Perturbation Theory Methods for the Semiconductor Plasma Diode Simulation

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***Abstract* — A technique for solving a nonlinear singularly perturbed boundary value problem of predicting the state of an electron-hole plasma in the active region of p-i-n (plasma) diodes is considered. The problem is formulated for system of equations of the electron and hole currents continuity and the Poisson's equation. The solution to the problem is sought by the asymptotic method of boundary corrections. It is shown that boundary corrections play a key role in forming the electric field in the active region of the diode. Under certain conditions, boundary corrections demonstrate non-monotonic behavior. The presence of boundary corrections makes it possible to solve problems of heat distribution in the semiconductor device under study, problems of the influence of external electromagnetic fields on electron-hole plasma, etc. A series of computer experiments were conducted.**

***Keywords*— perturbation method, singularly perturbed boundary value problem, asymptotic series, boundary function, p-i-n-diode.**

I. Introduction

One of the common methods for modeling the physical properties of semiconductor devices is to solve a system of equations for the continuity of diffusion-drift, recombination of the charge carriers currents and the Poisson`s equation with corresponding boundary and initial conditions to obtain information about the distribution of charge carriers ($n(\vec{r},t)$, $p(\vec{r},t)$, $\vec{r}$ is the spatial coordinates vector, t – time) and potential ($\varphi(x,t)$) in a certain active region of the device [1,2]. This systems of equations have a number of common properties, in particular: 1) they are nonlinear; 2) in normalized form the corresponding problems are singularly perturbed. These circumstances prompt the decision to involve the boundary function method [3-6] of perturbation theory [7,8] as instrumental tools.

The **purpose** of the paper to demonstrate the effectiveness of using the method of boundary functions of perturbation theory in a systematic approach to solving problems of semiconductor electronics using the example of a plasma diode.

II. Basis mathematical model of the studied system.

The operation of a semiconductor p-i-n-diode is based on the ability to control the conductivity of an electron-hole plasma formed in the active region (i-region) of such a device. The general formulation of the problem of modeling physical processes in the active region of the p-i-n-diode is as follows [1]:

$$-\frac{1}{e}\vec{\nabla}\cdot\vec{j}_p - R_p + G_p = 0\,,\quad \frac{1}{e}\vec{\nabla}\cdot\vec{j}_n - R_n + G_n = 0\,, \qquad (1)$$

$$\vec{j}_p = -e\mu_p p\vec{\nabla}\varphi - eD_p\vec{\nabla}p\,,\quad \vec{j}_n = -e\mu_n n\vec{\nabla}\varphi + eD_n\vec{\nabla}n\,,$$

$$div\left(\vec{\nabla}\varphi\right) = -e\left(p - n + N_d\right),$$

where $\vec{j}_p$, $\vec{j}_n$ are the holes and electrons current densities consisting of drift and diffuse components; N_d is a given function of the doping profile of the semiconductor material with impurities (donors or acceptors); e is the electron charge; D_p, D_n are the holes and electrons diffusion coefficients; , are the charge carrier mobilities; R_p, R_n, G_p, G_n are the recombination and generation rates of charge carriers respectively. The system of equations (1) is supplemented by the corresponding boundary and initial conditions.

In simplified case the mathematical model of electron-hole plasma description in the active region of a p-i-n-diode (only by one spatial coordinate - the case is typical for bulk diodes, $V = \{(x): 0 < x < w\}$) has the following form:

$$\begin{cases} \mu^2 \dfrac{\partial E}{\partial x} = -(p-n), \\ B_n \dfrac{\partial n}{\partial t} = \dfrac{\partial^2 n}{\partial x^2} + \dfrac{\partial n}{\partial x} E + n \dfrac{\partial E}{\partial x} - A_n n, \\ B_p \dfrac{\partial p}{\partial t} = \dfrac{\partial^2 p}{\partial x^2} - \dfrac{\partial p}{\partial x} E - p \dfrac{\partial E}{\partial x} - A_p p. \end{cases} \tag{2}$$

