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The Effect of Generation-Recombination Processes and of Injection Mechanisms on Current-Voltage Dependences in the Metal-Dielectric-Metal System
I. Carrier Generation

by

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Summary. A dielectric model in which electrons and holes are the charge carriers was studied. The space charge is formed by free electrons and holes as well as by trapped electrons. Carrier generation with two trapping states, in steady state and at constant voltage was considered in the assumed dielectric model. The considerations refer to the flat capacitor system. The charge injection mechanisms were described by the function of current density and field intensity at the electrodes. The effect of injection mechanisms in conditions of carrier generation on current-voltage relations was investigated.

1. Introduction. Among the problems of the theory of bipolar conductivity in a solid dielectric is the determination of the relation between negative charge carriers concentration and the concentration of positive charge carriers [1]. According to solid state theory [3] the negative and positive charge carriers may react with one another through trapping states. Two processes are possible here:

— recombination, i.e. the passage of negative charge carriers (electrons) from the conduction band to the valence band through the trapping states; or

— generation of electrons and holes, i.e. the passage of electrons from the valence band to the conduction band through the trapping states

In this approach the concentrations of free electrons and holes are related by a system of partial differential equations describing the kinetics of trapped electrons in the separate trapping states.

In this work it was assumed that the flow of electrons from the trapping level closest to the conduction band to the trapping level nearest to the valence band (and vice versa) through the trapping states between them may be replaced by the so called effective transition by introducing coefficients C_{12} and C_{21} into the equations. The purpose of this assumption is to avoid an excessive number of equations and coefficients. The transport of positive and negative charge carriers with the participation of trapping states is described by the continuity equation, the Gauss equation and equations describing generation-recombination processes [2]. After omitting diffusion currents and reducing the number of trapping states to two the charge carrier equations in the flat capacitor system take the form

$$\frac{\partial}{\partial x}(\mu_p pE+\mu_n nE)+\frac{\partial p}{\partial t}-\frac{\partial n}{\partial t}-\frac{\partial n_{t1}}{\partial t}-\frac{\partial n_{t2}}{\partial t}=0, \tag{1}$$

$$\frac{\varepsilon}{e_0}\frac{\partial E}{\partial x}=(p-p_0)-(n-n_0)-(n_{t1}-n_{t1,0})-(n_{t2}-n_{t2,0}), \tag{2}$$

$$\frac{\partial n}{\partial t}=\frac{\partial}{\partial x}(\mu_n nE)-c_n N_{t1} n+v_1 n_{t1}, \tag{3}$$

$$\frac{\partial n_{t1}}{\partial t}=c_n N_{t1} n-v_1 n_{t1}-c_{12} N_{t2} n_{t1}+c_{21} N_{t1} n_{t2}, \tag{4}$$

$$\frac{\partial n_{t2}}{\partial t}=c_{12} N_{t2} n_{t1}-c_{21} N_{t1} n_{t2}-C_p pn_{t2}+v_2 N_{t2}, \tag{5}$$

where $e_0 = 1.6\cdot 10^{-19}$ C, ε – high-frequency electric permeability, E – electric field intensity, x – distance of the point from the electrode, t – time; n, p, n_{t1}, n_{t2} – nonequilibrium concentrations of free electrons, holes and trapped electrons, respectively; N_{t1}, N_{t2} – trap concentrations of the first and second trapping level; μ_n, μ_p – mobility of electrons and holes, respectively; c_n, v_1, v_2, C_p, c_{12}, c_{21} – material coefficients; n_0, p_0, $n_{t1,0}$, $n_{t2,0}$ – equilibrium concentrations of free electrons, holes and of trapped electrons, respectively.

The equilibrium concentrations satisfy the neutrality condition

$$p_0 = n_0+n_{t1,0}+n_{t2,0}. \tag{6}$$

Equations (3)–(5) describe the passages of electrons from the conduction band through the trapping states into the valence band and vice versa. They are written for the case when the number of free spaces in the trapping states greatly exceeds the number of trapped electrons $N_{t1} \gg n_{t1}$ and $N_{t2} \gg n_{t2}$. The system of equations (1)–(6) describes the transition state of electric conductivity in a solid dielectric.

