Transport theory of Schottky barrier diodes

A.A.Klyukanov, P.A.Gashin, R.Scurtu

Semiconductor Physics Lab, Faculty of Physics, Moldova State University, 60 A. Mateevici str., Chisinau MD 2009,Republic of MoldovA
klukanov@usm.md

Abstract **— A microscopic many-body transport approach for electronic properties of spatially inhomogeneous systems is developed at the fully quantum-mechanical level by means of plane wavelets second quantization representation. It is obtained that current density is determined by the statistically averaged microscopic polarization dependent on the quantized positions and quantized momenta of charge carriers. At the semiclassical level the distribution function of electrons include many-body effects via drift , diffusion and thermionic emission as well as entirely quantum-mechanical tunneling through a Schottky barrier. Dependences of the current versus voltage on the thickness of semiconductor layer, the relaxation times in the neutral region and in the depletion layer, the width of Schottky barrier and the mean free paths are investigated. It is established that ideality factor n is a function of applied voltage V. The value of V at which I-V characteristics acquire an ohmic nature is depended on the parameters of semiconductors.**

Index Terms **— Schottky barrier, I-V characteristics, quantum mechanical transport theory, distribution function, plane wavelets second quantization representation.**

1. INTRODUCTION

Solar cells based on the thin film technology are important candidates for photovoltaic industry. One of the significant techniques for the device characterization is current versus voltage. Forward current, in many cases, can be described by exponential dependence with exponent index qV/nkT, where n is the so-called "ideality" factor lied in the range 1 to 2. Such simple formula does not cover the observed variety of experimental I-V characteristics of MOS structures. The measured I-V characteristics of MOS structures and their evolution at the temperature variation are governed by the thermionic-emission-diffusion Sze-Crowell theory [1,2]. But frequently experiment gives $n > 2$. To construct the theory one has to put into the consideration a number of simplifying assumptions. Here we consider an implication of difference kinetic theory, suggested in the reference [3], which, in a sense, allows us to consider of the validity of some theoretical assumptions. We discuss our analysis of basic equations for semiconductor-device operation in relation to other theoretical approaches.

Analysis of carrier's behavior under influences of applied electric field is described by the basic equations which include the Poisson equation, continuity equations and current-density equations. With account of drift and diffusion according to the both Ohm's law and Fick's law we have

$$j(x) = q\mu_n n(x)E(x) + qD_n \frac{dn(x)}{dx} \qquad (1)$$

where $E(x)$ is the intensity of the field, $n(x)$ is the concentration, D_n is the diffusion coefficient, $j(x)$ is the current density, x is coordinate and q is the charge of electrons. According to the Einstein relation valid for the nondegenerate semiconductors we have $D_n = \mu_n kT/q$. Here μ_n is the mobility, T is a temperature of device. It is well known that equation for current density (1) can easily be deduced by using of the classical Boltzmann equation solution in approximation of relaxation time $\tau(x,k_x)$

$$n(x,k_x) = n_e(x)n_e(k_x)f(x,k_x),\ n_e(k_x) = \left(\frac{\pi\hbar^2}{2mkT}\right)^{\frac{1}{2}} \exp\left(-\frac{\hbar^2 k_x^2}{2mkT}\right)$$

$$f(x,k_x) = 1 - \frac{\hbar k_x}{m}\left(\frac{qE(x)}{kT} + \frac{n'(x)}{n(x)}\right)\tau(x,k_x) \qquad (2)$$

Here m is the effective mass of electrons, $n_e(k_x)$ is the equilibrium distribution function. Other designations are standard. At small field intensities $n_e(x)$ is the thermodynamic equilibrium concentration of electrons and $f(x,k_x) \cong 1$. If one wants to investigate high field transport one may introduce the mobility depending of $E(x)$ [4]. We consider nonlinear current-voltage characteristics by means of concentration $n(x)$ as function of arbitrary field intensity $E(x)$. For semiconductor with depletion layer in the region of Schottky barrier distribution function can be represented in the form

$$n(x,k_x) = n(x)n_e(k_x)f(x,k_x)A^{-1}(x,V)T(x,k_x) \qquad (3)$$

Here $T(x,k_x)$ is the barrier-transmission coefficient, A(x,V)- normalizing factor, which can be determined from the equation for total number of electrons N

