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Carrier generation and the switching phenomenon: further theoretical description

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Abstract. In this paper the problem of the current flow between the two electrodes is further continued. The steady state of solid electric conduction with the two boundary conditions is analysed. The space charge is defined by free holes and electrons as well as by trapped electrons. As the interactions between free carriers, carrier generation is assumed. Under these conditions, it was found that the current–voltage characteristics can be discontinuous. The shape of these curves can be of ‘S’ or ‘N’ type.

1. Introduction

One of the electrical properties of the metal–solid (insulator or semiconductor)–metal system is the current–voltage characteristic. The shape of this curve is determined by the boundary and internal processes. The fundamental problem of the bipolar space charge theory is to identify the boundaries and the interior together.

The shape of the current–voltage characteristic can be ‘S’ or ‘N’ type with a negative differential resistance [1–14]. The most interesting case occurs when these curves are discontinuous (this property is called the switching effect of the current–voltage characteristic). Usually, the interior is characterized by a change in the total energy of the electron in the given material structure. There exist internal and external conditions in which the total energy of the electron increases (i.e. carrier generation occurs) [15–38]. In general, the internal processes determine a differential equation which makes a set of the electric field distributions. In order to find the ‘S’- or ‘N’-type curves, it is necessary to give the boundary conditions describing the mechanisms of carrier injection from the electrodes into a solid.

In [39, 40] we presented a model describing electric conduction with two boundary conditions. These analytical calculations show that there can exist two singular solutions for carrier generation conditions. In this paper we shall find the physical interpretation for singular solutions.

The purpose of this work is to explain the switching effect of the current–voltage characteristic.

2. The model system and the basic equations

In this paper we shall consider electric conduction in amorphous or impure crystalline solids. We shall assume that different defects exist in the given material structures. The atoms of

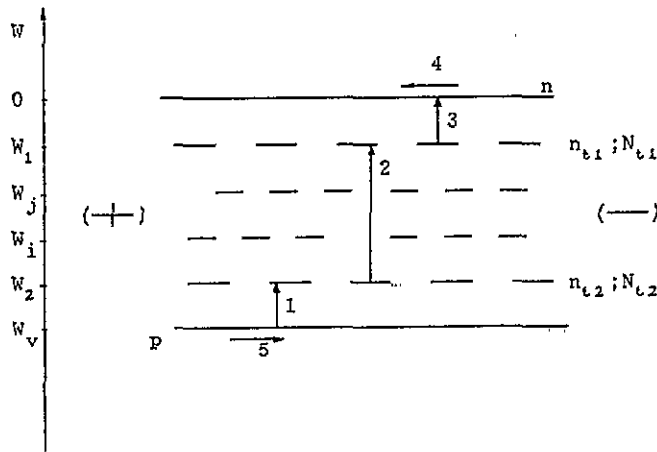


Figure 1. The energy diagram and allowed electron transitions caused by incident phonons and photons, where W is the total energy of the electron, W_v is the valence level, and (+) and (-) denote the anode and cathode, respectively: 1, $\nu_p N_{t2}$ with the hole activation energy denoted by $(W_2 - W_v)$; 2, $C_{21} n_{t2}$; 3, $\nu_n n_{t1}$ with the electron activation energy denoted by $-W_1$; 4, $\mu_n n E$; 5, $\mu_p p E$.

a solid can be displaced (the Schottky and Frenkl defects) or pollutants and impurities can occur. Also, different dislocations are possible. Under these conditions we shall assume that the concentration of atoms in space is possibly maximal. Thus, different electric-magnetic force interactions between adjacent atoms occur. These interactions determine a potential energy distribution of the electric field. We shall assume that microscopic regions (traps) exist in which the negative potential energy of the electric field is condensed. In these regions the total energy W is of the form

$$W_n = W_{p0} + \frac{n^2 \hbar^2}{8md^2} \quad n = 1, 2, \dots$$

or

$$W_n = W_{p0} + \frac{(n + \frac{1}{2})^2 \hbar^2}{8md^2} \quad n = 0, 1, 2, \dots$$

Here \hbar is the Planck constant, m is the electron mass, W_{p0} is a constant potential energy of the electric field and d denotes the microscopic distance. In the trapping region the total magnetic field is the sum of the magnetic fields of all the electrons and nuclei of the adjacent atoms surrounding the given trap. Thus, the Zeeman internal effect (the splitting of the total energy W_n) occurs and many allowed energy states are available for the valence electron in the band gap. When the temperature is sufficiently high, then the system of atoms becomes more chaotic since the kinetic energy of these atoms increases. Under these conditions the valence electrons can absorb additional kinetic energy and pass to a higher (trapping level) energy state. In this paper we shall assume that the valence and trapped electrons are permanently bombarded by phonons and photons. Absorbing the additional kinetic energy, the electrons can pass to the zero reference level in which these electrons become free. The empty energy state left by the electron determines the vacancy with the positive charge (hole). These allowed electron transitions define the hole-electron pair generation (figure 1). The empty energy state in the valence band can be occupied by the valence electron of an adjacent atom when an additional sufficiently high energy is given to these electrons by an external electric field. This property of the external electric field defines the vacancy

(hole) flow with the mobility μ_p . The same situation occurs in the conduction band. When additional kinetic energy is given to the free electron by the external electric field, the carrier flow with the mobility μ_n (figure 1) occurs. For the above internal processes, we shall find the equations describing the carrier flow between the two electrodes. To this end we make the following assumptions.