Independent variables x, t and unknown functions $E(x,t) = -\frac{d}{dx}\varphi(x,t)$, $n(x,t)$, $p(x,t)$ in the system of equations (2) are presented in normalized form – $\tilde{x} = \frac{x}{w}$ ($\tilde{x} \in [0,1]$), $\tilde{t} = \frac{t}{T}$ ($\tilde{t} \in [-\infty, \infty]$, periodic process: T is the period of the process), $\tilde{\varphi}(\tilde{x},\tilde{t}) = \frac{e\varphi(x,t)}{kQ_0}$, $\tilde{n}(\tilde{x},\tilde{t}) = \frac{n(x,t)}{N_i}$, $\tilde{p}(\tilde{x},\tilde{t}) = \frac{p(x,t)}{N_i}$ (the sign "~" is omitted from now on). Also in (1) the following notation is used: $\mu^2 = \frac{\varepsilon\varepsilon_0\kappa Q_0}{e^2 w N_i}$ (small parameter $\mu^2 \sim 10^{-4} \div 10^{-6}$); Q_0 – temperature (300º K); κ – Boltzmann constant; ε – relative dielectric constant; ε_0 – electrical constant; w is the characteristic size of the active region of the diode; N_i – constant, which determines the concentration of charge carriers in the intrinsic semiconductor, depends on the selected semiconductor material; $A_n = w^2 / D_n \tau_n^*$; $A_p = w^2 / D_p \tau_p^*$; D_n, D_p are the diffusion coefficients of electrons and holes, respectively; τ_n^*, τ_p^* - characteristic times of recombination of electrons and holes; $B_n = w^2 / D_n T$; $B_p = w^2 / D_p T$.

At the boundaries $x=0$ and $x=1$ under the action of the applied current and potential difference, charge carriers are injected into the active region. The injected flow has a diffusion character and its formation is influenced by the processes of surface recombination of electrons and holes. Used are boundary conditions of the form [1]:

$$\left.\frac{\partial n}{\partial x} - \gamma_n w n\right|_{x=0} = \frac{J(t)}{eD_n}\frac{w}{N_i}, \quad \left.-\frac{\partial p}{\partial x} - \gamma_p w p\right|_{x=0} = 0, \tag{3}$$

$$\left.\frac{\partial p}{\partial x} + \gamma_p w p\right|_{x=1} = -\frac{J(t)}{eD_p}\frac{w}{N_i}, \qquad \left.\frac{\partial n}{\partial x} - \gamma_n w n\right|_{x=1} = 0 ,$$

$$E\big|_{x=0} = 0 , \quad E\big|_{x=1} = 0 , \quad \int_0^1 E(x,t)\,dx = U(t),$$

where $J(t)$, $U(t)$ are specially specified periodic functions that determine the current density and voltage of the control signal, respectively, γ_n , γ_p - recombination coefficients of charge carriers at the contacts.

Note that the given problem is a non-linear non-stationary singularly perturbed boundary value problem of mathematical physics without initial conditions.

III. Asymptotics of the problem solution

To solve the problem, we successively use the method of boundary corrections of perturbation theory [3-8] and the Fourier method of separating variables. Guided by the methodology developed in the works [3,9], we propose to look for a solution in the following form:

$$\begin{aligned} n(x,t) &= N(x,t) + \underline{N}(\underline{\xi},t) + \overline{N}(\overline{\xi},t), \\ p(x,t) &= P(x,t) + \underline{P}(\underline{\xi},t) + \overline{P}(\overline{\xi},t), \\ E(x,t) &= \tilde{E}(x,t) + \underline{E}(\underline{\xi},t) + \overline{E}(\overline{\xi},t), \end{aligned} \tag{4}$$

where $N(x,t)$, $P(x,t)$, $\tilde{E}(x,t)$ are the regular components of the solution, which are presented in the form of asymptotic series in powers of the small parameter; $\underline{N}(\underline{\xi},t)$, $\underline{P}(\underline{\xi},t)$, $\underline{E}(\underline{\xi},t)$, $\overline{N}(\overline{\xi},t)$, $\overline{P}(\overline{\xi},t)$, $\overline{E}(\overline{\xi},t)$ - boundary corrections, respectively, in the vicinity of points $x=0$ and $x=1$ ($\underline{\xi} = x/\mu$, $\overline{\xi} = (1-x)/\mu$ - regularizing stretches), which are also given in the form of corresponding asymptotic series ($R_{E(s)}(x,t,\mu)$, $R_{n(s)}(x,t,\mu)$, $R_{p(s)}(x,t,\mu)$ - residual terms):

