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MODELLING OF SCHOTTKY CONTACTS FOR ADMITTANCE AND IMPURITY PROFILING MEASUREMENTS

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ABSTRACT

The paper presents a theory of a metal-semiconductor contact biased by dc voltage with superimposed small ac signal. Theoretical considerations based on general transport equations enabled to derive equations useful for admittance and impurity profiling measurements of materials properties.

1. Introduction

Schottky barrier contacts are essential parts of many semiconductor devices and also may serve as a valuable tool for extracting some important material parameters [1]. Mercury Schottky barrier makes this tool non-destructive [2]. Schottky barrier contact capacitance-voltage characteristics is used for extracting impurity profiles while in the case of admittance measurements one should measure C-V characteristics with test signal frequency and temperature as parameters [3]. Theory presented in the paper based on general transport equations enables to calculate structure admittance for various materials parameters.

2. Static characteristic

2.1. Transport equations

In the 1D case of Schottky barrier contact presented in Fig. 1, the value of total electric current density in semiconductor remains constant, therefore it is purposeful to assume it as a basic quantity. In order to describe the static characteristic of the considered structure the total current density J_o is defined as shown in Eq. (1).

$$J_o = \sigma_o E_o + \frac{1}{\beta}\left(\sigma_{no}\frac{1}{n_o}\frac{dn_o}{dx} - \sigma_{po}\frac{1}{p_o}\frac{dp_o}{dx}\right) \quad (1)$$

where σ_o is total conductivity, E_o is electric field intensity, σ_{no} (σ_{po}) is electron (hole) conductivity, n_o (p_o) is electron (hole) concentration, $\beta = q/kT$, k is Boltzmann constant, T is temperature, q is elementary charge.

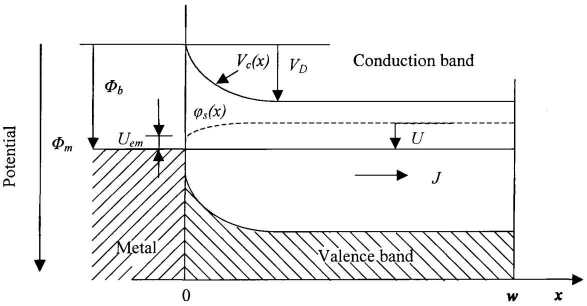

Fig. 1. Band model of Schottky barrier contact.

The first addend in Eq. (1) determines charge carriers convection, the second, electron and hole diffusion current. Equation (1) is a modification of Shockley's equations [4] defining the electron and hole currents.

The basic theory assumption is, that the constant value of current density J_o is given. The second assumption is the lack of excess charge carriers or very low carrier lifetime. In that case, from the law of mass action it results that:

$$\ln(n_o p_o) = \ln n_o + \ln p_o = \ln n_i^2 = const \quad (2)$$

where n_i is intrinsic carrier concentration.

By differentiating the above equation we obtain:

$$-\frac{1}{p_o}\frac{dp_o}{dx} = \frac{1}{n_o}\frac{dn_o}{dx}. \quad (3)$$

Substituting this equation to (1) we obtain formula:

$$J_o = \sigma_o E_o + \frac{1}{\beta}\frac{\sigma_o}{n_o}\frac{dn_o}{dx} \quad (4)$$

from which one can derive equivalent differential equations satisfied by n_o or p_o:

$$\frac{dn_o}{dx} = \beta n_o \left(\frac{J_o}{\sigma_o} - E_o \right). \qquad (5)$$

The space charge layer plays important role in the admittance and impurity profiling measurements, so one should formulate the Poisson's equation.

$$\frac{dE_o}{dx} = \frac{q}{\varepsilon_s}(p_o - n_o + N_D - N_A) \qquad (6)$$

where ε_s is dielectric constant, N_D and N_A are donor and acceptor concentrations, which are assumed to be fully ionized and dependent only on *x*-coordinate, but not dependent on concentrations n_o and p_o.

From Eq. (2) it is clear that to determine electron and hole concentration it is sufficient to give one of them. It is easy to obtain from Eq. (2) that:

$$p_o = \frac{n_i^2}{n_o} \qquad (7)$$

so, one can write the Poisson's equation in the form:

$$\frac{dE_o}{dx} = \frac{q}{\varepsilon_s}\left(\frac{n_i^2}{n_o} - n_o + N_D - N_A \right). \qquad (8)$$

Equations (5) and (8) determine the system of first--order non-linear differential equations which are satisfied by parameters n_o and E_o, being the functions of *x*-coordinate. The difference $N_D - N_A$ is treated as a given function $f(x)$.