$$N = 2S\sum_{x,k_x} n(x,k_x) = Sd\sum_x n(x,),\ A(x,V) =$$

$$\left(\frac{\hbar^2}{2\pi mkT}\right)^{1/2} \int_{-\infty}^{\infty} f(x,k_x)\exp\left(-\frac{\hbar^2 k_x^2}{2mkT}\right)T(x,k_x)dk_x \qquad (4)$$

where S-surface area, d-thickness of the semiconductor. In the neutral region $A(x,V) = 1, T(x,k_x) = 1$. Quantum transmission coefficient $T(x,k_x)$ can be calculated having applied the Wentzel–Kramers–Brillouin approximation for depletion region. On condition $U(x) < E$ one gets

$$T(x,k_x) = \exp\left(-\frac{x}{\lambda(x)}\right), \qquad (5)$$

If the inequality $U(x) > E$ is valid we have

$$T(x,k_x) = \frac{\exp(-\frac{2}{\hbar}\int_0^x \sqrt{2m(U(x)-E)dx})}{\left(1+\frac{1}{4}\exp(-\frac{2}{\hbar}\int_0^x \sqrt{2m(U(x)-E)dx})\right)^2} \qquad (6)$$

Here $U(x)$ is the potential and E is the total energy, $\lambda(x)$ is the mean free path of carriers. As the simple approximation the probability of electron emission over Schottky barrier is given by $T(x,k_x) = \exp(-x/\lambda)$ (5).

The dependence of the normalizing factor $A(0,V)$ on the applied voltage V is visualized in Fig.1.

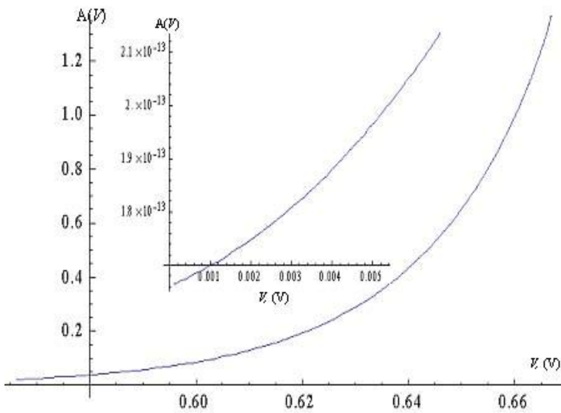

Fig.1. The computed normalizing factor $A(V)$ is shown as function of applied voltage V. Equation (4) is solved for a model with d=0.1 mm wide ZnSe semiconductor. For the calculation a temperature of 300 K, mobility $\mu_n = 0.053$ cm^2/V-s, $\lambda(0)/\Delta = 10$, $N_D = 10^{21} m^{-3}$ and effective mass $m_n = 0.2 m_0$ are used.

Insert shows that the value of $A(0,V)$ varies significantly from $1.66 \cdot 10^{-13}$ at $V = 0$ up to 1.4 at $V = 0.67$ V, such that one obtains very incorrect estimates of concentration $n(x)$ if one ignores the factor $A(0,V)$ variations and takes $A(x,V) = 1$.

It is common practice to assume the tunneling current proportional to the quantum transmission coefficient $T(x,k_x)$ multiplied by the equilibrium distribution function $n_e(k_x)$. In that case tunneling current is considered as additional quantum correction to the classical current, represented by the equation (1). It is not consistent theory if one has to remember what term he lost. We determine current density by the next equation

$$j(x) = -q\frac{\hbar}{m}\int_{-\infty}^{\infty}\frac{dk_x}{2\pi}2k_x n(x,k_x) \qquad (7)$$

where transmission coefficient is included into distribution function $n(x,k_x)$ (3) as multiplier. One would think that it is only the question of preferences. It is not so. Current density in depletion region is not the sum of tunneling, thermionic-emission and diffusion one from equation (1). We only have to know distribution function $n(x,k_x)$ (3) to calculate current density (7) without any assumption.

