

within the scope of the present model with the condition $r_* \neq r_0$ at the tube inlet. The results of such a calculation are shown in Fig. 4.

NOTATION

t , time; r , local value of radius; r_0 , tube radius; r_* , radial coordinate of interfacial surface; z , longitudinal coordinate; z_* , longitudinal coordinate of interfacial surface; z_{in} , length of inlet zone; L , tube length; T , temperature; T_* , temperature of phase change; T_0 , tube wall temperature; R , universal gas constant; E , energy of activation of viscous flow; Q_* , specific heat of the phase change; P , pressure; Q , liquid flow rate; α, γ, S, q , dimensionless parameters; G , difference in pressure drops calculated by various models; λ_1, λ_2 , thermal conductivities of the liquid and solid phases, respectively; ρ_l, c_l , density and heat capacity of liquid phase; v_z, v_r , axial and radial components of the liquid velocity; τ_{rz} , shear stress; η , viscosity; n_0 , preexponential multiplier.

LITERATURE CITED

1. S. V. Maklakov, A. M. Stolin, and S. I. Khudyaev, Zh. Prikl. Mekh. Tekh. Fiz., No. 4, 59-65 (1985).
2. S. V. Maklakov, A. M. Stolin, and S. I. Khudyaev, Zh. Prikl. Mekh. Tekh. Fiz., No. 4, 86-93 (1984).
3. O. Reynolds, Phil. Trans. R. Soc., 177, 157-234 (1886).

NUMERICAL ANALYSIS OF THE TRANSPORT PHENOMENON IN SEMICONDUCTOR DEVICES AND STRUCTURES.

5. THREE-DIMENSIONAL MODELING OF VLIS ELEMENTS

I. I. Abramov and V. V. Kharitonov

UDC 621.382.82.001:519.95

The high efficiency of a multidimensional numerical analysis of semiconductor devices is confirmed in an example of three-dimensional modeling of bipolar integral circuit structures.

A change in the configuration of the components in the plane of the crystal, i.e., their topology, is the approach approved in practice for improving the characteristics of LIC and VLIC elements. In this case, despite the possible significant machine time expenditures, the three-dimensional modeling of transport processes occurring in the elements [1, 2] is necessary in principle. Such an analysis in the preliminary stage of VLIC design permits complete investigation, without involving significant material expenditures, of the influence of different topological factors on the structure properties, which is extremely important for the engineer-developer in the creation of new optimized structures of elements and investigation of the influence of the changes made on the whole integrated circuit. As is known, this latter is realized by involving the programs of the circuit engineering design stage [2].

Traditionally it is considered that execution of a rigorous three-dimensional numerical analysis (coordinate solution of the problem mentioned) of just several stationary states of the element by solving the fundamental system of equations [3] is impossible in a reasonable time even on an ES-1060 type computer.

The inconsistency of such an assertion is shown in this paper. Results are cited for this that have been obtained for two fundamental kinds of bipolar structures of integrated circuits and that confirm the high efficiency of the universal program developed for three-dimensional numerical modeling of VLIC elements later designated "TREADE." Underlying it is the generalized and perfected method of previous papers [3-6].

Belorussian Institute of Railroad Transport Engineers, Gomel^{*}. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 53, No. 1, pp. 135-141, July, 1987. Original article submitted May 5, 1986.

The numerical solution of the fundamental system of equations [6] with the auxiliary relationships following directly for the current densities is realized in the three-dimensional modeling of transport phenomena in semiconductor devices:

$$j_n = -q\mu_n n \nabla(\psi + A\Delta V_g) + q\varphi_T \mu_n \nabla n, \quad (1)$$

$$j_p = -q\mu_p p \nabla[\psi - (1-A)\Delta V_g] - q\varphi_T \mu_p \nabla p. \quad (2)$$

Taking account of the effects of the high doping level is by one of the empirical models [7] with $\gamma_n = \gamma_p = 1$. Traditional boundary conditions [8] are utilized here.

In the preliminary stage a finite-difference approximation is realized for the fundamental system of equations with the boundary conditions and the appropriate initial data by using the G. I. Marchuk integral identity method in order to derive a hierarchy of models for the difference scheme coefficients. In the foreign literature the box integration method [8] is often used to construct difference schemes in the multidimensional case within the framework of the general integrointerpolation approach of A. N. Tikhonov and A. A. Samarskii [9]. It is important to note that these two methods result in different finite-difference approximations of the equations, as follows from the subsequent exposition.

Let us consider the generalization of the G. I. Marchuk method to the multidimensional case. Because of awkwardness, we present only the scheme to derive the fundamental integral identity and the form of the corresponding approximate problem in the two-dimensional case. The extension to the three-dimensional case is realized by an analogous method.