(I) As a model system, the planar capacitor (figure 2) with the anode at $x = 0$ for injecting holes and with the cathode at $x = L$ for injecting electrons will be considered.

(II) The potential barrier width is small in comparison with the mean free path and there are no surface states at the electrodes.

(III) The hole and electron mobilities are independent of the electric field intensity E .

(IV) The carrier diffusion is unimportant.

With these assumptions the carrier flow between the anode and the cathode will be described by the Gauss equation, the continuity equation, the generation equations and the field integral. In the planar capacitor system these equations are as follows:

$$\varepsilon \frac{\partial E(x, t)}{\partial x} = q\{p(x, t) - n(x, t) - n_{t1}(x, t) - n_{t2}(x, t)\} \quad (1)$$

$$\frac{\partial}{\partial x} \left\{ \mu_p p(x, t) E(x, t) + \mu_n n(x, t) E(x, t) \right\} + \frac{\partial p(x, t)}{\partial t} - \frac{\partial n(x, t)}{\partial t} - \frac{\partial n_{t1}(x, t)}{\partial t} - \frac{\partial n_{t2}(x, t)}{\partial t} = 0 \quad (2)$$

$$\frac{\partial n(x, t)}{\partial t} = v_n n_{t1}(x, t) + \frac{\partial}{\partial x} \{ \mu_n n(x, t) E(x, t) \} \quad (3)$$

$$\frac{\partial n_{t1}(x, t)}{\partial t} = C_{21} n_{t2}(x, t) - v_n n_{t1}(x, t) \quad N_{t1} \gg n_{t1} \quad (4)$$

$$\frac{\partial n_{t2}(x, t)}{\partial t} = v_p N_{t2} - C_{21} n_{t2}(x, t) \quad N_{t2} \gg n_{t2} \quad (5)$$

$$\int_0^L E(x, t) dx = V \quad V = \text{constant} > 0. \quad (6)$$

Here, q is the electric charge, t is the time, x is the distance from the electrode, ε is the dielectric constant, n and p are the free hole and electron concentrations, respectively, n_{t1} and n_{t2} are the concentrations of the trapped electrons, N_{t1} and N_{t2} are the concentrations of the energy states in the first and second trapping levels, respectively, v_n , v_p and C_{21} are the generation parameters, V is the applied voltage and L is the distance between the electrodes. The frequency parameters are of the form of the Boltzmann factors:

$$\begin{aligned} v_n &= v_0 \exp(W_1/kT) & v_p &= v_0 \exp((W_v - W_2)/kT) & C_{21} &= \langle C_{ij} \rangle \\ C_{ij} &= v_0 \exp(-W_{ij}/kT) & W_{ij} &= W_j - W_i > 0. \end{aligned} \quad (7)$$

Here, T is the temperature, k is the Boltzmann constant, $v_0 \approx 10^{12} \text{ s}^{-1}$ and $\langle \rangle$ denotes the mean value. The importance of the energy parameters is shown in figure 1. For these space charge conditions we shall examine the steady state and we shall find new current-voltage characteristics.

3. The solution of the problem

From (1)–(6) it follows that the electric field intensity $E(x)$ in the stationary state satisfies the following differential equation:

$$\frac{dE}{dx} = a_1 \frac{x - x_0}{E} - a_2 \quad (8)$$

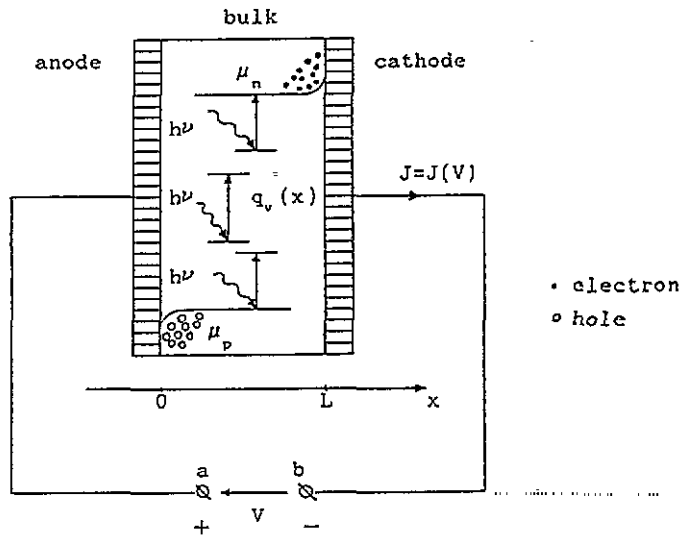


Figure 2. The planar capacitor system and the boundary and internal processes. Here, $h\nu$ denotes the total energy of a phonon and a photon; $q_v(x)$ is the space charge distribution and J is the total current density; a and b denote the voltage (or current) terminals.

