JOURNAL OF OPTOELECTRONICS AND ADVANCED MATERIALS Vol. 8, No. 4, August 2006, p. 1418 - 1423

Novel approach to the investigation of carriers' concentration in various semiconductor structures

RIFAT M. RAMOVIĆ*, RAJKO M. ŠAŠIĆ[a], PETAR M. LUKIĆ[b]
Faculty of Electrical Engineering, Bulevar kralja Aleksandra 73, Belgrade, Serbia
[a]*Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia*
[b]*Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade, Serbia*

In this paper modern approach to the investigation of carriers' concentration applicable to various semiconductor structures has been developed. The model has exploited transport equation with the quantum correction term included; this transport equation is a consequence of density matrix formalism and moment expansion of corresponding expressions. The achievements of this approach have been tested in the investigation of widely used semiconductor structures. The preliminary theoretical results have been compared with results available in the literature and previously formed knowledge related to this topic.

(Received June 12, 2006; accepted July 20, 2006)

Keywords: Carriers' concentration, Quantum well, Quantum correction

1. Introduction

The hastened progress of semiconductor devices has an inevitable consequence on their growing miniaturization which has surpassed micron dimensions and tends to realize nanometer ones. Compared to the usual picture, a lot of aspects are expected to be changed. Among these expectations the most important one is the appearance of quantum effects in the investigated space – time range. As a rule of a thumb, quantum effects are expected to become prominent when the sample size is of the order of thermal de Broglie wavelength of carriers or shorter [3].

So far the treatment of this problem consisted of self-consistent solution of one electron Schrödinger equation together with the Poisson's equation. The complex character of this approach has inspired numerous and less or more successful approximations; one of them is to assume simple profile quantum wells (mostly triangular or rectangular). Having determined wave function as described, the concentration is obtained according to equilibrium Fermi-Dirac distribution, considering only two lowest quantum levels occupied (electric quantum limit) [7].

This approach has some serious shortcomings. Firstly, at room temperatures and usual unintentional doping levels thermal energy is of the order of energy levels' distinction, so the ignorance of the higher levels contribution becomes questionable. Secondly, in the vicinity of strong barriers (and these are the regions of special interest) the conditions are far from those which recommend the use of Fermi-Dirac equilibrium distribution. Last, but not least, this approach makes it impossible to connect the region near strong barriers (where quantum effects are expected) and the "bulk" region (far inside the sample, satisfactory described by means of classical theory) and describe it in a unified manner [5]. All these reasons have inspired an attempt to construct a modern approach to the investigation of quantum effects in semiconductor samples of nanometer dimensions.

2. Theoretical background of the model

Quantum treatment of such devices can be developed in two directions. First of them is quantum description of carriers spatial distribution (it also describes the electric potential in the structure and the appearance of regions where the transport is assumed to occur); the other is quantum description of transport itself and usually exploits the quantum theory achievements to determine collision rate. This paper concerned only the first aspect.

Let us have a glance on evaluation of one electron wave function in the vicinity of heterojunction. Very often, "by hand" imposed boundary conditions demand that wave function at the barrier becomes equal to zero. In spite of the fact that the electric potential can't have any infinite discontinuity, one of the samples is assumed to be a barrier of infinite height. This is considered to be a quantum correction, as far as it has no classical counterpart. Quantum effects are therefore expected to be more prominent near strong barriers. This paper is an attempt to develop theoretical approach which will confirm these observations.

If quantum effects were neglected, Poisson's equation would remain the only one to be solved. If the total current is equal to zero (drift and diffusion components are assumed to cancel each other under equilibrium conditions) in stationary case, carriers distribution is described by the following classical equation (obtained by taking the moments of transport equation) [1, 3]:

$$k \cdot T \cdot \frac{dn}{dx} + n \cdot \frac{dU}{dx} = 0\,, \qquad U(x) = -e \cdot V(x), \quad 1(a)$$

$$\Phi t \cdot \frac{dn}{dx} - n \cdot \frac{dV}{dx} = 0\,, \qquad n(x) = n_0 \cdot e^{V(x)/\Phi_t}\,. \quad (1b)$$

For the sake of simplicity one dimensional problem is considered, $V(x)$ and Φ_t denote electrostatic and thermal potential respectively. The obtained result (1b) is usually explained as a consequence of the fact that carriers obey Maxwell-Boltzman statistics.

