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NUMERICAL ANALYSIS OF TRANSFER PHENOMENA IN SEMICONDUCTOR

DEVICES AND STRUCTURES.

1. UNIVERSAL PROGRAM FOR TWO-DIMENSIONAL MODELING

I. I. Abramov and V. V. Kharitonov
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A universal program for the two-dimensional numerical analysis of functionally integrated structures of integral circuits is described.

An important instrument of profound theoretical research of semiconductor devices and elements of integral circuits is comprised by programs of multidimensional numerical analysis. Their distinguishing feature is the possibility of analyzing structures of various design with an arbitrary number of p-n junctions. At present, several reports on programs of two-dimensional numerical analysis of this type have already appeared [1, 2]. However, according to existing information, it is fairly difficult to judge their potential and efficiency. The development of universal programs of three-dimensional analysis is evidently inexpedient at this point, because of the enormous time required to model even the simplest structures using current supercomputers [3]. Overall, the complexity of developing such programs depends primarily on a series of interrelated problems of methodological type: 1) the lack of universal procedures for choosing the initial approximation; 2) the low efficiency and reliability of well-known methods of numerical solution of the fundamental system of semiconductor-physics equations, including discretization methods.

In the present work, a universal program of two-dimensional numerical analysis of elements of PNAIIL integral circuits is described. To a definite extent, the above-noted complexities may be solved in developing this program. The results of computational experiments on EC-series computers are given, illustrating the possibilities of the program and its efficiency.

Description of the Program

Using the PNAIIL program, the fundamental system of semiconductor-physics equations is solved numerically in the two-dimensional approximation [4, 5]

$$\varepsilon\nabla^2\psi = -q(p - n + N_{\text{д}} - N_{\text{a}}), \tag{1}$$

$$\nabla\vec{j}_p = -qR, \quad \vec{j}_p = -q\mu_p p\nabla\Phi_p, \tag{2}$$

$$\nabla\vec{j}_n = qR, \quad \vec{j}_n = -q\mu_n n\nabla\Phi_n \tag{3}$$

with the auxiliary relations

$$n = n_i\gamma_n \exp(A\Delta V_g/\varphi_T)\exp[(\psi - \Phi_n)/\varphi_T],$$

$$p = n_i\gamma_p \exp[(1 - A)\Delta V_g/\varphi_T]\exp[(\Phi_p - \psi)/\varphi_T]. \tag{4}$$

The boundary condition models invoked are standard [3]. Provision is made for the use of the following models as the initial model information: 1) the Caughey–Thomas model [6] for mobilities μ_n and μ_p; 2) the Shockley–Reid–Hall model [7] and Auger recombination [8] for the

description of recombination—generation phenomena (R); 3) the Vol'fson—Subashiev [9], Slotboom-de Graaff [10], and Lanyon—Tuft [11] models, taking account of the high level of doping.

The PNAIIL program provides the basis for the method of numerical solution of the fundamental system of equations of [5], extended and refined for the case where the high level of doping and a series of other practically important situations are taken into account.* Discretization of Eqs. (1)-(4) is based on the Marchuk integral identity [12], using a series of physical assumptions. In the steady case, this leads to a finite—difference formulation for the continuity equations [13] and the Poisson equation [14]; in each case, a particular hierarchy of physical assumptions is invoked.

The following procedure is used in selecting the initial approximation in the program: the Fermi quasi-levels Φ_n and Φ_p are calculated according to the equations of [15] for regions of different type of conductivity; 2) the electrostatic potential ψ is determined by analytical solution of the Poisson equation, taking account of effects of the high level of doping, i.e., Eqs. (1) and (4), under the assumption of quasineutrality and thermal equilibrium over regions of the instrument with different types of conduction. In models in which the effects of a high level of doping depend explicitly on the concentration of the basic charge carriers N, it is assumed that $N = |N_d - N_a|$. It is of interest to consider some of the practically important situations briefly. Note that they could not be accompanied by the method of [15], in which contact was required in each of the regions. The most complex case is that in which there is no contact to the region G of p or n conduction surrounded by regions of the opposite type of conduction. In this situation, one of the following supplementary approaches is used at the preliminary stage of selection of an initial approximation: 1) a hypothetical contact is introduced at the surface of region G, with a potential equal to the potential at contact with one of the adjacent regions; 2) it is assumed that, in region G, the Fermi quasi-level of the basic carriers is equal to the theoretical Fermi quasi-level of the secondary carriers. Thus, the basic complexities are associated with determining the Fermi quasi-level of the basic carriers using the vector equations $\vec{\nabla\Phi_n}=0, \vec{\nabla\Phi_p}=0$. If there is one contact to each region of the same type of conduction but fundamentally different levels of doping, individual initial approximations corresponding to different Fermi quasi-levels of the basic charge carriers are considered in the selection process for the initial approximation. (For a single contact, no such sectioning is undertaken.) In the case when several contacts with different potentials are attached to the same region, the initial approximation is sectioned into regions of seemingly different levels of doping in the preliminary stage of the selection process. The initial approximation is then analyzed according to the above approach. Intermediate regions with linear variation in the Fermi quasi-level only of the basic carriers in one direction may be introduced here. Physically, this means that the flow of the basic-carrier current is one-dimensional and practically constant. If one contact is made of two regions of different conduction, it is divided into two adjacent contacts with equal potentials. This information, which is not in contradiction to the initial data, is used as the starting point in all subsequent stages of the calculation. All the remaining situations of practical importance may be treated using the given approaches.