$$\begin{pmatrix} n(x,t) \\ p(x,t) \\ E(x,t) \end{pmatrix} = \begin{pmatrix} \sum_{i=0}^{s} \mu^i n_i \\ \sum_{i=0}^{s} \mu^i p_i \\ \sum_{i=0}^{s} \mu^i E_i \end{pmatrix} + \begin{pmatrix} \sum_{i=0}^{s} \mu^i \underline{N}_i \\ \sum_{i=0}^{s} \mu^i \underline{P}_i \\ \sum_{i=-1}^{s} \mu^i \underline{E}_i \end{pmatrix} + \begin{pmatrix} \sum_{i=0}^{s} \mu^i \overline{N}_i \\ \sum_{i=0}^{s} \mu^i \overline{P}_i \\ \sum_{i=-1}^{s} \mu^i \overline{E}_i \end{pmatrix} + \begin{pmatrix} R_{n(s)} \\ R_{p(s)} \\ R_{E(s)} \end{pmatrix} . \tag{5}$$

Similarly to [5, 10], by sequentially substituting (4) and (5) into the system of equations (2), boundary conditions (3) and grouping regular component equations, corresponding boundary corrections, and equating coefficients with the same powers of the small parameter, we obtain the following sequence of tasks (for leading terms of asymptotics):

$$\begin{cases} p_0(x,t) - n_0(x,t) = 0, \\ \dfrac{\partial^2 n_0(x,t)}{\partial x^2} - A_n n_0(x,t) - B_n \dfrac{\partial n_0(x,t)}{\partial t} = -\dfrac{\partial}{\partial x}\big(n_0(x,t) E_0(x,t)\big), \\ \dfrac{\partial^2 p_0(x,t)}{\partial x^2} - A_p p_0(x,t) - B_p \dfrac{\partial p_0(x,t)}{\partial t} = \dfrac{\partial}{\partial x}\big(p_0(x,t) E_0(x,t)\big), \end{cases}$$

$$\left.\frac{\partial n_0(x,t)}{\partial x} - \gamma_n w n_0(x,t)\right|_{x=0} = \frac{J(t)}{eD_n}\frac{w}{N_i}, \tag{6.1}$$

$$\left.-\frac{\partial p_0(x,t)}{\partial x} - \gamma_p w p_0(x,t)\right|_{x=1} = \frac{J(t)}{eD_p}\frac{w}{N_i},$$

$$\left.-\frac{\partial p_0(x,t)}{\partial x} - \gamma_p w p_0(x,t)\right|_{x=0} = 0, \quad \left.\frac{\partial n_0(x,t)}{\partial x} - \gamma_n w n_0(x,t)\right|_{x=1} = 0;$$

$$\begin{cases} \dfrac{d\underline{E}_{-1}\left(\underline{\xi},t\right)}{d\underline{\xi}} = \underline{P}_0\left(\underline{\xi},t\right) - \underline{N}_0\left(\underline{\xi},t\right), \\ \dfrac{d^2\underline{N}_0\left(\underline{\xi},t\right)}{d\underline{\xi}^2} = -\dfrac{d}{d\underline{\xi}}\left(\left(n_0\left(0,t\right) + \underline{N}_0\left(\underline{\xi},t\right)\right)\underline{E}_{-1}\left(\underline{\xi},t\right)\right), \\ \dfrac{d^2\underline{P}_0\left(\underline{\xi},t\right)}{d\underline{\xi}^2} = \dfrac{d}{d\underline{\xi}}\left(\left(p_0\left(0,t\right) + \underline{P}_0\left(\underline{\xi},t\right)\right)\underline{E}_{-1}\left(\underline{\xi},t\right)\right), \end{cases} \qquad (6.2)$$

$$\lim_{\underline{\xi}\to\infty}\underline{E}_{-1}\left(\underline{\xi},t\right) = E^*\left(U\left(t\right)\right), \quad \left.\frac{d\underline{N}_0\left(\underline{\xi},t\right)}{d\underline{\xi}}\right|_{\underline{\xi}=0} = 0,$$

$$\lim_{\underline{\xi}\to\infty}\underline{N}_0\left(\underline{\xi},t\right) = 0, \quad \left.\frac{d\underline{P}_0\left(\underline{\xi},t\right)}{d\underline{\xi}}\right|_{\underline{\xi}=0} = 0, \quad \lim_{\underline{\xi}\to\infty}\underline{P}_0\left(\underline{\xi},t\right) = 0 .$$

The formulation of the problem for determining the characteristics of the volume charge in the vicinity of the point $x=1$ is similar to (6.2).

