begin{aligned}
E(0_+,t) &= U - \int_{0_+}^{1_-}(1-x)(p-n-n_t)\,dx\\
E(x,t) &= E(0_+,t) + \int_{0_+}^{x}(p-n-n_t)\,dx\\
E(1_-,t) &= E(0_+,t) + \int_{0_+}^{1_-}(p-n-n_t)\,dx
\end{aligned}$$

— the boundary equations:

$$\text{(22)}\quad \begin{aligned}
\varepsilon_r E(0_+,t) - E(0_-,t) &= \varepsilon_r q_{s|x=0}\\
E(1_+,t) - \varepsilon_r E(1_-,t) &= \varepsilon_r q_{s|x=1}
\end{aligned}$$

and

$$\text{(23)}\quad \frac{dq_s}{dt}_{|x=0} = f_0[E(0_-,t)] - [r_1p(0_+,t) + r_2n_t(0_+,t) + r_3n(0_+,t)]E(0_+,t)$$

$$\text{(24)}\quad \frac{dq_s}{dt}_{|x=1} = [r_1p(1_-,t) + r_2n_t(1_-,t) + r_3n(1_-,t)]E(1_-,t) - f_1[E(1_+,t)]$$

where f_0, f_1 — normalized emission current densities;

— the boundary conditions:

$$\text{(25)}\quad \frac{dp(0_+,t)}{dt} = \frac{1}{x_s}\left\{\frac{1}{\tau_{2s}} + f_0[E(0_-,t)] - r_1p(0_+,t)E(0_+,t) - \frac{p(0_+,t)n_t(0_+,t)}{\tau_{ps}}\right\}$$

$$\text{(26)}\quad \frac{dn(1_-,t)}{dt} = \frac{1}{x_s}\left\{-\frac{n(1_-,t)}{\tau_{ns}} + \frac{n_t(1_-,t)}{\tau_{1s}} - r_3n(1_-,t)E(1_-,t) + f_1[E(1_+,t)]\right\}$$

$$\text{(27)}\quad \frac{dn_t(1_-,t)}{dt} = \frac{1}{x_s}\left\{\frac{1}{\tau_{2s}} - \frac{p(1_-,t)n_t(1_-,t)}{\tau_{ps}} + \frac{n(1_-,t)}{\tau_{ns}} - \frac{n_t(1_-,t)}{\tau_{1s}} - r_2n_t(1_-,t)E(1_-,t)\right\}.$$

In Eqs (25)–(27), there are taken in the same values of the surface parameters τ_{2s} and τ_{ps} for surfaces $x = 0$ and $x = 1$. This assumption reduces the number of the dielectric' parameters. The generation-recombination parameters are described by the formulas:

$$\tau_1 = \tau_n \frac{n_{t,0}}{n_0}; \quad \tau_2 = \frac{\tau_p}{p_0 n_{t,0}}; \quad \tau_{1s} = \tau_{ns} \frac{n_{t,0}}{n_0}; \quad \tau_{2s} = \frac{\tau_{ps}}{p_0 n_{t,0}}. \tag{28}$$

There are taken in the following values of the initial conditions in the numerical calculation:

$$\begin{aligned} &p(x,0) = p_0 = 2; \quad n(x,0) = n_0 = 1; \quad n_t(x,0) = n_{t,0} = 1 \\ &q_s(t=0)_{|x=0} = 0; \quad q_s(t=0)_{|x=1} = 0. \end{aligned} \tag{29}$$

The functions $q_s(t)_{|x=0}$, $q_s(t)_{x=1}$ and the function $j(t)$

$$j(t) = \int_{0_+}^{1_-} [r_1 p(x,t) + r_2 n_t(x,t) + r_3 n(x,t)] E(x,t)\, dx \tag{30}$$

were defined in the present problem of the electric conduction.

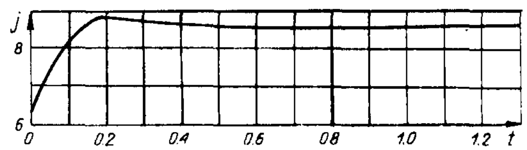

Fig. 1. Time-varying wave form of current density $j(t)$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 E^2(1_+, t)$; $a_0 = 0.2$; $a_1 = 0.5$; $r_1 = r_2 = 0.1$, $r_3 = 1$; $\tau_n = \tau_{ns} = \tau_2 = \tau_{2s} = 0.1$

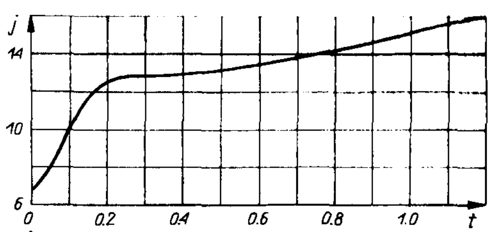

Fig. 2. Time-varying wave form of current density $j(t)$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 E^2(1_+, t)$; $a_0 = 0.2$; $a_1 = 0.5$; $r_1 = r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = \tau_2 = \tau_{2s} = 1$

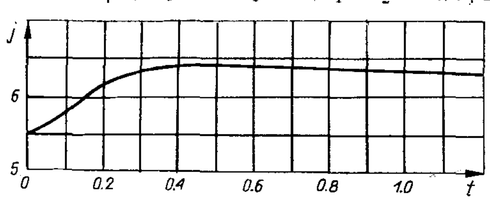

Fig. 3. Time-varying wave form of current density $j(t)$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t) \exp(-b_0 / E(0_-, t))$; $f_1 = a_1 E^2(1_+, t) \exp(-b_1 / E(1_+, t))$; $a_0 = 0.5$; $b_0 = 0.5$; $a_1 = 0.1$; $b_1 = 1$; $r_1 = 0$; $r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = 0.1$; $\tau_2 = \tau_{2s} = 1$

The numerical calculations were performed for selected functions of car-

rier emission f_0 and f_1 and $\varepsilon_r = 2$, $u = 5$, $x_s = 1$. The results are presented in the figures.