where

$$a_1 = \frac{(\mu_p + \mu_n)q v_p N_{I2}}{\varepsilon \mu_n \mu_p} \quad a_2 = \frac{q v_p N_{I2}}{\varepsilon} \left(\frac{1}{C_{21}} + \frac{1}{v_n} \right) \quad (8a)$$

and x_0 is a constant of integration. Equation (8) has the two singular solutions

$$E(x) = -2V_{01}(x - x_0)/L^2 \quad E(x) = 2V_{02}(x - x_0)/L^2 \quad (9)$$

where

$$V_{01} = \frac{L^2}{4} \left(a_2 + \sqrt{a_2^2 + 4a_1} \right) \quad V_{02} = \frac{L^2}{4} \left(-a_2 + \sqrt{a_2^2 + 4a_1} \right). \quad (9a)$$

The functions (9) are illustrated in figure 3. The voltage parameters V_{01} and V_{02} define the negative and positive space charge densities in the bulk. These functions (9) characterize the n-p-type material (figure 3(a)) or n-type material (figure 3(b)) or p-type material (figure 3(c)). It should be noted that the singular solutions contain only one constant of integration. Thus, in order to find the particular integral, we have to give only one boundary condition describing the mechanisms of hole and electron injection from the electrode $x = 0$ or $x = L$, respectively, into the bulk. These mechanisms can be described by $J = f_0[E(0)]$ as well as the $J = f_L[E(L)]$ where J is the steady-state current density, and f_0 and f_L are the boundary functions describing the carrier injection from the electrodes $x = 0$ or $x = L$, respectively, into the bulk. Therefore, the current-voltage characteristic determined by the integral condition (6) and the boundary function is of the form

$$J = f_L[(V - V_{01})/L] \quad V \geq V_{01} \quad (10)$$

$$J = f_0[(V - V_{02})/L] \equiv f_L[(V + V_{02})/L] \quad V \geq V_{02} \quad (11)$$

$$J = f_L[\alpha V/L] \quad V_0 \leq V < V_{TH} \leq V_{01} \quad (12)$$

where

$$\alpha = \frac{2\gamma(1+b\gamma)}{1+b\gamma^2} \quad V_0 = \frac{V_{01}V_{02}}{V_{01}+V_{02}} \quad V_{TH} = \frac{1+b\gamma^2}{1+b\gamma}V_{01} \quad (13)$$

$$b = \frac{V_{01}}{V_{02}} \quad \gamma = \frac{E(L)}{E(0)}$$

and

$$E(0) = (z_1^2 + z_1z_2)^{-1} \left\{ z_1L \pm \sqrt{z_1^2L^2 - (z_1^2 + z_1z_2)(L^2 - 2z_2V)} \right\} \quad (13a)$$

$$E(L) = (z_2^2 + z_1z_2)^{-1} \left\{ z_2L \pm \sqrt{z_2^2L^2 - (z_2^2 + z_1z_2)(L^2 - 2z_1V)} \right\} \quad (13b)$$

where

$$z_1 = \frac{L^2}{2V_{01}} \quad z_2 = \frac{L^2}{2V_{02}} \quad (13c)$$

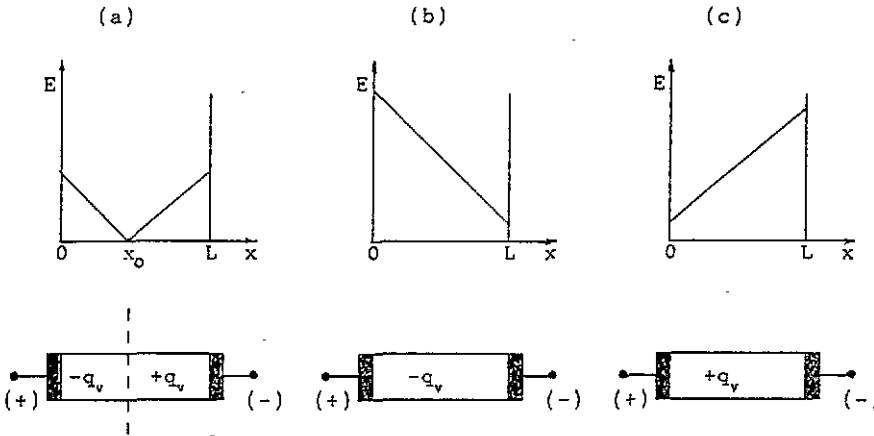


Figure 3. The interpretation of the singular solutions (9). (a) The system acts as an n-p junction. (b) A negative charge is distributed between the electrodes. (c) A positive charge is distributed between the electrodes.