II. QUANTUM MECHANICAL PLROBLEM ANALYSIS

To arrange our proofs that solution for distribution function can be represented in the form (3) we turn to account method of difference kinetic equations [3] considering discrete phase space by means of plane wavelets representation

$$|X,K_x\rangle = \Psi_{X,K_x}(x) =$$
$$\frac{1}{\sqrt{d_x}}\exp(iK_x x)\,\theta_+(X+\frac{d_x}{2}-x)\theta_-(x-X+\frac{d_x}{2}) \qquad (8)$$

Plane wavelet function $|X,K_x\rangle$ (8) is determined on the interval $[x-d_x/2, x+d_x/2)$. Position X and momentum K_x are quantized according to equation $K_x = \frac{2\pi}{d_x}n_x, X = d_x m_x$, where $n_x = 0,\pm1,...\pm\infty$, $m_x = 0,\pm1..\pm(d/2d_x - 1/2)$ are integers. The set of plane wavelet orthonormal functions $|X,K_x\rangle$ (8) is complete [3] and can be used as the second quantization basis allowing introducing the positively definite distribution function. The phase space model according to which dynamical variables $r, p = \hbar k$ specify the state of a classical system gives classical description (1) without accounting of effect of tunneling. For quantum systems a simultaneous specification of coordinates r and momenta p is not possible in view of Heisenberg uncertainty relations. A quantum mechanical description consists of a Hilbert space of states. According to the correspondence principle, the laws of quantum mechanics must reduce to those of classic in the limit where $\hbar$ tends to zero. This fundamental requirement views the equations of classical mechanics as limit of the Schrödinger equation. Analogously Boltzmann equation can be derived from the Schrödinger evolution of interacting particles. But classical description of homogeneous system is just the same as the quantum description if one uses a plane-waves representation. Thus some of the Boltzmann equation driving terms may be derived from the quantum mechanical many-body analysis for expectation value of microscopic polarization $P_{kk'}(t) = \langle a_k^+(t) a_{k'}(t) \rangle$ by making use a plane-waves representation in a fairly direct way in terms of creation a_k^+ and destruction a_k operators. In such a manner account of particles interaction with homogeneous electric field E leads to the drift term, represented in the form (2). But it is much more difficult to take into consideration the dependence of distribution function on position of particles which can not be considered in a plane-waves representation In order to develop kinetic theory with simultaneous listing of coordinates and momenta one has to introduce Wigner representation [5,6]. Wigner distribution function is derived from Greens function using the Wigner transform, which is

Fourier transform, with respect to the relative coordinate. This technique is useful in the systems that are not homogeneous. Wigner distribution function is reduced to classic Boltzmann function in the limit where $\hbar$ tends to zero. But for many Hamiltonians of interest Wigner distribution function is not positive definite and hence can not be interpreted as a probability density. We will use difference kinetic equation for microscopic polarization $P_{kk'}(t)$ given by the equation

$$\frac{\partial<\hat{P}_{kk'}(t)>}{\partial t}=\frac{i}{\hbar}<[\hat{H}(t),\hat{P}_{kk'}(t)]>+\left(\frac{\partial<\hat{P}_{kk'}(t)>}{\partial t}\right)_{coll} \quad (9)$$

which has been derived explicitly quantum mechanically [3] in a plane wavelets representation (8) with account of two-particle correlations. The set of ket vectors (8) was used as the second quantization basis allowing introducing the positively definite distribution function, which can be considered at $k=k'$ as density of particles of inhomogeneous system described by numbers of particles at quantized positions with quantized momenta. Difference kinetic equation for distribution function transforms into the classical Boltzmann equation in the limit, where expectation value of particles number varies little in $\Delta X = d_x$ and $\Delta K_x = 2\pi/d_x$. Using plane wavelets representation one gets for current density expression

$$j(x)=\frac{q\hbar}{mSd}\sum_{k_x}\left\{\frac{i}{2d_x}\sum_{k'_X}\cos\frac{d_x}{2}\Delta k'_x\left[P_{k'_xX-d_x,k}-P_{k,k'_xX-d_x}\right]-k_xP_{kk}\right\} \quad (10)$$