2.2. Boundary conditions

1) $x = w$

Assuming sufficiently large *w*, one can accept, that for $x = w$ space charge is equal zero, hence $dE_o/dx = 0$ and from Eq. (8) we obtain:

$$\frac{n_i^2}{n_o} - n_o = N_A - N_D, \quad (x = w) \qquad (9)$$

and then

$$n_o(w) = \left[\frac{1}{2}\sqrt{(N_D - N_A)^2 + 4n_i^2} + N_D - N_A \right]_{x=w}. \qquad (10)$$

2) $x = 0$

It is assumed, that Schottky barrier is formed on n-type and has an intimate contact with semiconductor. The surface states are neglected. According to [5] we obtain:

$$n_o(0) = N_c \left[\frac{J_o}{A^* T^2} + \exp(-\beta\phi_b) \right] \qquad (11)$$

where N_c is effective conduction band density of states, A^* is Richardson constant, ϕ_b is Schottky barrier height. This formula follows from emission-diffusion theory [6].

3. External ac-bias superimposed on structure static characteristic

3.1. Transport equations for ac components

When the external ac-bias is superimposed on static characteristic, the transport parameters are time dependent, so the total current density must contain the additional component – displacement current. In this instance total current *J* for the 1D case is dependent on time, but not on *x*-coordinate and can be presented as an expression:

$$J = \sigma E + \frac{1}{\beta}\frac{\sigma}{n}\frac{dn}{dx} + \varepsilon_s \frac{\partial E}{\partial t} = f(t) \qquad (12)$$

where σ – conductivity and *E* – electric field intensity, are transport parameters dependent on time and on *x*-coordinate.

From Eq. (12), which is a generalization of formula (4), one can derive differential equation of electron concentration *n* similarly to Eq. (5), and namely:

$$\frac{\partial n}{\partial x} = \beta n \left(\frac{J}{\sigma} - E - \frac{\varepsilon_s}{\sigma}\frac{\partial E}{\partial t} \right). \qquad (13)$$

Poisson's equation for *E* will have the form analogical to (8)

$$\frac{\partial E}{\partial x} = \frac{q}{\varepsilon_s}\left(\frac{n_i^2}{n} - n + N_D - N_A \right) \qquad (14)$$

because we think, that the law of mass action (2) is also valid for concentrations of time-dependent variables. Possible deviations from this law can last only for very short period of time of the order of lifetime which we assume as a close to zero.

In order to take into account ac bias of radial frequency ϖ superimposed on static characteristic we assume the following expressions specifying *J*, *n*, σ and *E*.

$$J = J_o + \Delta J = J_o + \hat{J}e^{i\varpi t}, \qquad (15)$$

$$n = n_o + \Delta n = n_o + \hat{n}e^{i\varpi t}, \qquad (16)$$

$$\sigma = \sigma_o + \Delta\sigma = \sigma_o + \hat{\sigma}e^{i\varpi t}, \qquad (17)$$

$$E = E_o + \Delta E = E_o + \hat{E}e^{i\varpi t} \qquad (18)$$

where $\hat{J}, \hat{n}, \hat{\sigma}, \hat{E}$ are complex amplitudes of ac components, dependent only on *x*-coordinate but not dependent on time.

The quantities J_o, n_o, s_o and E_o specify static characteristic discussed in Section 2.

In order to formulate the equations satisfied by $\hat{n}$ and $\hat{E}$ one should utilize Eqs. (13) and (14). The quantities ΔJ, Δn, $\Delta\sigma$ and ΔE are helpful in deriving these equations.

Corresponding transformations presented in Appendix A1 have been realized under following assumptions:

1. The given value $\hat{J}$ satisfies as inequality $|\hat{J}| << |J_o|$.
2. First order components are only taken into account. The components of frequency 2ϖ or greater are rejected.