The current-voltage characteristics (10)–(12) correspond to the $E(x)$ curves presented in figures 3(b), 3(c) and 3(a), respectively. The condition $V < V_{TH}(V)$ defines a set of values of the threshold voltages. The functions $\alpha(\gamma)$ and $V_{TH}(\gamma)$ are illustrated in figure 4. In this figure the characteristic parameters γ_1 , γ_2 and V'_{TH} are shown. These values depend on V_{01} and V_{02} in the following form:

$$\gamma_1 = \frac{1}{b}(-1 + \sqrt{1+b}) \quad \gamma_2 = 1 + \sqrt{1 + \frac{1}{b}} \quad V'_{TH} = 2(\sqrt{1+b} - 1)V_{02}. \quad (13d)$$

For $\gamma = \gamma_1$ we have $\alpha(\gamma) = 1$ and the threshold voltage $V_{TH}(\gamma_1)$ is equal to the minimum V'_{TH} . For $\gamma = \gamma_2$ the parameter α is equal to the maximum $\alpha_{max} = \alpha(\gamma_2) > 2$. The parameters α and V_{TH} are important for the switching effect. In order to show this property we have to use (10)–(13d). On this basis we can define the different current-voltage characteristics $J(V)$ for different values of γ and b . For example, if f_L is the Fowler-Nordheim function, then $J(V)$ has the form

$$J = \begin{cases} a(\alpha V)^2 \exp(-b_1/\alpha V) & V_0 < V < V_{TH} \\ a(V - V_{01})^2 \exp(-b_1/(V - V_{01})) & \text{for } V \geq V_{TH} \end{cases} \quad (14)$$

or

$$J = \begin{cases} a(\alpha V)^2 \exp(-b_1/\alpha V) & V_0 < V < V_{TH} \\ a(V + V_{02})^2 \exp(-b_1/(V + V_{02})) & \text{for } V \geq V_{02}. \end{cases} \quad (15)$$

Here, a and b_1 are the material parameters. The curves of (14) and (15) can explain the 'S' or 'N'-type switching effect. In figure 5 the current-voltage characteristics $J(V)$ are shown for different values of the ratios γ and b . The arrows indicate the change in the current density J with the voltage V . When $E(L)$ is equal to zero, i.e. $\alpha = 0$, then the system acts as a blocking diode (figure 5(a)). In this case, n-type conduction occurs. If $\alpha \ll 1$ and $b > 5/4$ or $\alpha \approx 1$ and $b = 5/4$, then the switching effect is possible for values of $V > V_{TH}$ (figures 5(b)–5(d)). Thus, in this case the condition $V > V_{TH}$ defines a transition from n-p-type conduction to p- or n-type conduction. For $\gamma \rightarrow 1^-$, i.e. $\alpha \approx 2$ and $V_{TH} \approx V_{01}$, transition from n-p-type conduction to p-type conduction is possible (figure 5(e)). In this case, if the threshold voltage V_{01} is great, then the switching effect cannot occur and the $J(V)$ curve is the Fowler-Nordheim function. In this case the system acts as an n-p junction.

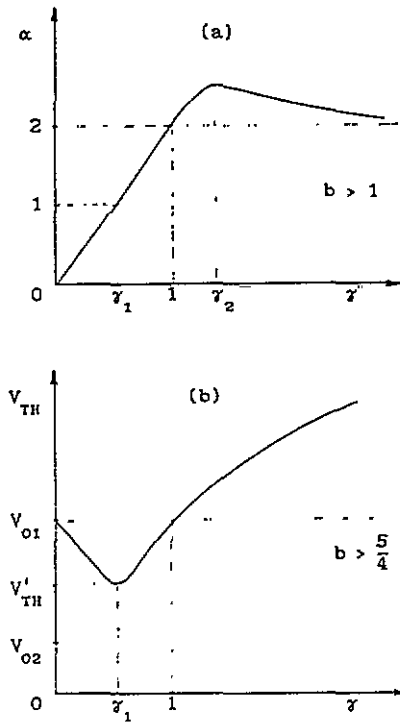


Figure 4. The importance of the parameters α and V_{TH} for the switching effect: (a) the shape of the function $\alpha = \alpha(\gamma)$; (b) the shape of the function $V_{TH} = V_{TH}(\gamma)$.