If the microscopic polarization $P_{kk'}=P_k^*P_{k'}$ varies little in $\Delta X = d_x$ and $\Delta K_x = 2\pi/d_x$ equation (10) transforms at $k=k'$ into the next one

$$j(x)=-\frac{q\hbar}{mSd}\sum_{k_x}\left\{k_xP_{kk}-\frac{i}{2}\left(P_k^*\frac{dP_k}{dx}-P_k\frac{dP_k^*}{dx}\right)\right\} \quad (11)$$

Second term in equation (11) has the form of the probability current and has no analog in classical theory. Indeed, using the same approximation we have for P_k kinetic equation which includes Schrödinger equation in the form

$$\frac{\partial P_k}{\partial t}=\frac{i}{\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-U(x)-\frac{\hbar^2k_x^2}{2m}\right)P_k+\frac{q}{\hbar}E(x)\frac{\partial P_k}{\partial k_x}+\frac{\hbar}{m}k_x\frac{\partial P_k}{\partial x} \quad (12)$$

Equation (12) shows that tunneling effect is described along with thermionic emission, drift in electric field and diffusion in the united approach for which one has to know nothing else but the solution of difference equation for microscopic polarization $P_{kk'}(t)$ (9, 12). We will resolve the transport problem by means of distribution function in the form (3).

III. NUMERICAL RESULTS AND DISCUSSION

Inserting $n(x,k_x)$ (3) into the equation for current density (7) and evaluating integral over k_x we obtain for current density at the metal-semiconductor interface $x=0$ the result

$$j(0)=\frac{1}{4}qn(0)v_TA^{-1}(0,V_\Delta)F(0,V_\Delta) \quad (13)$$

Here $V_\Delta = V - V_{d-\Delta}$. $V_{d-\Delta}$ is the parasitic voltage drop due to series resistance of neutral region. Function $F(0,V)$ is determined by the equation

$$F(x,V)=\frac{\hbar^2}{mkT}\int_{-\infty}^{\infty}k_xf(x,k_x)\exp\left(-\frac{\hbar^2k_x^2}{2mkT}\right)T(x,k_x)dk_x \quad (14)$$

Figure 2 depicts the main qualitative features of numerical results for function $F(0,V)$. In the limit where applied voltage tends to zero function $F(0,V)\to 0$. The value of function $F(0,V)$ varies from zero up to 7 . It can be shown that in the limit, where only thermionic current is taken into account one gets the well-known expression $F(0,V)=\exp(-qV_{bi}/kT)(\exp(qV/kT)-1)$. Here V_{bi} is the built-in potential.

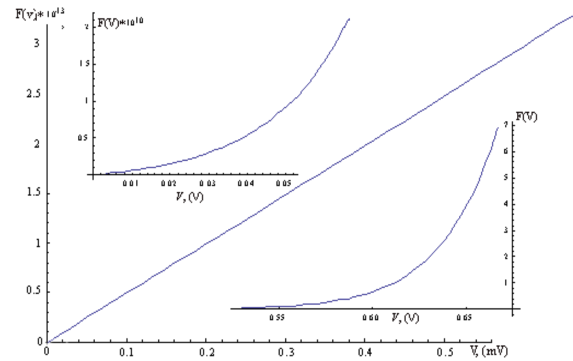

Fig.2. Calculated voltage-dependent function $F(0,V)$ for MOS structure. For the calculation the values of semiconductor's parameters given in the Fig.1 capture are used.

Considering neutral region, where expression for current density (1) is valid, we obtain the dependence of concentration on coordinate is represented by the equation

$$n(x)=e^{\frac{qu(x,x')}{kT}}\left\{n(x')+j(x)\int_{x'}^{x}e^{-\frac{qu(x_1,x')}{kT}}\frac{dx_1}{\mu_nkT}\right\} \quad (15)$$