After choosing the initial approximation for the variables Φ_n, Φ_p, ψ, matching of the bases of the fundamental variables with the fundamental system of equations used in the methods of solution is undertaken over the whole structure of the element. Five systemic methods of solving the fundamental system characterized by different regions and rates of convergence and preliminarily extended to the case where effects of a high level of doping are taken into account may be used for the calculation: 1) the Gummel method [16]; 2) the Seidman—Choo method [17]; 3) the method of [18]; 4) the two-step method of [5]; 5) the generalized two-step method [5]. The use of combined algorithms of the type in [18] and elsewhere is permitted. Thus, for the Gummel and Seidman—Choo methods, eliminating divergence entails using one of the methods of [5, 18] extended to the case where effects of high doping level are taken into account as the first complete iteration, beginning with the solution of the Poisson equation [5]. This means that the nonlinear Poisson equation is first solved for ψ by Newton's method, taking account of all the nonlinearities (no less than 2-3 times in accordance with the criterion

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*PNAIIL: Program on Numerical Analysis of Injection Logic Gates. The name of early versions of the program [5] characterized by more constricted possibilities (neglecting the effects of a high level of doping), is retained in later forms [4].
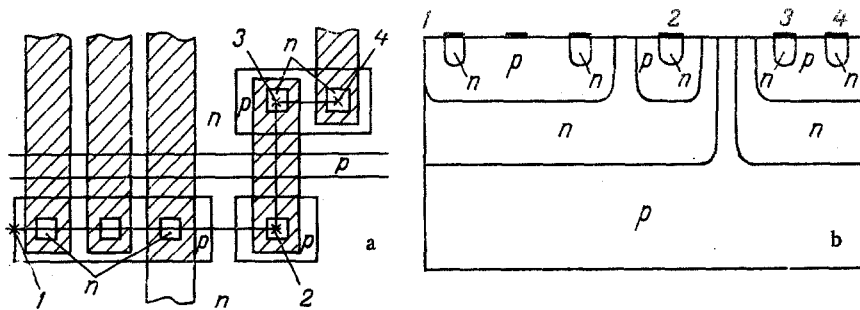
Fig. 1. Initial topology of LIS fragment (a) and structural diagram of fragment (b): 1-4) node points.

$|\delta\psi|_{\max l}/|\delta\psi|_{\max l+1} \geqslant K$ [18], where l is the number of the Newtonian iterations, or to complete convergence) at fixed $n_i\gamma_n\exp(A\Delta V_g/\varphi_T)\exp(-\Phi_n/\varphi_T)$ and $n_i\gamma_p\exp[(1-A)\Delta V_g/\varphi_T]\exp(\Phi_p/\varphi_T)$. In the first complete iteration of the methods of [5, 18], it is expedient (especially in analyzing metal–dielectric–semiconductor structures) also to damp the increment in electrostatic potential $\delta\psi$ in Newton's method by the procedure of [19]. Then the method used subsequently may be that corresponding to the user's desires or the most effective generalized two-stage method [5]. Note also that reordering of the stages of the given systemic methods,* and especially substitutions, particularly in the first iterations, may lead to change in their convergence properties [5]. These properties, however, are not unexpected for systemic methods of solving systems of ordinary differential equations [20].

Systems of linear equations are solved by the Chebyshev cyclic method [21], or the methods of [22, 23].

The universal PNAIIL program, in which the foregoing method is realized, is written in Fortran for EC-series computers (OC operational system). The program employs an input language permitting a convenient form of specification of initial information: 1) on models of mobility, recombination–generation, and effects of high doping level and their parameters; 2) on the structure of the element; 3) on the stress applied to the contact; 4) on the discretization grid; 5) on the methods of solution employed; and so on. The doping profile is specified by means of well-known analytical approximations or in tabular form. Parameters of program type (the accuracy of calculation parameters of the iterative methods of solving systems of linear equations, etc.) and a series of others from the foregoing description are built into the program; however, they may be specified by the user if desired.