4. Discussion

Usually the problem of the switching effect has been explained by the negative-differential-resistance (NDR) regime. The NDR problem has been analysed for perfect ($E(0) = E(L) = 0$) contacts as well as for the ohmic ($E(L) = 0$) and blocking ($J \propto E^2(0)$) contacts. With

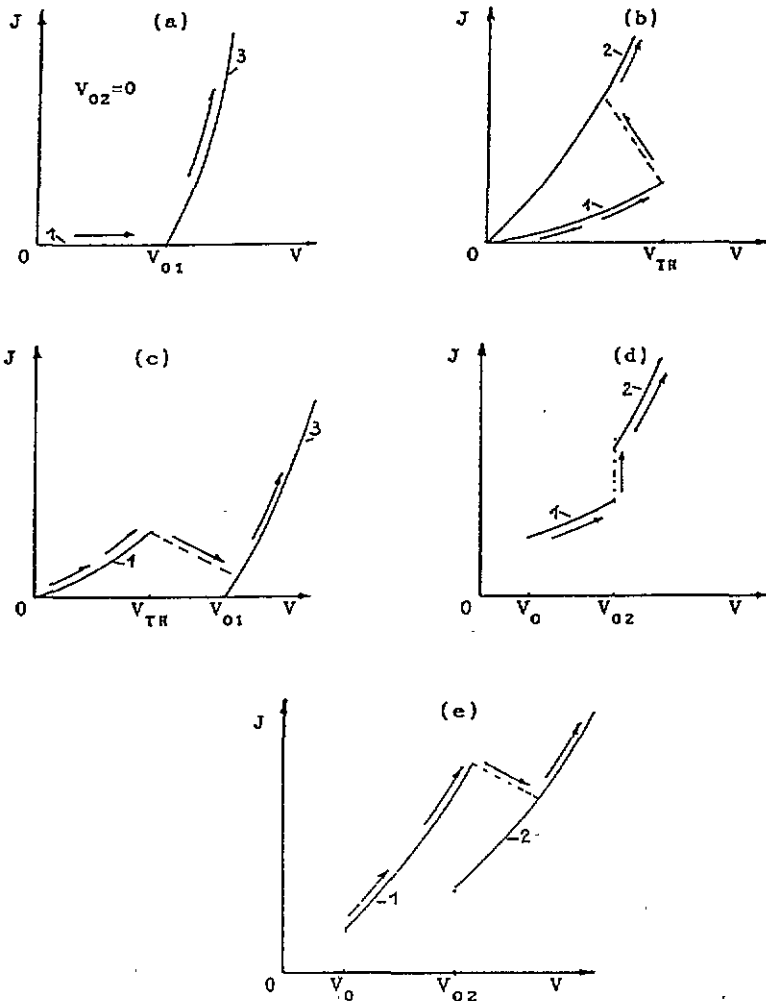


Figure 5. The current-voltage characteristics determined by the singular solutions (9) and by the Fowler-Nordheim boundary functions at $x = 0$ and $x = L$. (a) The system acts as a blocking diode (a case of the voltage source). (b) The 'S'-type switching effect occurs (a case of the current source and $V_{02} \approx 0$). (c) The 'N'-type switching effect occurs (a case of the voltage source and $V_{02} \approx 0$). (d) The 'S'-type switching effect occurs (a case of the voltage or current source). (e) The 'N'-type switching effect occurs (a case of the voltage source).

these boundary conditions, the 'S'-type characteristic with NDR has been obtained. From the regional approximation method it follows that the threshold voltage can be written as [30, 31]

$$V_{TH} = \frac{L^2 n_{R0}}{2\pi^{1/2}} \left(\frac{q\sigma_p v_p P_{R0}}{\epsilon \mu_p N_R} \right)^{1/2} \quad P_{R0} = N_R - n_{R0} \quad (16)$$

for the perfect contacts or [17, 18]

$$V_{TH} = \frac{L^2}{4\mu_n} \left(\frac{3n_{R0}}{\tau_n \tau_p n_0} \right)^{1/2} \left(\frac{\mu_n}{\mu_p} \right) \quad (16a)$$

for ohmic and blocking contacts. Here, σ_p is the recombination cross sections of a hole, v_p is the thermal velocity of a hole, N_R is the recombination centre concentration, n_{R0} and n_0 are the equilibrium concentrations of trapped and free electrons, respectively, and τ_n and τ_p are the electron and hole lifetimes, respectively. Referring to our considerations, we can ascertain that the $J(V)$ curves can be discontinuous (figure 5) and the threshold voltage V_{TH} is

$$V_0 \leq V_{TH} \leq V_{01} \quad \text{for } x_0 \in (0; L). \quad (17)$$

In general, referring to the planar capacitor system (figure 2), there exist the two following problems:

- (1) given V (the case of the voltage source), to find $J(V)$ (figures 5(a) and (5(c)–5(e));
- (2) given J (the case of the current source), to find $V(J)$ (figures 5(b) and 5(d)).