If quantum effects were included, it should be done obeying the principles of quantum statistics. According to the widely accepted quantum mechanical procedure, the equation of motion of density matrix is written [1]. After ensemble averaging the moment equations system is constructed. Assuming diagonal representation of density matrix operator and giving physical meaning to corresponding moments, the final system of equations, describing the most general quantum transport, is obtained [2]. The entire system will not be written here, except the equation which has drawn our attention [3]:

$$k \cdot T \cdot \frac{dn}{dx} + n \cdot \frac{d}{dx}(U + Q) = 0\,, \qquad (2a)$$

$$Q(x) = -\frac{\hbar^2}{2m^*} \cdot \frac{1}{\sqrt{n}} \cdot \frac{d^2\sqrt{n}}{dx^2}\,. \qquad (2b)$$

The obtained expression $Q(x)$ denotes quantum correction (to the electrostatic potential energy). Its shape suggests its strong influence in the region where the concentration abruptly changes (as usually happens in semiconductor samples) [2]. The equation (2a) also remiinds very much of the equation (1a) and can be rewritten as:

$$\Phi t \cdot \frac{dn}{dx} - n \cdot \frac{d}{dx}\{V(x) + q(x)\} = 0\,,\ Q(x) = -e \cdot q(x), \quad (3a)$$

$$q(x) = \frac{\hbar^2}{2m^* \cdot e} \cdot \frac{1}{\sqrt{n}} \cdot \frac{d^2\sqrt{n}}{dx^2}\,. \qquad (3b)$$

The integration of equation (3a) is straightforward. Its shape reminds very much of Boltzman distribution, although it has nothing to do with it:

$$n(x) = n_0 \cdot e^{\{V(x)+q(x)\}/\Phi_t}\,. \qquad (4)$$

Parameter n_0 is governed by boundary conditions and the nature of investigated device. The shape of equation (4) explicitely exibits the influence of "quantum potential $q(x)$". The equations (3a) and (3b) are coupled; therefore it is useful to put aside $q(x)$. After simple, but tedious procedure, a nonlinear second order differential equation with respect to carriers' concentration $n(x)$ is obtained [4]:

$$\frac{d^2n}{dx^2} - \frac{1}{2n}\left(\frac{dn}{dx}\right)^2 + \frac{4m^* e}{\hbar^2} \cdot n(x) \cdot \left\{V(x) - \Phi_t \cdot \ln\frac{n(x)}{n0}\right\} = 0\,. \quad (5)$$

The electrostatic potential $V(x)$, which obeys Poisson's equation, strongly governes the solution of equation (5), but that's beyond the scope of our investigation. Our goal is to consider simple shapes of $V(x)$ and thus reproduce the most frequent practical problems in order to investigate what the implications of equation (5) suggest [6].

3. Testing of the model in some interesting problems

I) One of first interesting questions is to find the solutions suggested by equation (5) in the absence of external voltage $V(x)$. Therefore, unintentionally p-doped semiconductor sample of large dimensions (far exceeding tens of nanometers), which abruptly ends in the plane x=0, is considered:

$$\frac{d^2n}{dx^2} - \frac{1}{2n} \cdot \left(\frac{dn}{dx}\right)^2 - \frac{4m^* \cdot e}{\hbar^2} \cdot \Phi_t \cdot n(x) \cdot \ln\frac{n(x)}{n_0} = 0\,. \quad (6)$$

There are also two boundary conditions to be satisfied in order to specify the problem:

$$n(0) = 0\,, \qquad \lim_{x \to +\infty} n(x) = n_0 = N_A \cdot e^{-2\Phi_F/\Phi_t}\,. \quad (7)$$

The first one is imposed "by hand" and denotes the border of the sample (infinite barrier height). The second one represents the fact that far from this border concentration reduces to its "bulk" value; the solution of (6) can be obtained as follows:

$$\frac{dn}{dx} = \sqrt{z(x)}\,, \qquad n(x) = n_0 \cdot \tilde{n}(x) \qquad (8)$$

what gives:

$$\frac{dz}{d\tilde{n}} - \frac{1}{\tilde{n}} \cdot z - \frac{8m^* \cdot e}{\hbar^2} \cdot \Phi_t \cdot \tilde{n} \cdot \ln\tilde{n} = 0\,. \qquad (9)$$

New parameter with the dimension of length should be introduced:

$$\lambda = \sqrt{\frac{\hbar^2}{8m^* \cdot e \cdot \Phi_t}}\,. \qquad (10)$$

This parameter is intended to show how deep quantum effects (edge effects) penetrate into "bulk". The equation (9) becomes:

$$\frac{dz}{d\tilde{n}} - \frac{1}{\tilde{n}} \cdot z - \frac{\tilde{n}}{\lambda^2} \cdot \ln \tilde{n} = 0 . \tag{11}$$