In analyzing the fragments of large integral systems (LIS), the following method may be used to prepare the initial data: 1) in each of the elements, according to their topology, two-dimensional structures in the vertical cross section are isolated, with the corresponding physicotopological parameters and a width in the third measurement equal to the width of one of the contacts (regions); 2) the two-dimensional structures obtained are arranged in a plane (in a structural diagram), retaining the connections between contacts corresponding to the electrical circuit of the LIS fragment. As a result of this arrangement, however, no account is taken of the completely three-dimensional effects characteristic of the real fragment topology. To a definite extent, this deficiency may be eliminated by adding basic elements of connecting type. An example of this transformation is shown in Fig. 1: a) initial topology of the fragment; b) structural diagram of fragment. The maximum possible number of p–n junctions of the structural diagram (assuming 10 points per p–n junction) for a memory capacity of 8 Mbyte (the total volume of the EC-1060 working store) is 200-400 in measuring y with the standard technological LIS and 3-5 in measuring x. It is understood that, in this case, the possibilities of the universal PNAIIL program are determined solely by the speed of the computer employed.

The output information of the program is: 1) two-dimensional distributions of the hole concentration p, electron concentration n, electrostatic potential ψ, and current densities in the structural diagram of the fragment; 2) currents through the contacts. On the basis of this information, various characteristics of the elements may be calculated.

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*The term "systemic" is similar to that used for special methods of solution of systems of ordinary differential equations [20]. The use of a more specific term — "methods of vectorial relaxation of systems" is also possible [5].
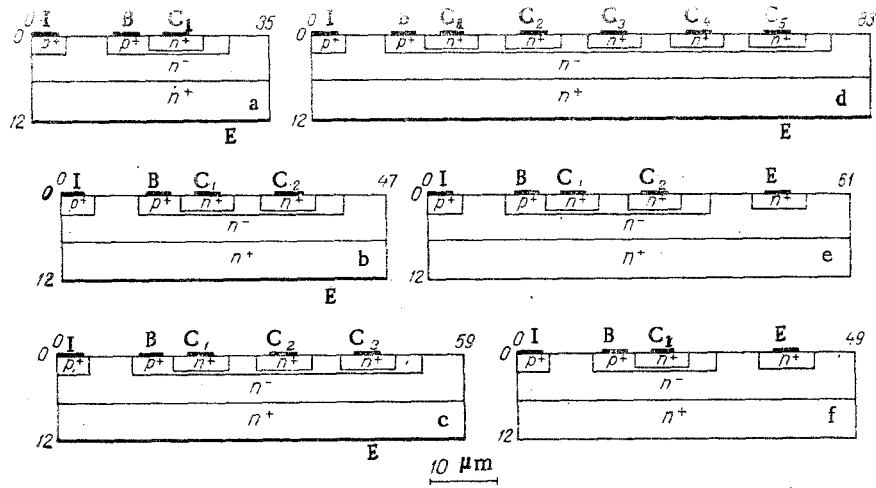
Fig. 2. ILS elements with injection supply under analysis.

Note, in conclusion, that new models of mobility, additional laws of recombination—generation (in this case, the Gummel method or generalized two-stage method of [5] is used) and, models of the effect of high doping level differing from the initial ones may easily be included in the program.

Results of Modeling

To illustrate the possibilities of the PNAIIL program, a series of computational experiments has been undertaken on the multidimensional numerical analysis of LIS elements with injectional supply in various configurations.

The elements under analysis are shown in the appropriate scale in Fig. 2. The doping levels of all the structures are the same for monotypic regions: epitaxial film, $n^- = 5 \cdot 10^{21}$ m^{-3}; latent emitter layer, $\sim 10^{25}$ m^{-3}; collector (contact regions of emitter) $\sim 10^{27}$ m^{-3}; base and injector, $\sim 5 \cdot 10^{24}$ m^{-3}. The results in Table 1 were obtained on EC-1022, EC-1035, EC-1040, and EC-1060 computers. For convenience of comparison and to permit extrapolational estimates of the time required to model even more complex structures, all the data are referred to the time data for the EC-1060 computer. This is accomplished by determining conversion coefficients. Thus, for one of the problems, the ratio of the time of operation of the central processor of an EC-1035 computer to the time of an EC-1060 computer is ~ 4.4.* The other conversion coefficients are determined analogously. The time for each of the computers may be estimated approximately using data on the speed of EC-series computers according to the Gibson scale [24]. Table 1 also gives information on the discretization grid. The first figure in the grid column corresponds to the number of grid points covering the structure in measuring x and the second gives the corresponding number of points in measuring y. In the shift column, the potential applied to the corresponding contact is shown. A forward shift is applied to the injector in all the experiments. The calculation accuracy is determined by the standard method [4]: $q|\delta\psi|_{max1}/kT \leqslant \varepsilon^*$. Results on the two-dimensional numerical calculation of the concentration of mobile carriers, fields, and current densities are not given in view of their unwieldiness. Comparison of the rates of convergence of the methods employed does not contradict [4, 5, 18], in broad outline.