In figure 5(a) the $J(V)$ curve is shown for $\alpha = 0$, i.e. $x_0 \rightarrow L-$. In this case we have $E(L) \rightarrow 0$. From (9) it follows that $E(L)$ is infinitesimal as $V_{02} \rightarrow 0$ (a negative space charge occurs). This condition is possible when $a_2^2 \gg 4a_1$, i.e.

$$\frac{\mu_n \mu_p}{\mu_n + \mu_p} \gg \frac{\varepsilon v_p}{q N_{t2}} \quad (18)$$

and

$$V_{01} \approx \frac{L^2 q N_{t2}}{\varepsilon} \quad \text{for } v_n \approx v_p \approx C_{21}. \quad (18a)$$

Hence, it follows that the negative space charge $\varepsilon dE/dx = -2\varepsilon V_{01}/L^2 = -2qN_{t2}$ is distributed in the bulk. Thus, the condition $\alpha = 0$ shows that the space charge of trapped electrons is dominant. In the particular case when $N_{t1} \approx N_{t2}$, then the total space charge is localized in the band gap. In other words, almost all the additional permissible energy states caused by the Zeeman internal effect are occupied. Note that the condition (18) determines a configuration of atoms in space (this property corresponds to the Schottky and Frenkl defects as well as to the different dislocations). Also, the condition $\alpha = 0$ occurs when the boundary function f_L is monotonic and the inverse function f_L^{-1} satisfies the condition $f_L^{-1}(0) = 0$. For instance, if f_L is the Schottky function, then the condition $\alpha = 0$ is not satisfied. When carriers are less mobile ($a_2^2 \approx 4a_1$ or $a_2^2 < 4a_1$) and a low level of carrier injection from the electrodes $x = 0$ and $x = L$ occurs, then carrier generation has an important influence on electric conduction. This property is characterized by $\alpha > 0$ and $x_0 \in (0, L)$. The condition $x_0 \in (0, L)$ defines the threshold voltage V_{TH} . If $\alpha \ll 1$, then the voltage parameter V_{02} is very small. In this case we can assume that $V_0 \approx V_{02} \approx 0$ (figures 5(b) and 5(c)). In these figures, curves 1 are for $\alpha > 0$ and $x_0 \in (0, L)$. For this current flow the space charge density $q_v(x)$ has the form

$$q_v(x) = \begin{cases} -q_v & \text{for } \begin{cases} x \in (0, x_0) \\ x \in (x_0, L) \end{cases} \\ +q_v & \end{cases} \quad -q_v = -2\varepsilon V_{01}/L^2 \quad +q_v = 2\varepsilon V_{02}/L^2. \quad (19)$$

The distribution (19) is possible for a low level of carrier injection. The function $q_v(x)$ is discontinuous at the plane $x = x_0$ and the planar capacitor system acts as an n-p junction (figure 3(a)). Curves 2 (in figure 5) can occur when a positive charge $+q_v$ (figure 3(c)) is distributed between the electrodes (the case of a high level of hole injection). Similarly, if a negative charge $-q_v$ (figure 3(b)) is distributed between the electrodes, then curve 3 (in figure 5) occurs (high level of electron injection). Thus, for $V > V_{TH}$ (this condition defines a new configuration of atoms) the distribution $q_v(x)$ becomes continuous and $q_v(x) \equiv -q_v$ (transition from curve 1 to curve 3 in figure 5(c)) or $q_v(x) \equiv +q_v$ for $x \in (0, L)$ (transition

from curve 1 to curve 2 in figures 5(b), 5(d) and 5(e)). In the particular case when carriers are not too mobile, then we can have $4a_1 \gg a_2^2$ (this condition determines a configuration of atoms in space), i.e. $V_{01} \rightarrow V_{02}$. In this case the threshold voltage V_{01} can take the following form:

$$V_{01} \approx \frac{1}{2}L^2\sqrt{a_1} = \frac{1}{2}L^2\sqrt{\frac{(\mu_n + \mu_p)qv_pN_{i2}}{\epsilon\mu_n\mu_p}}. \quad (20)$$

A switching effect can occur when the threshold voltage V_{01} is not too great. If this value is very great (e.g. $L \gg 10^{-4}$ cm and $N_i \geq 10^{17}$ cm $^{-3}$), then the current-voltage characteristic is described by (12) (curve 1 in figure 5). Generally, from our considerations it follows that the switching effect is a singularity of electric conduction and n- or p-type space charge regions are determined by a configuration of atoms in space (this property is equivalent to a distribution of permissible energy states in the band gap) and by the mechanisms describing carrier injection from the electrodes into the bulk.