Its solution is known in the literature:

$$z(\tilde{n}) = \tilde{n} \cdot \left\{ C + \frac{\tilde{n} \cdot \ln \tilde{n} - \tilde{n}}{\lambda^2} \right\}. \tag{12}$$

If the modified boundary conditions (8):

$$\lim_{x \to +\infty} \tilde{n}(x) = 1 \quad \text{and} \quad z(1) = 0 \tag{13}$$

are imposed, the equation (12) becomes:

$$z(\tilde{n}) = \frac{\tilde{n}}{\lambda^2} \cdot \{1 + \tilde{n} \cdot \ln \tilde{n} - \tilde{n}\}, \tag{14}$$

or:

$$\frac{d\tilde{n}}{dx} = \frac{1}{\lambda} \cdot \sqrt{\tilde{n}(1 + \tilde{n} \cdot \ln \tilde{n} - \tilde{n})} . \tag{15}$$

This equation must be integrated numerically; but for our purpose it's quite satisfactory to introduce the approximation:

$$\tilde{n} \cdot (1 + \tilde{n} \cdot \ln \tilde{n} - \tilde{n}) \approx 0.7(1 - \tilde{n})^2 \cdot \tilde{n} . \tag{16}$$

Now, the equation (15) is easily integrated:

$$\tilde{n}(x) = \frac{\left(e^{\frac{\sqrt{0.7} \cdot x}{\lambda}} - 1 \right)^2}{\left(e^{\frac{\sqrt{0.7} \cdot x}{\lambda}} + 1 \right)^2}, \tag{17a}$$

or:

$$n(x) = N_A \cdot e^{-2\Phi_F / \Phi_t} \cdot \frac{\left(e^{\frac{\sqrt{0.7} \cdot x}{\lambda}} - 1 \right)^2}{\left(e^{\frac{\sqrt{0.7} \cdot x}{\lambda}} + 1 \right)^2} . \tag{17b}$$

The parameter λ is given in Table 1 for several various semiconductor materials and two typical values of temperature (T = 300 K, T = 77 K). The distinction between various semiconductor materials is introduced through their effective masses.

Table 1. Values of λ-parameter for various semiconductor materials and typical temperatures.

Material m^*/m_0	Si 0.41/0.29	GaN 0.20	GaAs 0.067	InAs 0.022
T=300 K	λ=0.946 nm λ=1.130 nm	λ=1.354 nm	λ=2.35nm	λ=4.093nm
T=77 K	λ=1.830 nm λ=2.23 nm	λ=2.67 nm	λ=4.54nm	λ=8.080nm

Without quantum correction in equation (5) no boundary condition can be imposed. The λ-parameter explicitely shows the depth of penetration of quantum (edge) effects into "bulk". Also the hierarchy among various semiconductor materials with respect to quantum effects is restored (Fig. 1. – at least in Si, more in GaN, even more in GaAs and most in InAs). The smaller effective mass, the bigger value of λ-parameter, so quantum effects penetrate deeper into "bulk". The same holds for temperature - lower value causes the increase of λ-parameter and more expressed quantum effects.

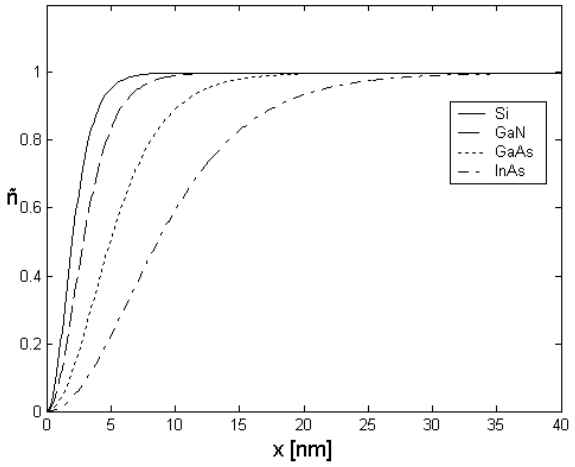

Fig. 1. The evaluated profile of carriers' concentration for various semiconductors.

It is possible to determine "semi-penetration length", i. e. distance from the border where the concentration is half of that in the "bulk". It is clear from Table 1 that all these lengths are of the order on nm, i. e. for samples of corresponding dimensions quantum-mechanical treatment becomes necessary.