After a number of simple manipulations each of the three fundamental equations to be solved (electron and hole continuity and Poisson equation) can be represented in the general form

$$-\frac{\partial}{\partial x} p^M \frac{\partial \varphi^M}{\partial x} - \frac{\partial}{\partial y} p^M \frac{\partial \varphi^M}{\partial y} + q^M \varphi^M = f^M, \quad (3)$$

where for the continuity equation of the electrons

$$p^M = -\mu_n n_{in} \varphi_T \exp(\psi/\varphi_T), \quad q^M = 0, \quad \varphi^M = \exp(-\Phi_n/\varphi_T), \quad f^M = R, \quad (4)$$

of holes

$$p^M = \mu_p n_{ip} \varphi_T \exp(-\psi/\varphi_T), \quad q^M = 0, \quad \varphi^M = \exp(\Phi_p/\varphi_T), \quad f^M = -R \quad (5)$$

and for Poisson equation

$$p^M = -\varepsilon, \quad \varphi^M = \psi, \quad q^M = 0, \quad (6)$$

$$f^M = q \{n_{in} \exp[(\psi - \Phi_n)/\varphi_T] - n_{ip} \exp[(\Phi_p - \psi)/\varphi_T] - N_d + N_a\}.$$

We realize construction of the difference scheme for (3) in the main $\{x_i\}$, $\{y_j\}$ and auxiliary $\{x_{i+1/2} = (x_i + x_{i+1})/2\}$, $\{y_{j+1/2} = (y_j + y_{j+1})/2\}$ meshes of the spatial discretization.

We use (3) in two forms

$$-\frac{\partial}{\partial x} p^M \frac{\partial \varphi^M}{\partial x} + q^M f^M = f_1^M, \quad (7)$$

$$-\frac{\partial}{\partial y} p^M \frac{\partial \varphi^M}{\partial y} + q^M f^M = f_2^M, \quad (8)$$

where

$$f_1^M = f^M + \frac{\partial}{\partial y} p^M \frac{\partial \varphi^M}{\partial y}, \quad f_2^M = f^M + \frac{\partial}{\partial x} p^M \frac{\partial \varphi^M}{\partial x}.$$

Let us apply the G. I. Marchuk [10] method first to the relationship (7). We consequently obtain

$$-J_{i+1/2,i}^M + J_{i-1/2,i}^M + (\Delta y_j)^{-1} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} (q^M \varphi^M - f_1^M) dx dy = 0, \quad (9)$$

where $\Delta y_j = y_{j+1/2} - y_{j-1/2}$,

$$J_{i-1/2, j}^M = \Delta y_j \left\{ \int_{y_{j-1/2}}^{y_{j+1/2}} \left[\int_{x_{i-1}}^{x_i} (p^M)^{-1} dx \right] dy \right\}^{-1} [\Phi_{i, j}^M - \Phi_{i-1, j}^M - (\Delta y_j)^{-1} \int_{y_{j-1/2}}^{y_{j+1/2}} dy \int_{x_{i-1}}^{x_i} (p^M)^{-1} dx \int_{x_{i-1/2}}^x (q^M \psi^M - f_1^M) d\xi]. \quad (10)$$

To derive the main integral identity we expand one of the integrals in the left side of (9)

$$\int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} f_1^M dx dy = \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} f^M dx dy + (J_{i, j+1/2}^M - J_{i, j-1/2}^M) \Delta x_i, \quad (11)$$

where $\Delta x_i = x_{i+1/2} - x_{i-1/2}$. The well-known property of multiple integrals was used here.

To find $J_{i, j-1/2}^M$ ($J_{i, j+1/2}^M$) in (11) and (9), an analogous approach is used as for the derivation of (10), however with the just essential difference that (8) is the initial equation in this case. Let us note that the relationships obtained as a result of such manipulations although awkward are exact integral identities or balance equations.

It is easy to show that

$$A^h \varphi^h = f^h \quad (12)$$

can be used as an approximate problem for $q^M = 0$ (case under consideration), where for each inner node of the spatial discretization mesh (i, j)

$$(A^h \varphi^h)_{i, j} = -(\Delta x_i)^{-1} \left\{ \frac{\Phi_{i+1, j}^h - \Phi_{i, j}^h}{(\Delta y_j)^{-1} \int_{y_{j-1/2}}^{y_{j+1/2}} \left[\int_{x_i}^{x_{i+1}} (p^M)^{-1} dx \right] dy} - \frac{\Phi_{i, j}^h - \Phi_{i-1, j}^h}{(\Delta y_j)^{-1} \int_{y_{j-1/2}}^{y_{j+1/2}} \left[\int_{x_{i-1}}^{x_i} (p^M)^{-1} dx \right] dy} \right\} - (\Delta y_j)^{-1} \left\{ \frac{\Phi_{i, j+1}^h - \Phi_{i, j}^h}{(\Delta x_i)^{-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left[\int_{y_j}^{y_{j+1}} (p^M)^{-1} dy \right] dx} - \frac{\Phi_{i, j}^h - \Phi_{i, j-1}^h}{(\Delta x_i)^{-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left[\int_{y_{j-1}}^{y_j} (p^M)^{-1} dy \right] dx} \right\},$$

$$(f^h)_{i, j} = (\Delta x_i \Delta y_j)^{-1} \int_{y_{j-1/2}}^{y_{j+1/2}} \left[\int_{x_{i-1/2}}^{x_{i+1/2}} f^M dx \right] dy.$$

Comparison with the box integration method ([11], say) shows that the G. I. Marchuk method is a more general and flexible instrument for the construction of difference schemes because of the possibility of utilizing different approximations for double integrals of p^M .