Where $u(x,x')=\varphi(x)-\varphi(x')$. Electric potential $\varphi(x)$ is determined by the distributions of electrons and shallow impurities according to the Poisson equation. In the depletion layer formula (15) is no longer valid. The approach [2] has been derived from the boundary condition near the metal-semiconductor interface, where equation (15) fails. In the neutral region potential $\varphi(x)$ is the linear function of x, accordingly

$$j(d)=q\mu_nE(d)n(d),(d-\Delta)E(d)=V_{d-\Delta} \quad (16)$$

Equation of continuity $j(0)=j(d)$ can be easily resolved in the limit, where applied voltage $V\to 0$ and $j(0)\approx V_\Delta$. In view of $V_\Delta = V - V_{d-\Delta}$ one gets at arbitrary applied voltage expression for current density

$$j=q\mu_nn(d)\frac{V}{d-\Delta}\left(1+\frac{4\mu_nV_\Delta}{(d-\Delta)v_T}\frac{n(d)}{n(0)}\frac{A(V_\Delta)}{F(V_\Delta)}\right)^{-1} \quad (17)$$

Further analytical expression for the above equation is difficult, and the results can be obtained by numerical

calculation. Some of the parameters of theory expressed by the Eq.(17) $V_{bi}, \mu_n, m_n, d, N_D, T$ are well established, others such as relaxation time $\tau(d) = \mu_n m_n / q$, at the semiconductor surface $x = d$ and $\tau(d) v_T = \lambda(d)$, $\pi\lambda(d)/2d$ can be calculated. But effective width of barrier Schottky Δ and relaxation time $\tau(0)$ can be only estimated. Figure 3 displays the I-V characteristics computed by using different values of parameter $\lambda(0)/\Delta$, where $\lambda(0) = \tau(0) v_T$ is the mean free path of electrons at the interface $x = 0$.

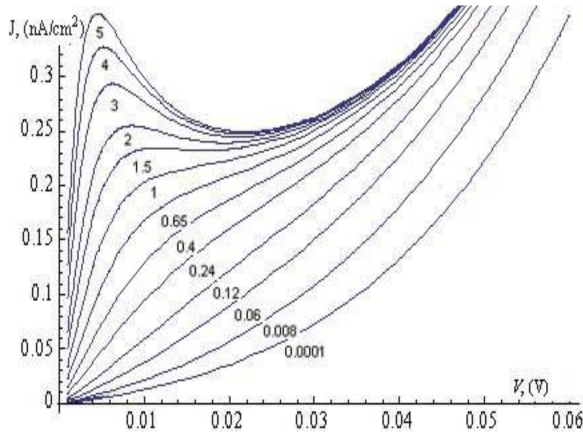

Fig.3. Theoretical I-V characteristics of different MOS structures for $\pi\lambda(d)/2d = 0.008$. The curves are obtained assuming simple rectangular barrier model with incising parameter $\lambda(0)/4\Delta = 0.0001$, 0.02, 0.06, 0.12, 0.24, 0.4, 0.65, 1, 1.5, 2, 3, 4, 5.

Calculated values of typical current-voltage characteristics show that in the region of small electric field $V < 0.1$V current reaches its maximum if parameter $\lambda(0)/4\Delta > 1.4$. At high voltage $V > 0.1$V the ratio $A(0,V)/F(0,V)$ do not depend on parameter $\lambda(0)/\Delta$, therefore all curves showing in the Fig.3 merge into one. But at a fixed value of $\lambda(0)/\Delta$ and different $\lambda(d)/d$ a curves $j(V)$ at $V > 0.1$V depend on parameter $\lambda(d)/d$ according to Fig.4. If applied voltage is in the range $0.5\text{V} > V > 0.1\text{V}$ the current density obey the exponential dependence on V due to the Boltzmann distribution and ideality factor at $0.5\text{V} > V > 0.1\text{V}$ is equal approximately to one $n \cong 1$.