Note, that leading terms of the asymptotics (zero) make the main contribution to the problem solution Problems. Problem statements for the first and following members of the asymptotics have a similar form.

An important feature of this approach to modeling physical processes in a p-i-n diode is the ability to separate it into components that are convenient to interpret. For example, the system of equations (6.1) is easily reduced to the classical equation of ambipolar diffusion [1], which explains the formation of electron-hole plasma in the active region of a p-i-n diode and the appearance of an active component of impedance. Solutions to the system of equations (6.2) (first obtained in [9]) model the behavior of charge carriers in the zones of n-i, p-i contacts (space charge regions), which determine the reactive component of impedance, the distribution of electric field components in the system under study, and the mechanisms of thermal heating.

It was found that under certain conditions, the boundary functions demonstrate non-monotonic behavior (experimental fact), the theoretical description of which is not reflected in the literature. This issue remains to be studied in detail.

It should be noted that the algorithm for solving the problem using the asymptotic method is an example of the application of general system methods for studying complex systems – decomposition and synthesis. This is already evident at the level of solving the basic problem (1). When calculating, for example, temperature fields, the basic system of equations must be supplemented with the heat conductivity equation; when considering the processes of influence of external electromagnetic fields on the state of plasma – with the system of Maxwell equations. Separately, it is necessary to note the complication of the basic model in cases of solving the corresponding problems in areas of complex geometry or conducting optimization measures. Accordingly, the construction and use of a mathematical model of a p-i-n diode must be carried out using methods of system analysis.

IV. Analysis of results and conclusions

From the standpoint of the system approach, it is necessary, in particular, to determine the goals of modeling and, accordingly, select the components of the mathematical model that forms the network structure (Fig. 1), and assess the required level of adequacy of the results with the selected model layout.

Note that in each of the subproblems formed, it is possible to single out both singularly perturbed and regularly perturbed equations, which are solved using the corresponding asymptotic methods. In our opinion, in this case (solving problems of semiconductor electronics), the use of perturbation theory methods will be more effective than, for example, the use of computational methods. This conclusion is based on the fact that the sought functions in the boundary zones of the studied area have large gradients. As a result, the computational algorithm will be resource-intensive. In addition, some problems (similar to (6)) of the recurrent sequence of problems, which are obtained by perturbation theory methods, may have an exact analytical solution.

Несколько типичных модельных графиков распределений исследуемых характеристик в активной области структур показано на рис. 2-6 (заимствованы с работ [10-12]). Результаты получены на основе анализа базовой модельной задачи.

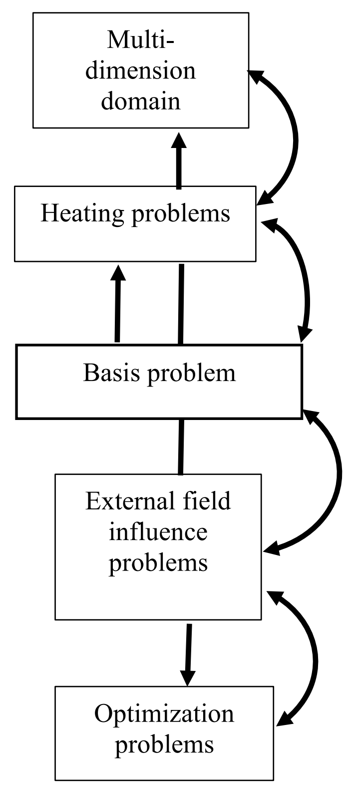


Fig. 1.