The current-voltage characteristics presented in figure 5 are obtained by experiment. In figure 5(a) the shape of the function $J(V)$ is typical for PcZn, PcCu, Se, As:Se, PcNi, SiC, ZnTe and halogen glass of composition 12 at.% Si-9.76 at.% Ge-29.9 at.% As-47.7 at.% Te. This characteristic defines one of the properties of the solar cell system. In figures 5(b)-5(e), the current-voltage characteristics are typical for the different insulator and semiconductor materials such as ZnS, CdS, Se, As:Se, SiO₂, Al₂O₃, GaAs, anthracene (amorphous structure), polyethylene, Ge and Si. Usually, as the material electrodes, Au, Ag, Cu, Al, In, Sn, Ta, Zn and others have been used. For example, the metal-solid-metal system has been realized by structures such as In/InP/In, Ta/halogen glass/Ta, Sn/GaAs/Sn, Al/Al₂O₃/Au, Al/SiO₂/Al, In/CdS/Ta, In/CdS/Au, In/PcZn/Au and Au/PcZn/Al.

Now, let us discuss the boundary problem for (1)-(6). By combining (1)-(5), the equations describing the free carrier flow can be written as

$$\frac{\partial n}{\partial t} - \mu_n E \frac{\partial n}{\partial x} - \frac{\mu_n q}{\epsilon} n(p - n - n_{i1} - n_{i2}) - v_n n_{i1} = 0 \quad (21)$$

$$\frac{\partial p}{\partial t} + \mu_p E \frac{\partial p}{\partial x} + \frac{\mu_p q}{\epsilon} p(p - n - n_{i1} - n_{i2}) - v_p N_{i2} = 0. \quad (22)$$

Using the theory of characteristics for (21) and (22), we can write the ordinary equations for free electron flow as

$$\begin{aligned} \frac{dx_n(t)}{dt} &= -\mu_n E(x_n(t), t) \\ \frac{dn(x_n(t), t)}{dt} &= f_n(x_n(t), t) \end{aligned} \quad f_n = \frac{\mu_n q}{\epsilon} n(p - n - n_{i1} - n_{i2}) + v_n n_{i1} \quad (21a)$$

and for free hole flow

$$\begin{aligned} \frac{dx_p(t)}{dt} &= \mu_p E(x_p(t), t) \\ \frac{dp(x_p(t), t)}{dt} &= f_p(x_p(t), t) \end{aligned} \quad f_p = -\frac{\mu_p q}{\epsilon} p(p - n - n_{i1} - n_{i2}) + v_p N_{i2}. \quad (22a)$$

From (21a), (22a) and (4)-(6) it follows that the current flow between the anode $x = 0$ and the cathode $x = L$ is determined by the initial conditions $p(x_p(0), 0)$, $n(x_n(0), 0)$, $n_{i1}(x, 0)$ and $n_{i2}(x, 0)$ and by the boundary conditions $p(0, t)$ and $n(L, t)$ for $E(x, t) > 0$ in the

region $x \in (0, L)$ and $t \geq 0$. In order to obtain the singular solutions (9) (figure 3(b) and 3(c)), we must have the following boundary condition [39]:

$$\begin{aligned} p(0, t) &= \frac{\mu_n}{q(\mu_n + \mu_p)} \left[\frac{f_L[E(L, t)]}{\mu_n E(0, t)} + \varepsilon \left(a_2 - \frac{2V_{01}}{L^2} \right) \right] \\ n(L, t) &= \frac{\mu_n}{q(\mu_n + \mu_p)} \left[\frac{f_L[E(L, t)]}{\mu_n E(L, t)} - \varepsilon \frac{\mu_p}{\mu_n} \left(a_2 - \frac{2V_{01}}{L^2} \right) \right] \end{aligned} \quad (23)$$

or

$$\begin{aligned} p(0, t) &= \frac{\mu_n}{q(\mu_n + \mu_p)} \left[\frac{f_0[E(0, t)]}{\mu_n E(0, t)} + \varepsilon \left(a_2 + \frac{2V_{02}}{L^2} \right) \right] \\ n(L, t) &= \frac{\mu_n}{q(\mu_n + \mu_p)} \left[\frac{f_0[E(0, t)]}{\mu_n E(L, t)} - \varepsilon \frac{\mu_p}{\mu_n} \left(a_2 + \frac{2V_{02}}{L^2} \right) \right]. \end{aligned} \quad (24)$$

Here, the boundary functions f_0 and f_L describe the mechanisms of carrier injection from the electrodes into the bulk. The boundary function $p(0, t)$ described by (23) and $n(L, t)$ described by (24) determine the singular solution shown in figure 5(a). On this basis we ascertain that the current-voltage characteristics (10)–(12) are valid. Instead of μ_p in (22a), we can make use of $-\mu_p$ (the valence electron mobility and $\mu_p < 0$). Under this condition, the characteristics (22a) describe the valence electron flow from the cathode $x = L$ to the anode $x = 0$. This is expressed by f_L in (11). From (23) and (24) it follows that the condition $\alpha = 0$ (i.e. the $J(V)$ curve shown in figure 5(a) occurs) is possible when the boundary functions satisfy the following conditions:

$$|f_0(0)/0| < \infty \quad |f_L(0)/0| < \infty. \quad (25)$$

For example, these conditions are satisfied by the Fowler–Nordheim function and by the power functions, i.e. $f_{0,L}(E_{0,L}) \propto E_{0,L}^k$ and $k \geq 1$.