Taking advantage of results of Appendix A1 we can write:

$$\frac{\partial \hat{n}}{\partial x} = \beta\left\{\frac{J_o}{\sigma_o}\left[1 - q\frac{n_o}{\sigma_o}\left(\mu_n - \frac{p_o}{n_o}\mu_p\right)\right] - E_o\right\}\hat{n} - \\ -\beta n_o\left(1 - \frac{\varepsilon_s}{\sigma_o} i\varpi\right)\hat{E} + \frac{\beta n_o}{\sigma_o}\hat{J}, \tag{19}$$

$$\frac{\partial \hat{E}}{\partial x} = \frac{q}{\varepsilon_s}\left(\frac{n_i^2}{n_o^2} + 1\right)\hat{n}. \tag{20}$$

The above formulas form set of linear ordinary differential equations which are satisfied by complex amplitudes $\hat{n}$ and. $\hat{E}$ Coefficient of $\hat{n}$ and $\hat{E}$ are functions of n_o and E_o, which should be calculated by solving Eqs. (5) and (6), specifying static characteristic. The parameters n_o and E_o are functions of argument x. The amplitude of alternating current density $\hat{J}$ is a quantity independent on x, what follows in the case of 1D, from the continuity equation of total current density. The value of current density $\hat{J}$ have to be given and for calculation simplification can be specified by real number.

3.2. Boundary conditions for ac external bias

1) $x = w$

It is assumed that, in the vicinity of $x = w$, sufficiently distant from structure depletion space carriers concentrations are independent on time. So in that case one should accept condition:

$$\hat{n}(w) = 0. \tag{21}$$

2) $x = 0$

Boundary condition (11) can be generalized to obtain relation between concentration n and current J.

$$n(0) = N_c\left[\frac{J}{A^* T^2} + \exp(-\beta\varphi_b)\right]. \tag{22}$$

Substracting from this expression relation (11) we obtain according to formulas (15) and (16):

$$\Delta n(0) = N_c\frac{\Delta J}{A^* T^2} \tag{23}$$

and

$$\hat{n}(0) = N_c\frac{\hat{J}}{A^* T^2}. \tag{24}$$

4. The structure under an applied voltage

4.1. Static voltage

According to results of [4] introducing here common level φ_{so} for electrons and holes, the current density J_o can be determined also in the following way:

$$J_o = -\sigma\frac{d\varphi_{so}}{dx}. \tag{25}$$

The above expression is fully equivalent to relation (1) and enables to determine the difference $\varphi_{so}(0) - \varphi_{so}(w)$. In order to obtain complete voltage on the structure one should add the voltage U_{emo} as it results from energy diagram presented in Fig. 1.

Then the static voltage U_o applied to structure is equal:

$$U_o = E_{emo} + J_o\int_o^w\frac{dx}{\sigma_o} \tag{26}$$

where:

$$U_{emo} = \frac{1}{\beta}\ln\left(1 + \frac{J_o}{A^* T^2}\exp\beta\varphi_b\right) \tag{27}$$

in accordance with Eq. (37) derived in [5].

4.2. Alternating bias voltage

In the general case we have

$$J = -\sigma\frac{d\varphi}{dx} + \varepsilon_s\frac{\partial\Delta E}{\partial t} \tag{28}$$

hence:

$$\frac{d\varphi}{dx} = -\frac{J}{\sigma} + \frac{\varepsilon_s}{\sigma}\frac{\partial\Delta E}{\partial t}. \tag{29}$$

Taking into account only variables one can obtain:

$$\frac{d\Delta\varphi}{dx} = -\frac{\Delta J}{\sigma_o} + J_o\frac{\Delta\sigma}{\sigma_o^2} + \frac{\varepsilon_s}{\sigma_o}\frac{\partial\Delta E}{\partial t} \tag{30}$$

so the voltage connected with Fermi level is given in the form:

$$\Delta U_{Ferm} = -\int_o^w\frac{d\Delta\varphi}{dx} = \int_o^w\frac{\Delta J}{\sigma_o}dx - J_o\int_o^w\frac{\Delta\sigma}{\sigma_o^2}dx - \\ -\varepsilon_s\int_o^w\frac{1}{\sigma_o}\frac{\partial\Delta E}{\partial t}dx \tag{31}$$

while the voltage increment ΔU_{em} resulting from emission characteristic (formula (37) [5]) is given by:

$$\Delta U_{em} = \frac{1}{\beta}\ln\left[1 + \frac{J_o + \Delta J}{A^* T^2}\exp(\beta\varphi_b)\right] - \\ -\frac{1}{\beta}\ln\left[1 + \frac{J_o}{A^* T^2}\exp(\beta\varphi_b)\right] = \\ = \frac{1}{\beta}\ln\frac{1 + \frac{J_o + \Delta J}{A^* T^2}\exp(\beta\varphi_b)}{1 + \frac{J_o}{A^* T^2}\exp(\beta\varphi_b)} \cong \\ \cong \frac{1}{\beta}\frac{\frac{\Delta J}{A^* T^2}\exp(\beta\varphi_b)}{1 + \frac{J_o}{A^* T^2}\exp(\beta\varphi_b)} \tag{32}$$

passing to complex amplitudes one can obtain:

$$\hat{U}_{em} = \frac{1}{\beta}\frac{\frac{1}{A^{*}T^{2}}\exp(\beta\varphi_b)}{1+\frac{J_o}{A^{*}T^{2}}\exp(\beta\varphi_b)}\hat{J} = \\ = \frac{\hat{J}}{\beta[A^{*}T^{2}\exp(-\beta\varphi_b)+J_o]} \tag{33}$$

because total eternal bias on the structure is given by $U = U_o + \hat{U}^{i\varpi t}$,

where $\hat{U} = \hat{U}_{Ferm} + \hat{U}_{em}$, therefore

$$\hat{U} = \frac{\hat{J}}{\beta[A^{*}T^{2}\exp(-\beta\varphi_b)+J_o]} + \int_o^w \frac{\hat{J}}{\sigma_o}dx - \\ - J_o\int_o^w \frac{\hat{\sigma}}{\sigma_o^2}dx - \varepsilon_s\int_o^w \frac{1}{\sigma_o}\frac{\partial \varDelta E}{\varDelta t}dx = \\ = \frac{\hat{J}}{\beta[A^{*}T^{2}\exp(-\beta\varphi_b)+J_o]} + \hat{J}\int_o^w \frac{dx}{\sigma_o} - \\ - J_o\int_o^w \frac{\hat{\sigma}}{\sigma_o^2}dx - \varepsilon_s i\overline{\varpi}\int_o^w \frac{\hat{E}}{\sigma_o}dx. \tag{34}$$

The amplitude of variable component of the voltage as a function of variable component of the current is dependent on the static current J_o, Schottky barrier height, temperature, total conductivity σ_o, angular frequency ϖ and variable components of the conductivity and electric field intensity. Using Eq. (34) one can calculate structure admittance as:

$$\hat{Y} = \frac{\hat{J}}{\hat{U}}. \tag{35}$$

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Appendix A1

In order to obtain equations satisfied by Δ*n* and Δ*E* in linear approximation, one should find increments of particular functions occurring in Eqs. (13) and (14).

Equation (13)

LHS of Eq. (13)

$$\Delta\left(\frac{\partial n}{\partial x}\right) = \frac{\partial \Delta n}{\partial x}. \tag{A1.1}$$

RHS of Eq. (13)

a)

$$\varDelta\beta n\frac{J}{\sigma} = \beta\frac{\partial}{\partial n}\left(n\frac{J}{\sigma}\right)_o \varDelta n + \beta\frac{\partial}{\partial\sigma}\left(n\frac{J}{\sigma}\right)_o \varDelta\sigma + \\ + \beta\frac{\partial}{\partial J}\left(n\frac{J}{\sigma}\right)_o \varDelta J = \beta\frac{J_o}{\partial_o}\varDelta n + \\ + \beta n_o J_o\left(-\frac{1}{\sigma_o^2}\right)\varDelta\sigma + \beta\frac{n_o}{\sigma_o}\varDelta J, \tag{A1.2}$$

b)

$$\varDelta(-\beta nE) = -\beta\frac{\partial}{\partial n}(nE)_o\varDelta n - \\ - \beta\frac{\partial}{\partial E}(nE)_o\varDelta E = -\beta E_o\varDelta n - \beta n_o\varDelta E, \tag{A1.3}$$

c)

$$-\varDelta\left(\beta n\frac{\varepsilon_s}{\sigma}\frac{\partial E}{\partial t}\right) = -\beta n_o\frac{\varepsilon_s}{\sigma_o}\frac{\partial\varDelta E}{\partial t} = \\ = -\beta n_o\frac{\varepsilon_s}{\sigma_o}\hat{E}\overline{\varpi}e^{i\overline{\varpi}t} = -\beta n_o\frac{\varepsilon_s}{\sigma_o}i\overline{\varpi}\varDelta E. \tag{A1.4}$$

$\Delta\sigma$ has not been taken into account in case c), because the obtained product $\Delta\sigma\Delta E$ as a second order term has been discharged, moreover we take advantage of denotation (18).