In this work we consider the stationary state of conductivity in the metal-dielectric-metal system at constant voltage

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

where U is the voltage applied to the electrodes and L the distance between electrodes. The stationary state is described by equations (1)–(7), assuming zero values of derivatives over time

(8) $$e_0 \mu_p pE + e_0 \mu_n nE = j; \quad j = \text{const}$$

(9) $$\frac{\varepsilon}{e_0} \frac{dE}{dx} = p - n - n_{t1} - n_{t2}$$

(10) $$\frac{d}{dx} (\mu_n nE) = C_n n - \nu_1 n_{t1}$$

(11) $$C_n n - \nu_1 n_{t1} = C_{12} n_{t1} - C_{21} n_{t2}$$

(12) $$C_{12} n_{t1} - C_{21} n_{t2} = C_p pn_{t2} - \nu_2 N_{t2}$$

where j is the transport current density, $C_n = c_n N_{t1}$, $C_{12} = c_{12} N_{t2}$ and $C_{21} = c_{21} N_{t1}$. In this work we intend to determine the current-voltage dependence $j = j(U)$ or $U = U(j)$ in conditions of carrier generation.

The relation between current density and voltage depends not only on the interior of the dielectric but also on mechanisms of charge injection from the electrodes into the dielectric. The charge injection mechanisms were described by functions of current density and field intensity next to the electrodes $j = f_0 [E(0)]$ and $j = f_L [E(L)]$.

2. Problem solution. We get the current-voltage dependence from equations (7)–(12). The analytical determination of function $j = j(U)$ or $U = U(j)$ with given injection mechanisms is usually a fairly complex problem. In some cases, depending on the dielectric's interior, the problem can be solved. In what follows we consider two cases of dielectric interior leading to the analytical determination of the current-voltage characteristic.

2.1. *Generation of electron-hole pairs.* In this case we must assume in equations (10)–(12) zero values of parameters $C_n = C_p = C_{12} = 0$. From this we get the relations

(13) $$n_{t2} = \frac{\nu_2 N_{t2}}{C_{21}}; \quad n_{t1} = \frac{\nu_2 N_{t2}}{\nu_1}; \quad \nu_2 \leqslant C_{21}.$$

After introducing new variables A_1 and A_2 and taking into consideration (13), equations (8)–(10) take the form

(14) $$rA_1 + A_2 = 1 \qquad r = \mu_p/\mu_n,$$

(15) $$\frac{\varepsilon \mu_n E}{j} \frac{dE}{dx} = A_1 - A_2 - \frac{e_0 \mu_n \nu_2 N_{t2}}{j} \left(\frac{1}{C_{21}} + \frac{1}{\nu_1} \right) E,$$

$$\frac{dA_2}{dx} = -\frac{e_0 \nu_2 N_{t2}}{j}, \tag{16}$$

where

$$A_1 = \frac{e_0 \mu_n pE}{j}; \quad A_2 = \frac{e_0 \mu_n nE}{j}. \tag{17}$$

The solution of (16) is the following function $A_2(x)$

$$A_2(x) = -\frac{e_0 \nu_2 N_{t2}}{j}(x-L)+A_2(L). \tag{18}$$

Hence, on the basis of (14) and (15), we obtain a differential equation describing the distribution of electric field intensity $E(x)$

$$\frac{dE}{dx} = \alpha_1 \frac{(x-x_0)}{E} - \alpha_2, \tag{19}$$

where

$$\begin{gathered} \alpha_1 = \frac{(r+1)\, e_0 \nu_2 N_{t2}}{\varepsilon \mu_p}; \quad \alpha_2 = \frac{e_0 \nu_2 N_{t2}}{\varepsilon}\left(\frac{1}{C_{21}}+\frac{1}{\nu_1}\right), \\ x_0 = L + \frac{[(r+1)\, A_2(L)-1]\, j}{(r+1)\, e_0 \nu_2 N_{t2}}. \end{gathered} \tag{20}$$

Performing the substitution $y = x - x_0$ in equation (19) we get the homogeneous equation

$$\frac{dE}{dy} = \frac{\alpha_1 y}{E} - \alpha_2. \tag{21}$$

Hence the general integral of equation (19) is of the form

$$\left|\frac{E}{x-x_0} - z_1\right|^{\gamma_1} \left|\frac{E}{x-x_0} - z_2\right|^{\gamma_2} = C\,|x-x_0|; \quad C = \text{const}, \tag{22}$$

where

$$\begin{gathered} z_{1,2} = -\frac{\alpha_2}{2} \pm \frac{1}{2}(\alpha_2^2+4\alpha_1)^{1/2}; \quad z_1 > 0; \quad z_2 < 0, \\ \gamma_1 = \frac{-z_1}{z_1 - z_2}; \quad \gamma_2 = \frac{-z_2}{z_2 - z_1}. \end{gathered} \tag{23}$$

