ON ONE METHOD OF SEMICONDUCTOR STRUCTURE CALCULATION

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At present the computer simulation of semiconductor structures is attracting a great deal of attention in connection with an intensive development of electronic engineering. Within the framework of this simulation, new efficient methods of solving the set of equations describing processes taking place in semiconductors are constantly being developed. One of the first and most efficiently described methods was method [1] later used by many authors with reference to various semiconductor systems. Nowadays there is a great amount of works dealing with both the One- (1D) and Two-dimensional(2D) calculations of a set of equations for holes and electrons and Poisson's equation for the electrostatic potential.

In the 1D case the system is written as follows:

$$\frac{dP}{dt} + \frac{1}{q}\frac{dJ_p}{dx} = - R \qquad (1)$$

$$\frac{dN}{dt} - \frac{1}{q}\frac{dJ_n}{dx} = - R \qquad (2)$$

$$\frac{d^2\varphi}{dx^2} = - \frac{4\pi q}{\varepsilon}(p-N+\Gamma) \qquad (3)$$

$$J_n = - q\mu_n N \frac{d\varphi}{dx} + qD_n \frac{dN}{dx} \qquad (4)$$

$$J_p = - q\mu_p P \frac{d\varphi}{dx} - qD_p \frac{dP}{dx} \qquad (5)$$

with the following boundary condition:

$$P(0)N(0) = P(1)N(1) = N_i^2; \Gamma(x) = N_d(x) - N_a(x);$$

$$\Gamma(0) + P(0) - N(0) = \Gamma(1) + P(1) - N(1) = 0 ;$$

$$\varphi(0) = V - \frac{kT}{q} \ln(P(0)/N_i); \varphi(1) = \frac{kT}{q} \ln(N(1)/N_i);$$

Here N,P - electron, hole concentrations; φ - electrostatic potential; $\Gamma(x)$ - doping function; q - electronic charge; J_n, J_p -hole and electron current densities; μ_p, μ_n - drift mobilities of holes and electrons; D_p, D_n - diffusion constants; R - recombinations rate; l - diode length; V - diode voltage; N_i - electron density of the intrinsic semiconductor; k - Boltzmann's constant; T - temperature; ε - dielectric constant; N_d , N_A - donor and acceptor concentrations.

The dependence of carrier mobility on the doping impurity concentration and the electric field was taken according to [1] , and the recombination rate was set proceeding from model [2] .

Previously various methods had been used when approximating the initial set (1)-(5) by the finite difference circuit. Thus, for example, the replacement of variables suggested in [4] was made in [3], and the problem was solved on an explicit circuit, whide, however, led to great restriction on the τ. In paper [5] when obtaining a finite difference analogue of continuity equations method [1] was used and, to solve them simultaneously with Poisson's equation, Newton's iteration method was used. The authors [6] proposed an iteration process based on the introduction of adjusting members into right and the left parts of the difference analogues of equations (1)-(3), allowing to reduce significantly the restriction by an integration step τ which is reduced to the form $4\pi\sigma\tau<1$ (where $\sigma = q(\mu_n N + \mu_p P)$ - conductance).

The present paper dwells upon an iteration method of solving the (1)-(5) set, which can be written as:

$$\frac{P^{i+1} - P_o}{\tau} + \frac{1}{q}\frac{dJ_p^*}{dx} = - R_o$$

$$\frac{N^{i+1} - N_o}{\tau} - \frac{1}{q}\frac{dJ_n^*}{dx} = - R_o$$

$$J_p^* = -q\mu_p^i P^{i+1} \frac{d\varphi^{i+1}}{dx} - q D_p^i \frac{dP^{i+1}}{dx}$$

$$J_n^* = -q\mu_n^i N^{i+1} \frac{d\varphi^{i+1}}{dx} + q D_n^i \frac{dN^{i+1}}{dx}$$

$$\sigma^* = q(\mu_n^i N^{i+1} + \mu_p^i P^{i+1}), \rho_o = \Gamma + P_o - N_o ;$$

$$\frac{d}{dx}(1+4\pi\tau\sigma^*)\frac{d\varphi^{i+1}}{dx} = - \frac{4\pi q}{\varepsilon}\rho_o + \frac{d}{dx}D_p^i \frac{dP^{i+1}}{dx} -$$

$$- \frac{d}{dx} D_n^i \frac{dN^{i+1}}{dx} \qquad (7)$$

Here i - iteration number, index "0" means that the corresponding variables are taken from the step prior in time. This method differs from those mentioned above in the fact that not Poisson's equation was used to find the electric field potential, but equation (7) which is the corollary of the set (1)-(5) [7]. A similar replacement was first used in the computer simulation of electric discharges in gas [8]. In going to the difference kind of continuity equations method [1] was used, It should be emphasised that to provide algorithm convergency the difference analogue of equation (7) should be an exact algebraic corollary of the difference continuity equations. At each time moment simultaneous iterations of continuity equations and equations for finding the potential (7) were made. Input from iterations was made when the following requirement was met:

$$\| \varphi^i + \frac{4\pi q}{\varepsilon} \rho^i \| \ll 1 \qquad (8)$$

The time-dependent step τ was automatically increased if requirement (8) was met under a given number of iterations (of the whole set of equations).