Connecting formulas (A1.1) – (A1.4) in accordance to Eq. (13) one can obtain:

$$\frac{\partial\varDelta n}{\partial x} = \beta\frac{J_o}{\sigma_o}\varDelta n - \beta n_o J_o\frac{1}{\sigma_o^2}\varDelta\sigma + \beta\frac{n_o}{\sigma_o}\varDelta J - \\ - \beta E_o\varDelta n - \beta n_o\varDelta E - \beta n_o\frac{\varepsilon_s}{\sigma_o}i\overline{\varpi}\varDelta E = \\ = \beta\left(\frac{J_o}{\sigma_o} - E_o\right)\varDelta n - \beta n_o\frac{J_o}{\sigma_o^2}\varDelta\sigma - \\ - \beta n_o\left(1 - \frac{\varepsilon_s}{\sigma_o}i\varpi\right)\varDelta E + \frac{\beta n_o}{\sigma_o}\varDelta J. \tag{A1.5}$$

Now it is needed to determine the relationship between $\Delta\sigma$ and Δn.

Applying mass action law one can obtain:

$$\Delta(np) \cong n_o\Delta p + p_o\Delta n = 0 \tag{A1.6}$$

hence:

$$\Delta p = -\frac{p_o}{n_o}\Delta n \tag{A1.7}$$

and then:

$$\Delta\sigma = q(\mu_p\Delta n + \mu_p\Delta p) = q\left(\mu_n - \mu_p\frac{p_o}{n_o}\right)\Delta n \tag{A1.8}$$

where $\mu_n(\mu_p)$ is electrons (holes) mobility.

Substituting (A1.8) into (A1.5) one can obtain:

$$\begin{aligned}\frac{\partial \Delta n}{\partial x} &= \beta\left\{\frac{J_o}{\sigma_o}\left[1-\frac{n_o}{\sigma_o}q\left(\mu_n-\frac{p_o}{n_o}\mu_p\right)\right]-E_o\right\}\Delta n - \\ &-\beta n_o\left(1-\frac{\varepsilon_s}{\sigma_o}i\varpi\right)\Delta E+\frac{\beta n_o}{\sigma_o}\Delta J\end{aligned} \tag{A1.9}$$

where Δn, ΔE are searched variables, ΔJ is given quantity, J_o, σ_o, E_o, n_o are quantities calculated for static characteristic. Replacing variables Δn, ΔE, ΔJ through expressions occurring in (15) – (18) and removing common factor $e^{i\varpi t}$ we have:

$$\begin{aligned}\frac{\partial \hat{n}}{\partial x} &= \beta\left\{\frac{J_o}{\sigma_o}\left[1-q\frac{n_o}{\sigma_o}\left(\mu_n-\frac{p_o}{n_o}\mu_p\right)\right]-E\right\}\hat{n} - \\ &-\beta n_o\left(1-\frac{\varepsilon_s}{\sigma_o}i\varpi\right)\hat{E}+\frac{\beta n_o}{\sigma_o}\hat{J}.\end{aligned} \tag{A1.10}$$

Equation (14)

LHS of Eq. (14)

$$\Delta\left(\frac{\partial E}{\partial x}\right)=\frac{\partial \Delta E}{\partial x}. \tag{A1.11}$$

RHS of Eq. (14) is obtained as follows:

$$\begin{aligned}&\frac{q}{\varepsilon}\Delta\left(\frac{n_i^2}{n}-n+N_D-N_A\right)= \\ &=\frac{q}{\varepsilon}\frac{\partial}{\partial n}\left(\frac{n_i^2}{n}-n+N_D-N_A\right)_o\Delta n= \\ &=-\frac{q}{\varepsilon}\left(\frac{n_i^2}{n_o^2}+1\right)\Delta n.\end{aligned} \tag{A1.12}$$

In that case we have:

$$\frac{\partial \Delta E}{\partial x}=-\frac{q}{\varepsilon}\left(\frac{n_i^2}{n_o^2}+1\right)\Delta n. \tag{A1.13}$$

Making use of denotations in Eqs. (16) and (18) one can obtain:

$$\frac{\partial \hat{E}}{\partial x}=-\frac{q}{\varepsilon}\left(\frac{n_i^2}{n_o^2}+1\right)\hat{n}. \tag{A1.14}$$