II) The other case to be discussed here should give more realistic character to the structure described in the

previous section. It will be investigated what kind of solution is suggested by this model in the presence of external voltage. If the border (plane x=0) is subject to positive voltage bias V_0 (referent level is far in the "bulk"), the following spatial dependence of electrostatic potential in the structure is expected [7]:

$$V(x) = V_0 \cdot e^{-\alpha \cdot x}, \quad \alpha > 0, \tag{18}$$

what, together with the starting equation, gives:

$$\frac{d^2\tilde{n}}{dx^2} - \frac{1}{2\tilde{n}} \cdot \left(\frac{d\tilde{n}}{dx}\right)^2 + \frac{4m^* \cdot e}{\hbar^2} \cdot \tilde{n}(x) \cdot \left\{V_0 \cdot e^{-\alpha \cdot x} - \Phi_t \cdot \ln \tilde{n}(x)\right\} = 0 \cdot \tag{19a}$$

$$n(x) = N_A \cdot e^{-2\Phi_F / \Phi_t} \cdot \tilde{n}(x), \lim_{x \to +\infty} \tilde{n}(x) = 1. \tag{19b}$$

The goal of this paper is only to discuss asymptotic behaviour of the solution of equation (19a), whose following form is assumed:

$$\tilde{n}(x) = 1 + K \cdot e^{-\beta \cdot x}, \beta > 0. \tag{20}$$

Together with the substitutions:

$$\lambda^2 = \frac{\hbar^2}{8m^* \cdot e \cdot \Phi_t}, V_0 = \Phi_t \cdot \tilde{V}_0, \tag{21}$$

the equation (19a) becomes:

$$\frac{d^2\tilde{n}}{dx^2} - \frac{1}{2\tilde{n}} \cdot \left(\frac{d\tilde{n}}{dx}\right)^2 + \frac{\tilde{n}(x)}{2\lambda^2} \cdot \left\{\tilde{V}_0 \cdot e^{-\alpha \cdot x} - \ln \tilde{n}(x)\right\} = 0 \cdot \tag{22}$$

Combining expressions (18), (20) and (22) and considering only first order terms containing $e^{-\alpha x}$, $e^{-\beta x}$ (terms containing $e^{-2\alpha x}$, $e^{-2\beta x}$, $e^{-(\alpha+\beta)x}$ are of higher order and therefore neglected) the interesting conclusion is obtained:

$$\beta^2 \cdot K \cdot e^{-\beta \cdot x} + \frac{\tilde{V}_0}{2\lambda^2} \cdot e^{-\alpha \cdot x} - \frac{K}{2\lambda^2} \cdot e^{-\beta \cdot x} \cong 0, \tag{23}$$

and:

$$\alpha = \beta, \tag{24a}$$

$$K = \frac{\tilde{V}_0}{1 - 2\lambda^2 \cdot \alpha^2}. \tag{24b}$$

To include higher order terms the assumptions (18) and (20) are not sufficient and they have to be modified. But the mentioned assumptions permit some qualitative conclusions.

1. $2\lambda^2 \cdot \alpha^2 > 1 \Rightarrow \alpha > \frac{1}{\lambda \cdot \sqrt{2}} \Rightarrow \quad e^{-\alpha \cdot x} < e^{-\frac{x}{\lambda \cdot \sqrt{2}}}$

The potential decreases faster than the penetration of quantum effects occurs and therefore K<0. Therefore is $\tilde{n}(x)$ smaller than its asymptotic value in the whole $x \geq 0$ range (Fig. 2. curve a).

2. $2\lambda^2 \cdot \alpha^2 < 1 \Rightarrow \alpha < \frac{1}{\lambda \cdot \sqrt{2}} \Rightarrow \quad e^{-\alpha \cdot x} > e^{-\frac{x}{\lambda \cdot \sqrt{2}}}$,

The potential decreases slowlier than the penetration of quantum effects occurs and K>0; far away from the border concentration decreases to unity ($\tilde{n}(x) \to 1^+$). It actually means that the region exists where the concentration exceeds its "bulk" value. Due to the boundary condition $\tilde{n}(0)$=0, concentration has a shape shown in Fig. 2. curve b; i. e. in the vicinity of the border conduction channel with the considerably increased carriers concentration is formed, as expected from theoretical and practical knowledge concerning unipolar devices [5].