Moreover, equation (21) has two singular solutions

$$E = z_1 y = z_1 (x-x_0); \quad E = z_2 y = z_2 (x-x_0). \tag{24}$$

Point $x = x_0$ is the singular point of the general integral (22). In agreement with (20), the position of point $x = x_0$ depends on the value of the integration constant $A_2(L)$ (dimensionless density of electron transport current at the electrode $x = L$). In the case of singular solutions (24), when the integration constant $A_2(L)$ satisfies the condition $A_2(L) > \frac{1}{r+1}$, $x_0 > L$ and one must assume the solution $E = z_2(x - x_0)$ since $z_2 < 0$. From this, on the basis of the voltage condition (7), there results the relation between voltage and field intensity at the electrode $x = L$

$$U = \frac{z_2(L-x_0)^2}{2} - \frac{z_2 x_0^2}{2} = \frac{(2E(L) - z_2 L) L}{2}. \tag{25}$$

It results from (25) that the current-voltage characteristic $j = f(U)$ is determined by the mechanism of charge injection from electrode $x = L$ into the dielectric described by the function of current density j and electric field intensity $E(L)$, $j = f_L[E(L)]$

$$j = f_L\left(\frac{U}{L} - \frac{|z_2| L}{2}\right); \quad U \geqslant \frac{|z_2| L^2}{2}. \tag{26}$$

For example, when next to the electrode $x = L$ there occurs the Schottky effect, $j = a \exp\left(bE^{1/2}(L)\right)$ $(a, b = \text{const})$, the relation (26) takes the form

$$j = a \exp\left\{b\left(\frac{U}{L} - \frac{|z_2| L}{2}\right)^{1/2}\right\}. \tag{27}$$

It is worth noting that the integration constant $A_2(L)$ depends on the boundary value of $E(L)$

$$A_2(L) = \frac{e_0 \nu_2 N_{t2} E(L)}{|z_2| j} + \frac{1}{r+1}; \quad E(L) = z_2(L - x_0). \tag{28}$$

Since $A_2(L) < 1$ and $j = f_L[E(L)]$, the boundary values of $E(L)$ must satisfy the condition

$$E(L) < \frac{r |z_2| f_L[E(L)]}{e_0 (r+1) \nu_2 N_{t2}}. \tag{29}$$

Hence, on the basis of (25) and (26) we find that in the case of the tunnel effect, $j = aE^2(L) \exp\left(-b/E(L)\right)$, and of the Schottky effect, $j = a_1 \exp\left(b_1 E^{1/2}(L)\right)$, where a, b, a_1 and b_1 are constant, there exists the lowest value of voltage U_g, that for all the voltage values $U \geqslant U_g$ the current-voltage dependence (26) is correct. It is noteworthy that the boundary values of carrier concentrations $n(L)$ and $p(0)$ are determined by the mechanism of charge injection from electrode $x = L$ into the dielectric

$$p(0) = \frac{\mu_n}{e_0(\mu_n + \mu_p)} \left\{\frac{f_L[E(L)]}{\mu_n E(0)} + \varepsilon(\alpha_2 + z_2)\right\}, \tag{30}$$

$$n(L)=\frac{\mu_n}{e_0(\mu_n+\mu_p)}\left\{\frac{f_L[E(L)]}{\mu_n E(L)}-\frac{\varepsilon\mu_p}{\mu_n}(\alpha_2+z_2)\right\}, \tag{31}$$

with the boundary value $E(0)=E(L)-z_2 L$. It results from (30) and (31) that a negative charge of constant density $^-q_v=\varepsilon z_2$ may be formed in the entire dielectric, in steady state, when only one electrode injects carriers.

Similar considerations are performed when $A_2(L)<\frac{1}{r+1}$, i.e. when $x_0<L$. In this case solutions exist when $x_0<0$ and one must assume the singular solution $E=z_1(x-x_0)$. The current-voltage dependence then has the form

$$j=f_L\left(\frac{U}{L}+\frac{z_1 L}{2}\right);\qquad U\geqslant\frac{z_1 L^2}{2}. \tag{32}$$

The weak inequality (32) ensures the positive sign of the distribution of electric field intensity $E(x)$ in the entire interval $0\leqslant x\leqslant L$. Similarly as before it is concluded that a positive charge of constant density $^+q_v=\varepsilon z_1$ may arise in the soild dielectric in steady state when only one electrode is injecting carriers.