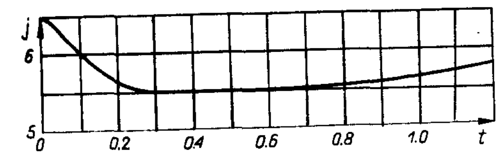

Fig. 4. Time-varying wave form of current density $j(t)$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t) \exp(-b_0 / E(0_-, t))$; $f_1 = a_1 \exp(b_1 E^{1/2}(1_+, t))$; $a_0 = 0.2$; $b_0 = 1$; $a_1 = 1$; $b_1 = 0.1$; $r_1 = r_3 = 0.1$; $r_2 = 1$; $\tau_n = \tau_2 = 10$; $\tau_{ns} = \tau_{2s} = 0.1$;

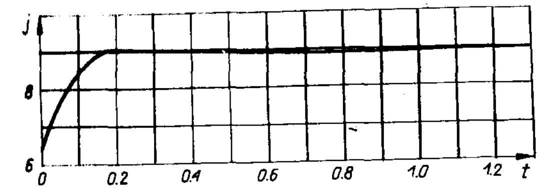

Fig. 5. Time-varying wave form of current density in the system of normalized variables
$f_0 = 0$; $f_1 = a_1 E^2(1_+, t) \exp(-b_1 / E(1_+, t))$; $a_1 = 0.5$; $b_1 = 1$; $r_1 = r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = \tau_2 = \tau_{2s} = 0.1$

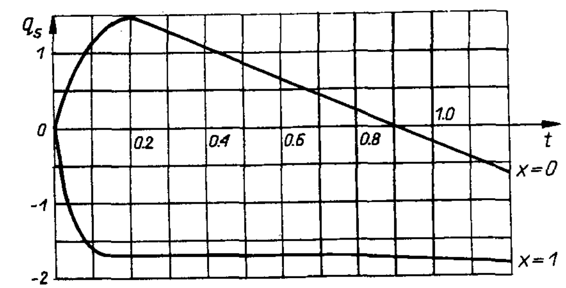

Fig. 6. Time-varying wave form of surface-charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 E^2(1_+, t)$; $a_0 = 0.2$; $a_1 = 0.5$; $r_1 = r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = \tau_2 = \tau_{2s} = 1$

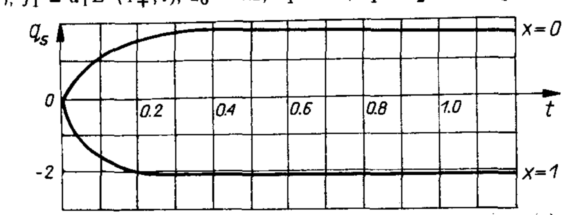

Fig. 7. Time-varying wave form of surface-charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t)$; $f_1 = a_1 E^2(1_+, t)$; $a_0 = 0.2$; $a_1 = 0.5$; $r_1 = r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = \tau_2 = \tau_{2s} = 0.1$

3. Conclusion. The model of the electric conduction presented in the work can be applied for an investigation of the nonhomogeneous dielectric structures which are made by the vapour deposition of metal, of semiconductor or another dielectric material on the dielectric surface (the thickness of deposited film is small in comparison with the thickness of the dielectric base).

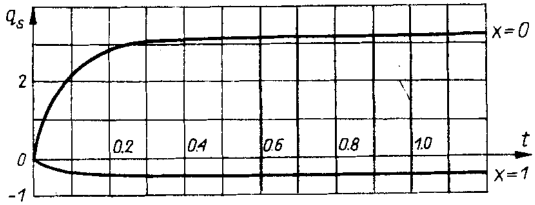

Fig. 8. Time-varying wave form of surface-charge density $q_s(t)_{|x=0}$ and $q_s(t)_{|x=1}$ in the system of normalized variables
$f_0 = a_0 E^2(0_-, t)\exp(-b_0/E(0_-, t))$; $f_1 = a_1 E^2(1_+, t)\exp(-b_1/E(1_+, t))$; $a_0 = 0.5$; $b_0 = 0.5$; $a_1 = 0.1$; $b_1 = 1$; $r_1 = 0$; $r_2 = 0.1$; $r_3 = 1$; $\tau_n = \tau_{ns} = 0.1$; $\tau_2 = \tau_{2s} = 1$

The heterogeneity of the dielectric surface can be characterized by the parameter q_s. Numerous numerical calculations allow to ascertain that the system may attain the steady state in a case of the finite time-constants of the generation-recombination processes. Thus, the current changes are slow after some time. The trap states have an effect on the asymptotic stability of the $j(t)$ and $q_s(t)$ curves. According to [1], we ascertain that including the third mobility μ_t and the surface traps usually do not vary the character of the function $j(t)$ and $q_s(t)$.

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