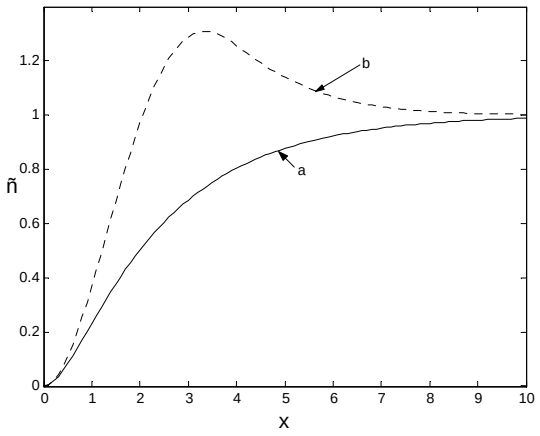

Fig. 2. Normalized concentration for V_0>0 external bias. A qualitative picture.

It is worth mentioning that the channel creation is not exclusively governed by the magnitude of applied voltage, but also depends on α-parameter. Therefore it is more accurate to conclude that the conditions of channel creation mostly depend on quantum well profile, i. e. on the quasi-electric field strength [6].

III) In this section the described aproach is applied to the problem of carriers contained in a quantum well of finite width (2L) with infinite barrier heights and zero potential energy inside. The equation to be solved inside the quantum well is the same as in problem I, but with different boundary conditions (the concentration $n(x)$ is an even function with respect to the center of the well, so only the region $x \geq 0$ will be considered):

$$\frac{d^2n}{dx^2}-\frac{1}{2n}\cdot\left(\frac{dn}{dx}\right)^2-\frac{4m^*\cdot e}{\hbar^2}\cdot\Phi_t\cdot n(x)\cdot\ln\frac{n(x)}{n_0}=0\,. \quad (25a)$$

$$n(L)=0\,,\left.\frac{dn}{dx}\right|_0=0\,. \quad (25b)$$

One of the interesting features of equation (25a) is that it can be normalized by an arbitrary value n_0 and modified into dimensionless form:

$$\frac{d^2\tilde{n}}{dx^2}-\frac{1}{2\tilde{n}}\cdot\left(\frac{d\tilde{n}}{dx}\right)^2-\frac{\tilde{n}\cdot\ln\tilde{n}}{\lambda^2}=0\,, \quad (26a)$$

$$n(x)=n_0\cdot\tilde{n}(x)\,, \quad (26b)$$

with modified boundary conditions too:

$$\tilde{n}(L)=0\,,\left.\frac{d\tilde{n}}{dx}\right|_0=0\,. \quad (27)$$

The boundary condition (26b) is expected because it enables the evaluation for an arbitrary amount of carriers in the quantum well. Together with the mentioned ones it is suitable to introduce an additional boundary condition (due to a special constraint, as explained later):

$$\tilde{n}(0)=p<1\,. \quad (28)$$

The solution of (26a) is analytical, as mentioned before:

$$\left(\frac{d\tilde{n}}{dx}\right)^2=\frac{\tilde{n}}{2\lambda^2}\cdot\{C+\tilde{n}\cdot(\ln\tilde{n}-1)\}\,, \quad (29)$$

what together with (27) gives:

$$\left(\frac{d\tilde{n}}{dx}\right)^2=\frac{\tilde{n}}{2\lambda^2}\cdot\{\tilde{n}\cdot(\ln\tilde{n}-1)-p\cdot(\ln p-1)\}\,, \quad (30)$$

under the expectation $\tilde{n}(x)\le p$, $\forall x$. The equation (30) can be rewritten as follows:

$$\frac{d\tilde{n}}{dx}=-\frac{1}{\lambda\cdot\sqrt{2}}\cdot\sqrt{\tilde{n}\cdot\{\tilde{n}\cdot(\ln\tilde{n}-1)-p\cdot(\ln p-1)\}}\,,\quad x\in[0;L]. \quad (31)$$

If our goal is to avoid numerical integration of (31), in the region $0.5<p<1$, the following approximation works:

$$\frac{d\tilde{n}}{dx}=-\frac{2}{\lambda\cdot\sqrt{2}}\cdot\sqrt{\tilde{n}\cdot\left\{\sqrt{p\cdot(2-p)}-\frac{\tilde{n}}{\sqrt{p\cdot(2-p)}}\right\}^2}\,. \quad (32)$$

The integration of the equation (32), together with the boundary condition (27), is straightforward:

$$\tilde{n}(x)=p\cdot(2-p)\cdot\frac{\left(e^{\frac{L-x}{\lambda\cdot\sqrt{2}}}-1\right)^2}{\left(e^{\frac{L-x}{\lambda\cdot\sqrt{2}}}+1\right)^2}\,. \quad (33)$$