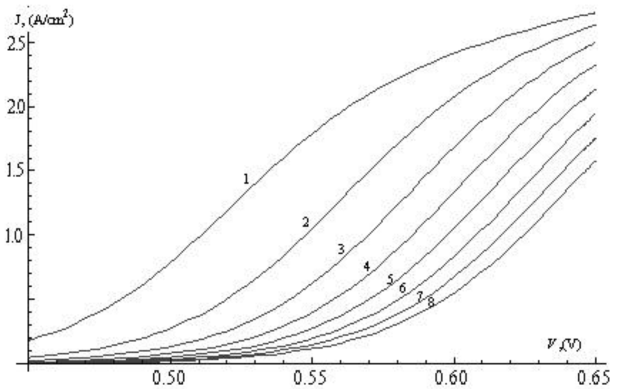

Fig.4. Same as Fig.3, but in the high electric field $V > 0.4$V for $\lambda(0)/4\Delta = 0.1$. and $\pi\lambda(d)/2d$: 1-0.0004, 2-0.0016, 3-0.0036, 4-0.0064, 5-0.01, 6-0.0144, 7-0.0196, 8-0.0256.

Fig.5 and 6 are a plots of ideality factor n versus V.

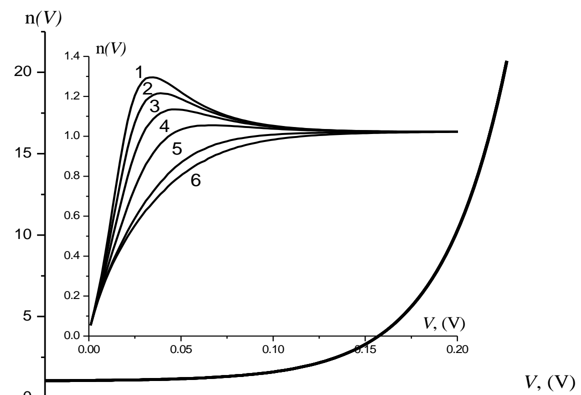

Fig.5. Ideality factor $n(V)$ calculated with using of Eq.(17) at different values of $\lambda(0)/4\Delta =$ 1-0.2, 2-0.15, 3-0.1, 4-0.05, 5-0.01, 6-0.0001 and $\pi\lambda(d)/2d = 0.008$.

As it is clear from figures 5 and 6 the magnitude of $n(V)$ increases with increasing of V at small V. Then at $0.4\text{V} > V > 0.1\text{V}$ the value of $n(V)$ reaches $n \cong 1$. In the region of high voltage $V > 0.4$V $n(V)$ increases again. This effect is visualized in Fig.6. The value of V at which I-V characteristics acquire an ohmic nature is shifted to the smaller V as parameter $\pi\lambda(d)/2d$ decreases.

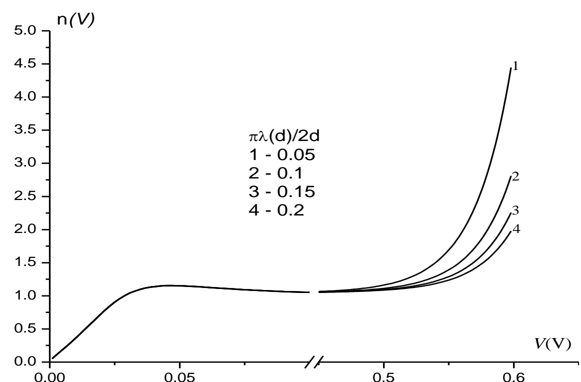

Fig.6. Ideality factor n(V) versus applied voltage at different values of $\pi\lambda(d)/2d$: 1-0.05, 2-0.1, 3-0.15, 4-0.2, for $\lambda(0)/4\Delta = 0.1$

We can conclude that it is possible to phenomenologically

adjust the parameters of the theory, Eq.(17), to reproduce the main signatures of the results for the I-V characteristics of Schottky barrier diodes.

REFERENCES

[1] S.M.Sze, Kwok K.Ng. Physics of semiconductor devices. Hoboken. New Jersey. 2007

[2] C. R. Crowell and S. M. Sze, “Current Transport in Metal-Semiconductor Barriers,” Solid-State Electron., 9, 1035 (1966).

[3] A.A.Klyukanov. Difference Boltzmann Equation. arXiv: 1106.5616v1 [math-ph].(2011).

[4] E.M.Conwell “High field transport in semiconductors” Academic Press. New York and London.1967.

[5] T.Chen, Comm.Math.Phys. V.267, 355-392, (2006).

[6] K.S.Gibbons, M.G.Hoffman, W.K.Wootters. Phys. Rev. A, 70, 062101 (2004)