Overall, the data in Table 1 indicate sufficiently broad potential and also high efficiency and reliability of the PNAIIL program. These results on the efficiency of the program may be very approximately compared for the element in Fig. 2a with the data of [3] on modeling a similar structure using the more efficient non-Soviet STEPSOLVING method for solving the fundamental systems of equations. Thus, for the PNAIIL program, the time required is 6.5 min for the EC-1060 computer with a speed of 1,300,000 operations/sec according to Gibson and 1.4-2 min for the CYBER-175 computer with a speed of around 10 million operations/

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*The results are given with respect to the data for an EC-1060 computer in which some of the means for increasing the speed are switched off, thereby increasing the time by a factor of ~ 1.6.

TABLE 1. Time Required to Model Elements

Structure (Fig.)	Grid	Shift, V	EC-1060 Time, min	Accuracy $\varepsilon^\bullet$
2a	25 × 60	$VI = 0.7$; $VB = VC_1 = VE = 0$	6.5	0.003
2b	25 × 78	$VI = 0.7$; $VB = VC_1 = 0$; $VC_2 = VE = 0$	8	0.007
2b	25 × 78	$VI = 0.7$; $VB = 0.67$; $VC_1 = VC_2 = 0.01$; $VE = 0$	8.3	0.007
2b	25 × 78	$VI = 0.7$; $VB = VC_2 = 0.67$; $VC_1 = 0.01$; $VE = 0$	8	0.007
2b	25 × 78	$VI = 0.7$; $VE = 0$; $VB = VC_1 = VC_2 = 0.67$	8	0.007
2c	25 × 100	$VI = 0.7$; $VB = VE = 0$; $VC_1 = VC_2 = VC_3 = 0$	11.7	0.003
2c	25 × 100	$VI = 0.7$; $VB = 0.67$; $VE = 0$; $VC_1 = VC_2 = VC_3 = 0.01V$	20.7	0.003
2c	25 × 100	$VI = 0.7$; $VB = VC_2 = 0.67$; $VC_1 = VC_3 = 0.01$; $VE = 0$	20.2	0.003
2c	25 × 100	$VI = 0.7$; $VB = VC_1 = VC_2 = VC_3 = 0.67$; $VE = 0$	20	0.003
2c	25 × 100	$VI = 0.7$; $VE = 0$; $VC_2 = 0.01$; $VB = VC_1 = VC_3 = 0.67$	20	0.003
2c	25 × 100	$VI = 0.8$; $VB = VE = 0$; $VC_1 = VC_2 = VC_3 = 0$	28.4	0.003
2d	25 × 144	$VI = 0.7$; $VB = VE = 0$; $VC_1 = VC_2 = VC_3 = 0$; $VC_4 = VC_5 = 0$	16.6	0.003
2e	25 × 99	$VI = 0.7$; $VB = VE = 0$; $VC_1 = VC_2 = 0$	15.6	0.003
2f	25 × 80	$VI = 0.7$; $VB = 0$; $VE = VC_1 = 0$	13.4	0.003

sec according to Gibson using the STEPSOLVING method [24].* These data indicate the sufficiently high accuracy of the PNAIIL universal program. Regrettably, such a comparison of the time required to model other I^2L structures is not possible, since data on multidimensional numerical analysis of most of them are published here for the first time.

NOTATION

ψ, electrostatic potential; n, p, electron and hole concentrations; N_d, N_a, donor and acceptor concentrations; R, amount by which the recombination rate exceeds the generation rate; $\vec{j}_n$, $\vec{j}_p$, electron and hole current density vectors; μ_n, μ_p, electron and hole mobilities; q, electron charge; ε, dielectric permittivity of material; Φ_n, Φ_p, electron and hole Fermi quasi-levels; n_i, intrinsic concentration; φ_T, temperature potential (0.0258 V at T = 300°K); ΔV_g, total narrowing of forbidden-band width; A, asymmetry coefficient in narrowing; γ_n, γ_p, degrees of electron and hold degeneracy; $\delta\psi$, perturbation of the electrostatic potential ψ relative to which the linearized Poisson equation is formed; V_I, V_B, V_E, V_{C1}, V_{C2}, V_{C3}, V_{C4}, V_{C4}, voltages (potentials) applied to the contacts of the injector (I), base (B), emitter (E), and collectors (C1-C5).

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