The previously mentioned constraint with respect to p is the equation (28) and is used to extract p:

$$p=2-\frac{\left(e^{\frac{L}{\lambda\cdot\sqrt{2}}}+1\right)^2}{\left(e^{\frac{L}{\lambda\cdot\sqrt{2}}}-1\right)^2}\,. \quad (34)$$

Obviously $p<1$ is satisfied; the other condition $p>0.5$ implies:

$$L\ge 2.3\sqrt{2}\lambda=3.25\lambda\,,2L\ge 6.25\lambda\,. \quad (35)$$

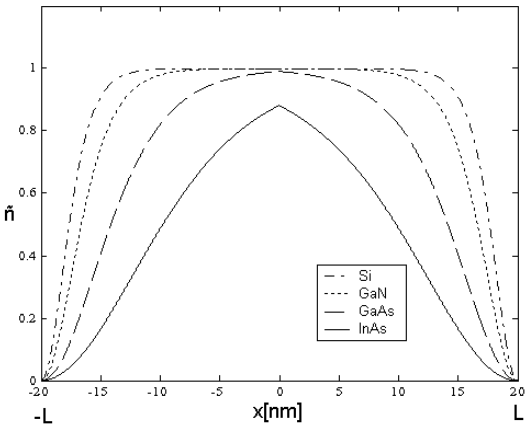

Fig. 3. Carriers' concentration profile in quantum well with infinite barrier height for various semiconductor materials.

i.e. the minimal width of quantum well surely exists, if our goal is to safely use approximation (32). Numerical results are exposed in Table 2. For smaller values of quantum well width, the integration of equation (31) must be performed numerically.

Table 2. Minimal quantum well width for various semiconductor materials.

Material	Si	GaN	GaAs	InAs
$(2L)_{min}$	6.15 nm	8.80 nm	15.28 nm	26.60 nm

In Fig. 3 the concentration profiles in one-dimensional quantum well, for various semiconducor materials, at room temperature T=300 K, are shown. Only if InAs quantum well of investigated width is considered, the approximation (32) must be slightly improved (extremely strong quantum effects).

4. Conclusions

The suggested approach was successful in fulfilling the goals described in Introduction (natural connection between different sections of semiconductor sample, as well as the application of tools of quantum statistical physics). The successful estimation how deep quantum effects penetrate into semiconductor sample has also been performed (several tens of nm), together with the established hierarchy among various materials with respect to the outstanding appearence of quantum effects (at least in Si, more in GaN, even more in GaAs, most in InAs). It was also confirmed that quantum effects were stronger at lower temperatures than at higher ones (approximately twice stronger at T=77 K than at T=300 K). It is also interesting to pay attention to the former statement that quantum effects become prominent if the sample dimensions are of the order of de Broglie thermal length λ_D [3]. The thermal de Broglie length is approximately ten times bigger than λ (penetration length introduced in this paper), what very well coincides with our estimation $(2L)_{min} \approx 6.5\lambda$.

Described approach is of great theoretical significance. The expression (4) is very similar to the classical one, and the only difference is expressed by a term generating quantum correction. The equation (5) may be solved together with the Poisson's one in a self-consistent procedure, where the solution of problem I can be considered starting itteration.

References

[1] G. J. Iafrate, H. L. Grubin, D. K. Ferry, J. Phys. (Orsay, Fr) **42**, C7 – 307 (1981).
[2] C. Philippidis, D. Bohm, R. D. Kaye – Nuovo Cimento Soc. Ital. Fis. B [11], 71B, 75 (1982).
[3] Cheng T. Wang, Introduction to Semiconductor Technology – GaAs and Related Compounds, John Wiley & Sons, pp. 1– 26 (1990).
[4] R. Šašić, R. Ramović, D. Tjapkin, A Simple 2D Analytical Model of HEMT – Proceedings of MIEL '95, pp. 709– 712 (1995).
[5] Patric Roblin, Hans Rohdin, High-speed heterostructure devices – Cambridge University Press, Cambridge, U. K. (2002).
[6] R. Šašić, D. Čevizović, R. Ramović, Influence of the Semiconductor Doping Level on the Carrier Surface Density in AlGaN/GaN MODFET Channel – Materials Science Forum, **413**, 39-44 (2003).
[7] P. M. Lukić, R. M. Ramović, R. M. Šašić, J. Optoelectron. Adv. Mater. **7**(3), 1911-1618 (2005).

*Corresponding author: ramovic@etf.bg.ac.yu