From (12) it follows that the current-voltage characteristic is not defined for the voltages $V < V_0$ (figure 5). This property can be explained by a change in the configurations of atoms in space. When the given material structure is permanently bombarded by photons, a part of this energy is absorbed by the rotators and oscillators. By quantum mechanics, the energy W_{rot} of the rotator and the energy W_{osc} of the double (linear) oscillator are of the form

$$W_{rot} = \frac{\hbar^2}{2I} l(l+1) \quad W_{osc} = h\nu_{osc} \left(k + \frac{1}{2} \right) \quad l, k = 0, 1, 2, \dots \quad (26)$$

Here, I denotes the moment of inertia, l is the orbital quantum number and ν_{osc} is the frequency of the oscillator. The phonon can absorb a portion of energy when $\Delta l = 1$ and $\Delta k = 1$ (Δ denotes the difference). Thus, the photon energy $h\nu_{phot}$ absorbed by the phonon is of the form

$$h\nu_{phot} = \frac{\hbar^2}{I} (l+1) + h\nu_{osc} \quad \text{for } \Delta l = 1 \text{ and } \Delta k = 1. \quad (26a)$$

This relation is valid when the Compton effect for the phonon is neglected. Also, either $\Delta l = 1$ and $\Delta k = 0$ (the function $\nu_{phot} = \nu_{phot}(l)$ defines a spectrum of the rotator) or $\Delta k = 1$ and $\Delta l = 0$ (the spectrum of the oscillator). The rotator and oscillator characterize interactions between the given atom and the adjacent atoms in the bulk. Thus, the new (higher-)energy states are occupied by the phonon. In other words, the condition $V < V_0$ denotes that there exists a configuration of atoms (i.e. the energy levels occupied by the rotators and oscillators are sufficiently great) for which the mobility parameters μ_n and μ_p (figure 1, arrows 4 and 5) do not exist.

Also, for the condition $V < V_0$ we must assume that special photoelectrochemical and thermal processes at the electrodes occur [16, 25, 41–43].

On this basis, we ascertain that there exist boundary and internal conditions in which the metal–solid (insulator or semiconductor)–metal system can act as a solar cell. This property, in particular, is observed for materials such as Si, SiC, PcZn, PcCu, CdS, CdSe, As_2S_3 , $As_2S_3:Sb_2S_3$, As_2Se_3 and TiO_2 .

Now, let us find the relation between the general integral in (8) and the singular solutions of this equation. From (8) it follows that the general solution is of the form $E(x) = E(x, A, B)$ where A and B are constants of integration. A particular integral is found by the use of the boundary values of $E(0)$ and $E(L)$. Therefore, for this problem, the space charge density distribution $q_v(x) = \varepsilon dE(x)/dx$ is written as

$$q_v(x) = q_v(x, E(0), E(L)) \quad J = f_0[E(0)] \quad J = f_L[E(L)]. \quad (27)$$

In the case of the singular solutions (9), the space charge density distribution is uniform, i.e.

$$q_v(x) \equiv -2\varepsilon V_{01}/L^2 \text{ or } q_v(x) \equiv 2\varepsilon V_{02}/L^2.$$

On this basis we ascertain that the particular integral $E(x)$ and the singular solutions (9) are separated. Therefore, in terms of (27), the current–voltage characteristics presented in figure 5 cannot be obtained [39].

5. Conclusions

In the above we have obtained new and simple solutions for carrier generation. These solutions are as follows.

(1) The system can act as a blocking diode with the current–voltage characteristic showed in figure 5(a). This $J(V)$ curve occurs when carriers are very mobile, the boundary function f_L is monotonic and the inverse function f_L^{-1} satisfies the condition $f_L^{-1}(0) = 0$. In this case the total space charge is localized in the band gap.

(2) In the case when carriers are not too mobile, the solutions (10)–(13d) define the ‘S’- or ‘N’-type switching effect for $V > V_{TH}$. There exists a function $a_2 = f(a_1)$ (this is a condition for a configuration of atoms in space) which defines the values of the threshold voltages $V_{TH} \in (V_0, V_{01})$. The condition $V > V_{TH}$ defines the transition from a low level of carrier injection to a high level of electron or hole injection.

(3) When the threshold voltage $V_{TH} = V_{01}$ is very great, then the current–voltage characteristic has the form $J = f_L(2V/L)$ and the switching effect does not occur.

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