The further considerations will concern the general integral (22). To this end we additionally assume the equality of coefficients $v_1=v_2=C_{21}$ and a strong inequality of parameters $4\alpha_1\gg\alpha_2^2$, which leads to a limitation of hole mobility $\mu_p\ll\frac{\varepsilon v_2(r+1)}{e_0 N_{t2}}$. Given these assumptions, the general integral (22) takes the form

$$\left|\frac{E}{x-x_0}-\alpha_1^{1/2}\right|^{-1/2}\left|\frac{E}{x-x_0}+\alpha_1^{1/2}\right|^{-1/2}=C\,|x-x_0| \tag{33}$$

whence, after unraveling, we obtain the distribution of electric field intensity $E(x)$

$$E(x)=[K+\alpha_1(x-x_0)^2]^{1/2};\qquad K=\text{const};\qquad K>0. \tag{34}$$

After substituting (34) in the voltage condition (7) we get the relation between voltage U and boundary values $E(0)$, $E(L)$ and integration constants K and x_0

$$U=\frac{1}{2}\left\{\frac{K}{\alpha_1^{1/2}}\ln\left|\frac{E(L)+\alpha_1^{1/2}(L-x_0)}{E(0)-\alpha_1^{1/2}x_0}\right|+(L-x_0)E(L)+x_0 E(0)\right\}. \tag{35}$$

If the singular point $x=x_0$ lies inside the interval $0<x_0<L$, then the value $E(x_0)$ may be defined as $E^2(x_0)=K$. From (34) there result formulas defining the values of parameters x_0 and K

$$x_0 = \frac{E^2(0) - E^2(L) + \alpha_1 L^2}{2\alpha_1 L},$$

(36)

$$K = E^2(0) - \frac{(E^2(0) - E^2(L) + \alpha_1 L^2)^2}{4\alpha_1 L^2}; \quad E(0) > \alpha_1^{1/2} x_0.$$

From (35) and (36) is results that the current-voltage characteristic is described by the mechanism of charge injection from electrode $x = 0$ into the dielectric described by the function $j = f_0[E(0)]$, and by the mechanism of charge injection from the electrode $x = L$ into the dielectric described by the function $j = f_L[E(L)]$. In a particular case when functions f_0 and f_L are identical $j = f_0[E(0)] \equiv f_L[E(L)]$, i.e. $E(0) = E(L)$, then $x_0 = L/2$. After substituting $x_0 = L/2$ in (34) we may obtain an expression for space charge density $q_v = \varepsilon \frac{dE}{dx}$ in the dielectric

(37) $$q_v = \frac{\varepsilon\alpha_1 (x - L/2)}{E}; \quad E > 0.$$

Hence it results that a negative charge $q_v < 0$ is distributed in region $0 \leqslant x < L/2$, and a positive charge $q_v > 0$ in region $L/2 < x \leqslant L$, making the dielectric behave like an n-p junction. The current-voltage dependence of the emergent n-p junction is defined parametrically by the system of functions

(38) $$U = \frac{\alpha_1^{-1/2}}{2}\left(E^2(L) - \frac{\alpha_1 L^2}{4}\right) \ln \left| \frac{E(L) + \frac{1}{2}\alpha_1^{1/2} L}{E(L) - \frac{1}{2}\alpha_1^{1/2} L} \right| + \frac{1}{2} LE(L),$$

and $j = f_L[E(L)]$.

It is worth noting that if $E(L) \gg (1/2)\,\alpha_1^{1/2} L$, then (38) adopts the formula $j = f_L(U/L)$. For example when f_L is the Schottky function, the current--voltage characteristic is described by the formula $j = a \exp\{b(U/L)^{1/2}\}$ where a and b are constant. Similarly, in the case of the tunnel effect $j = a_1 (U/L)^2 \exp(-b_1 L/U)$ where a_1 and b_1 are constant.

2.2. *Absence of electron exchange between the first and the second trapping level.* In this case one must assume in equations (10)–(12) zero values of parameters $C_{12} = C_{21} = 0$. After introducing new variables A_1, A_2, A_3 and A_4 defined by the formulas

(39) $$A_1 = \frac{e_0 \mu_n pE}{j}; \quad A_2 = \frac{e_0 \mu_n nE}{j}; \quad A_3 = \frac{e_0 \mu_n n_{t1} E}{j};$$

$$A_4 = \frac{e_0 \mu_n n_{t2} E}{j},$$

we get the relations

$$A_2(x) = A_2(L) = \text{const}; \quad A_1 = (1-A_2)\,\mu_n/\mu_p; \quad A_3 = A_2/\theta_n; \tag{40}$$
$$\theta_n = v_1/C_n; \quad A_4 = \frac{\theta_p (e_0 \mu_n E)^2}{A_j j^2}; \quad \theta_p = v_2 N_{t2}/C_p.$$