The technique of solving the nonlinear singularly perturbed boundary value problem of forecasting the state of electron-hole plasma in the active region of p-i-n (plasma) diodes, which is based on the use of asymptotic methods (in particular, the

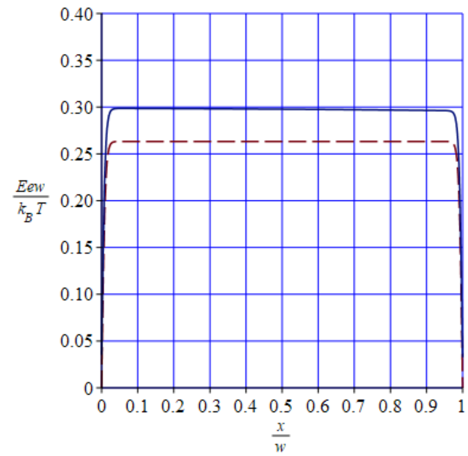


Fig. 2. Typical distribution of the electrostatic field strength in the active region of the p-i-n-diode (the total contribution of the main components of the regular component and boundary corrections is shown, stationary case)

boundary function method) has proven its effectiveness. If, with respect to the distribution of the concentration of charge carriers, the corrections are significant only in relatively narrow contact zones, then they play a key role in the formation of the electric field in the investigated region. The presence of boundary corrections to the electric potential distribution function provides the possibility of solving derivatives (to the basic) comple problems (for example, the problem of heat

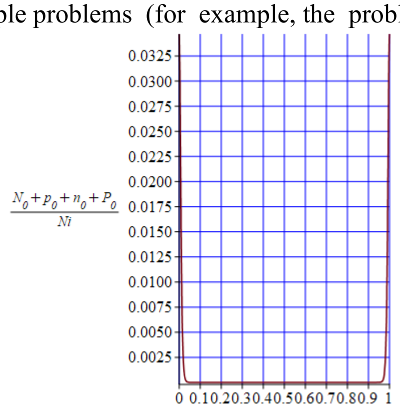


Fig. 3. Typical distribution of charge carrier concentration in the active region of the diode (the total contribution of the main components of the regular component and boundary corrections is shown, stationary case)

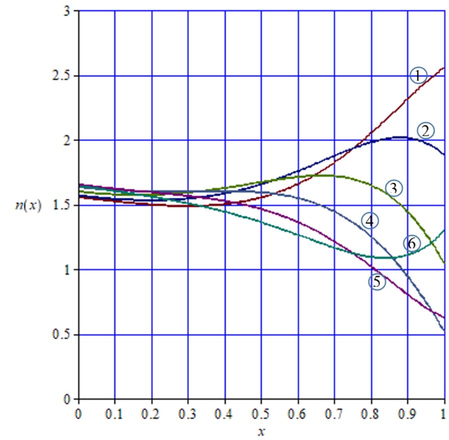
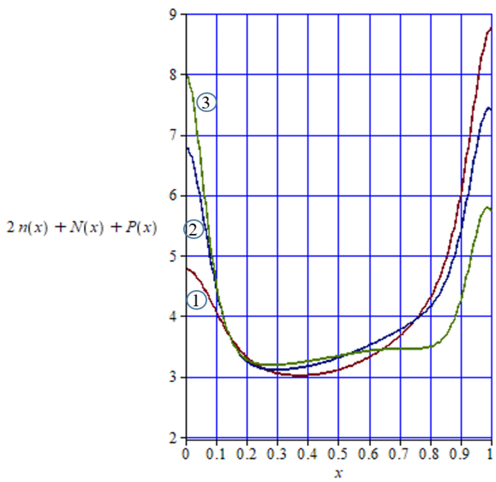


Fig. 4. Plasma concentration distributions in the diode active region in the development of the oscillatory process – regular parts of the asymptotics (1-0, 2-1/8T, 3-1/4T, 4-3/8T, 5-T/2, 6-5/8T)



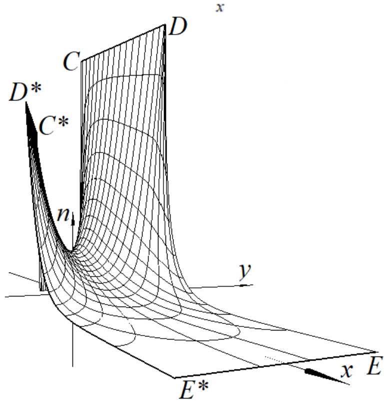


Fig. 6. Distribution of the concentration of charge carriers in the active region of the integrated p-i-n-structures (wedge-shaped contact region, stationary case)

distribution in the studied semiconductor device, the problem of the influence of external electromagnetic fields on electron-hole plasma, etc.). Boundary corrections play the role of connecting elements in the system of model problems.

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Fig. 5. The diode active region charge concentration distributions taking into account the boundary corrections in the oscillatory process development (1-0, 2-1/8T, 3-1/4T)

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