To control an accuracy of the algorithm described, calculations were made with decreasing the mesh step h_k, and particularly with increasing the number of meshpoints K_o along the space coordinate (from 60 to 120), changes in the steady-state current being less than 1%.

Besides, the case when diode potential equals zero was tested. Shifting the point of reading out the potential so that $\varphi(0) = 0$, one can express hole and electron concentrations as follows [9] :

$$P = N_a \cdot \exp(- \frac{q}{kT} \varphi)$$

$$N = N_d \cdot \exp(\frac{q}{kT} (\varphi - \varphi_b)), \quad \varphi_b = \varphi_n - \varphi_p$$

φ_n, φ_p - Fermi quasipotential for electrones and holes. Poisson's equation (3) takes the form:

$$\frac{1}{4\pi q} \varepsilon \frac{d^2\varphi}{dx^2} = - \rho(\varphi), \quad \rho(\varphi) = P - N + \Gamma \qquad (9)$$

It is difficult to solve this equation rigorously, and, since the electrostatic potential is known to have, in equilibrium, the configuration shown in Fig.1, this dependence was approximated by an expression:

$$\varphi(x) = (1 - 1/(1 + \exp(C(x - x_o)))) \cdot \varphi_b \qquad (10)$$

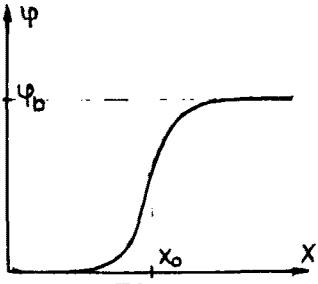

Fig.1

Substituting (10) into (9) and determining $\Gamma(x)$ we got an analytical solution for N, P, φ of the set (1)-(5), where x_o - midpoint of the diode. The results of the test calculations showed that the maximal difference between an analytical solution and a calculated one for N(x) and P(x) was less than 2% in the transition region and less than 10 % in the distribution tails(close to x=0 and x=1).

The test calculations assemblage demonstrated a satisfactory accuracy of the suggested algorithm for solving the set of equations (1)-(5), with the average solving time being 1.5-2 minutes of computer time on BECM-6 computer (at K_o=60 and the V=0.4 v). Transition parameters were taken from paper [3]

In the present paper a number of calculations were made aimed at choosing an algorithm for construction of a nonuniform mesh along the space coordinate. They showed that the best result was obtained on a nonuniform mesh with an automatic frequency control,i.d., a mesh thickening in the areas of steep density gradients of carriers. At the initial moment (t=0) a mesh thickening in the junction region was designated:

$$h_k = A(1- \exp(- C\cdot|x-x_o| -\mathcal{E}_2)),$$

where A - constant calculated from standardization; C, $\mathcal{E}_2$ - varied constants, determining the maximal and minimal step h_k. Then the mesh was constructing according to [10] at each moment of time. The reconstruction of the mesh was stopped as soon as a condition was reached:

$$\frac{1}{K_o}\left\{\sum_{K=0}^{K_o}\left(\frac{N_k^i - N_k^{i-1}}{\tau} + \frac{P_k^i - P_k^{i-1}}{\tau}\right)\right\} \ll 1$$

and after that calculations were made on the stationary nonuniform mesh up to reaching the steady state.

Comparison of the results of calculating the set of equation (1)-(5) on a nonuniform mesh and those on a uniform mesh with a large number of mesh points (K_o=120) showed that a significant reduction of the number of meshpoints on an nonuniform mesh was possible which slightly affected the accuracy of calculation of integral characteristics. Thus, with introduction of a nonuniform mesh with 40 mesh points, magnitude changes of the steady-state current were less than 0.5%, with K_o= 20 - $<$5%(V=0.4v).

One should point out the influence of doping impurity magnitudes (N_d and N_A) and applied potential V on the characteristics of the above mentioned algorithm and the choice of an irregular mesh.