Relations (40) result from (39) and from equations (8)–(12). Taking into consideration (39), (40) and (9) we get differential equations describing the distribution of electric field intensity

$$\frac{\varepsilon\mu_n E}{j}\frac{dE}{dx} = \alpha - \frac{\theta_p}{A_1}\left(\frac{e_0 \mu_n}{j}\right)^2 E^2; \quad \alpha = A_1 - A_2 - A_3 = \text{const}, \tag{41}$$

the general integral of which is of the form

$$E(x) = \{\alpha_0 j^2 + C_2 \exp(-2\beta_0 x/j)\}^{1/2}, \tag{42}$$
$$\alpha_0 = \frac{\alpha A_1}{\theta_p (e_0 \mu_n)^2}; \quad \beta_0 = \frac{\theta_p e_0^2 \mu_n}{A_1 \varepsilon}; \quad C_2 = \text{const}.$$

It is noteworthy that the solution of (42) contains two integration constants $A_2(L)$ and C_2 which are determined on the basis of boundary values $E(0)$ and $E(L)$.

The determination of the functional dependence between voltage U and boundary values $U = U(E(0), E(L))$ is a complex problem since it additionally requires the solution of the transcendental equation

$$E^2(0) = \alpha_0 j^2 + C_2, \tag{43}$$
$$E^2(L) = \alpha_0 j^2 + C_2 \exp(-2\beta_0 L/j).$$

The problem may be solved numerically. In a particular case when $\alpha_0 = \alpha = 0$, the constants A_1 and A_2 take the values

$$A_2 = \frac{1}{1+r\theta}; \quad A_1 = \frac{\theta}{1+r\theta}; \quad \theta = 1 + \frac{1}{\theta_n}, \tag{44}$$

and the solution (42) assumes the simpler form

$$E(x) = E(0)\exp(-\beta_0 x/j). \tag{45}$$

Hence we obtain the relation between boundary values $E(0)$ and $E(L)$

$$E(0) = E(L)\exp(\beta_0 L/j). \tag{46}$$

After substituting distribution (45) of the voltage integral (7) we get

$$U = \frac{j}{\beta_0}(E(0) - E(L)). \tag{47}$$

It results from (46) and (47) that the current-voltage characteristic is defined if there is given the injection mechanism at electrode $x = L$ described by the function of current density and electric field intensity $j = f_L [E(L)]$. After taking into consideration (46), (47) and the function $j = f_L [E(L)]$ we get the current-voltage dependence in parametric form

$$U = \frac{jE(L)}{\beta_0} (\exp(\beta_0 L/j) - 1) \quad j = f_L [E(L)].$$

In the case of large values of current density j the characteristic (48) assumes the formula $j = f_L (U/L)$. For example, when f_L is a linear function $j = \sigma_L E(L)$, $\sigma_L = \text{const}$, the characteristic (48) takes the form

(49) $$U = \frac{j^2}{\sigma_L \beta_0} (\exp(\beta_0 L/j) - 1),$$

and for large values of j it becomes the Ohm law $j = \sigma_L U/L$.

3. Conclusions. The performed analysis indicates that the form of function $j = j(U)$ or $U = U(j)$ depends on the dielectric's interior and on the mechanisms of carrier injection from the electrodes into the dielectric. In the case of carrier generation in stationary state a positive or a negative charge of constant density may arise when only one electrode is injecting carriers. In this case the current-voltage characteristic is of the form $j = f_L (U - U_{01})$ or $j = f_L (U + U_{02})$ respectively, where U_{01} and U_{02} denote the minimum voltage value and f_L is the function describing the mechanism of electron injection from the electrode into the dielectric. When both electrodes inject carriers and the functions describing the injection mechanism are identical, one half of the dielectric is charged negatively and the other is charged positively; accordingly, the dielectric behaves like an *n-p* junction. In the boundary case the current-voltage characteristic assumes the formula $j = f_L (U/L)$.

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Б. Сьвистач, **Влияние процессов генерации-рекомбинации и механизмов инжекции на вольтамперные характеристики соотношения металл-диэлектрик-металл, I. Генерация носителей**

В статье исследуется модель диэлектрика, в котором содержатся свободные электроны и дырки. Объемный заряд определяется концентрацией свободных носителей и захваченных электронов. В предложенной модели диэлектрика анализируется генерация носителей в случае двух уровней прилипания, в стационарном сосотоянии, при постоянном напряжении. Результаты достигаются в системе плоского конденсатора. Механизмы инжекции заряда описываются по функции плотности тока и напряженности электрического поля на контактах электрод-диэлектрик. Изучается влияние механизмов инжекции в условиях генерации носителей на вольтамперные характеристики.