Let's consider the case of a forward bias. The thickness of the barrier layer (for abrupt junction) can be written as:

$$L_o = \left(\frac{2\varepsilon}{q} (\varphi_c - V) \frac{N_d + N_a}{N_d N_a} \right)^{1/2} \qquad (11)$$

and electron, hole concentration on the barrier layer boundaries with P- and N-regions as:

$$N_p = N_{po} \cdot \exp\left(\frac{qV}{kT}\right), \quad P_n = P_{no} \cdot \exp\left(\frac{qV}{kT}\right), \qquad (12)$$

here N_{po}, P_{no} - equilibrium concentrations of minority carriers, $\varphi_c = kT \ln(N_d N_A / N_i^2)/q$ - contact potential. The holes which have drifted to the N-region, diffusing in-depth, recombine, on account of which their concentration decreases:

$$P_n(x) = P_{no} + P_{no}\left(\exp\left(\frac{qV}{kT}\right) - 1\right)\exp\left(-\frac{x - x_o}{L_p}\right), \text{ for } x > x_o$$

$$N_p(x) = N_{po} + N_{po}\left(\exp\left(\frac{qV}{kT}\right) - 1\right)\exp\left(\frac{x - x_o}{L_n}\right), \text{ for } x < x_o$$

Where $L_p = \sqrt{D_p \tau_p}$, $L_n = \sqrt{D_n \tau_n}$ (τ_p, τ_n - characteristic lifetimes of holes and electrones in the N- and P-regions accordingly).

From (11) and (12) one can see that with increasing the forward bias the injected carriers concentration grows sharply, and the barrier layer thickness decreases. Due to imposing an "ohmness" condition on the contacts for sufficiently high applied voltages ($V \sim \varphi_c$) in boundary regions at comparatively small intervals $\Delta x \ll 1$ great changes in minority carriers concentration are achieved (up to 10^{10}), i.e. the influence of boundaries is felt. The slowing down of the convergence rate in this case can be explained by the fact that at $V \to \varphi_c$ a significant contribution is made by higher harmonic of solution whose damping is going on at comparatively slower rates. It should be noted that the use of a nonuniform mesh, stationary throughout the stages of calculation, may lead to a significant error for the simple reason that at changing the magnitude of the applied voltage gradient regions of hole and electron densities, influencing significantly the steady-state solution, move along the X axis, whereas it is in those regions the maximal decreasing of step h_k should be achived. Note that a nonuniform stationary mesh is not applicable whatsoever in case of time-dependent boundary con-

dition. Besides, an algorithm for calculation of the set of equations(1)-(5) was considered, in which finite-difference analogues of continuity eigen equations for electrons and holes rather than method [1] were used to find N(x) and P(x):

$$\frac{dP}{dt} - \frac{d}{dx}\mu_p P \frac{d}{dx} - \frac{d}{dx}D_p \frac{dP}{dx} = -R$$

$$\frac{dN}{dt} + \frac{d}{dx}\mu_n N \frac{d}{dx} - \frac{d}{dx}D_n \frac{dN}{dx} = -R$$

Electrostatic potential φ was calculated from (7). It was found that such an algorithm not only fails to gain time compared with above mentioned, but also leads to a grave error. To avoid further significant approximation errors(connected with the availability of regions with large gradients which in this case directly enter difference equations, as distinct from method [1]), fine fractioning of the mesh in the gradient regions and an increase of meshpoints K_o up to 300–400 is necessary, which leads to a significant increase of computer time.

It should be pointed out that the algorithm of solving the set (1-2,7) is convenient for 2D problems, unlike algorithm [5] where at each moment of time transformation of large-scale matrices $3(K \cdot M)^2$ (K,M - the number of fractioning the integrated region) is required. Algorithm convergence (1-2,7) is slightly aggravated compared with metod [5] .

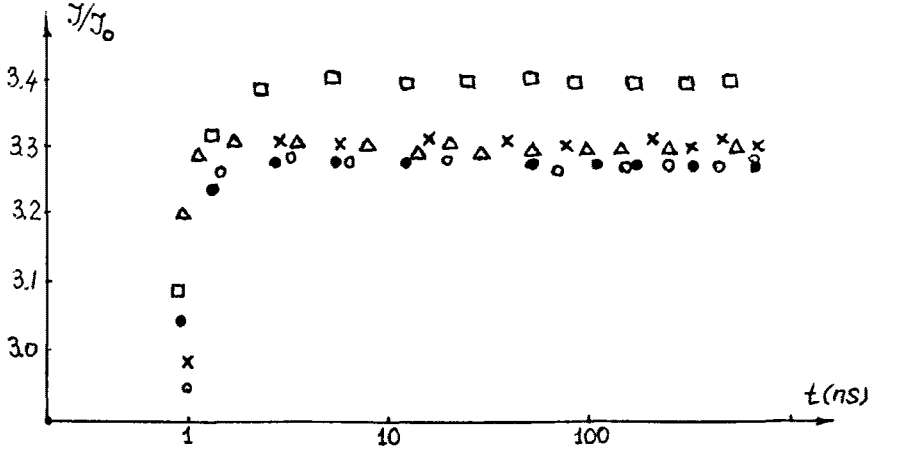

Fig.2 Dependence of current versus time, calculated on the different mesh. V = 0.4v, junction parameters from [3]. Uniform mesh: o - K_o= 120, × - K_o= 60; nonuniform mesh: • - K_o= 60, Δ - K_o= 40, □ - K_o= 20; $J_o = q\mu E_o n_o$; $E_o = E(t=0)$, $n_o = \frac{E_o}{4\pi q \ell}$.

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