Difference schemes for the electron and hole continuity equations and the Poisson equations are obtained by substitution of appropriate values of p^M , φ^M , q^M , f^M from relationships (4)-(6) into equations of the form (12). After this, physical propositions from the following set are relied upon (in the box) to approximate the integrals in an expression of the type (12): 1) a weak change in $\mu_p n_{ip} \varphi_T$ ($\mu_n n_{in} \varphi_T$); 2) constancy of the Fermi quasilevel; 3) linear changes in the concentration, chemical and electrostatic potentials recombination. It is interesting to note that if the initial fundamental system of equations is considered in a box, then two assumptions about the constancy of the Fermi quasilevel and on the linearity of the change in electrostatic potential will correspond separately to the underlying physical approximations of the theory of semiconductor devices on quasiequilibrium ($j_p \approx 0$, $j_n \approx 0$) and

quasineutrality ($\nabla \epsilon \nabla \psi \approx 0$). However, it must be recalled that in the case under consideration these assumptions are used to construct the difference scheme by using an approximate problem of the form (12) and not in the initial continuity of the model. On the whole, reliance on the conservation laws (conservative schemes) and physical assumptions assures elevated accuracy and stability of the finite-difference approximation of the fundamental system of equations. In the one-dimensional case the presence of these properties is proved rigorously for the approximate problem [10]. The methods of approximating integrals in expressions of the type (12) and the derivation of a hierarchy of models for the difference scheme coefficients do not differ especially essentially in any way from those described in [3, 12] for the continuity equations and in [13] for the Poisson equation; consequently, we do not consider them. Unfortunately, because of the extreme awkwardness it is not possible to present a list of the difference scheme coefficients for each of these equations.

As a result of the finite-difference approximation of the fundamental system of equations in the basis of the variables ϕ_n, ϕ_p, ψ , we obtain a general difference scheme in the three mesh vectors $\{\psi_t\}, \{\phi_{nt}\}, \{\phi_{pt}\}$, where the subscript t runs through values in all nodes of the fundamental three-dimensional spatial discretization mesh covering the device. Later (for simplicity), we write ψ, ϕ_n, ϕ_p , and omit the subscript t .

After the manipulations considered above, quasilinearization of the discrete analog of the Poisson equation is realized with respect to $\delta\psi$ for fixed $\phi_n, \phi_p, n_{in}, n_{ip}$. The general form of the matrix equation after the return passage to the ψ, n, p variables corresponds to (10) in [5]. The electron and hole continuity equations are also quasilinearized with respect to δn and δp for fixed ψ only after an analogous return passage of the equations to the basis of the n, p, ψ variables by using the relations (4) from [6]. Equations of the form (11) and (12) from [5] will be the result. The solution of the matrix equations obtained will be realized by the method elucidated in [5]. It is necessary to recall here that in each iteration of methods difference-scheme coefficients and more accurately the appropriate quasilinearized equations can be calculated by different formulas from the preliminarily derived hierarchy of models for each of them. The method of [6, 14] is used to select the initial approximation. The solution of the systems of linear algebraic equations that occur is realized by using the three-dimensional versions of the cyclic method of Chebyshev and Buleev [4].

At the present time, two promising and mutually supplementing tendencies were noted in the development of program support for the solution of problems of two-dimensional numerical modeling of VLIC elements, namely: 1) creation of program complexes for effective and economical computation of different elements in which the specifics of their operation is taken into account [15], 2) development of general-purpose programs permitting simulation of the structure with an arbitrary quantity of p-n junctions [6, 14]. The development of the latter aspect in the three-dimensional case is continued in this paper.

The method described was the basis for the general-purpose program of a three-dimensional numerical analysis of the semiconductor devices and structures "TREADE" written in the language FORTRAN-IV for electronic computers of the ES series (operation system OS). The insertion and list of initial information is analogous to [6]. We just note here that not required in the program "TREADE," as compared with "PNAIIL" [6], is the preliminary transformation of the initial data about the real structure of the VLIC element, which can also, generally speaking, have an arbitrary quantity of p-n junctions. However, it is conceivable that its real possibilities are entirely and completely determined by the calculational resources of the electronic computer being utilized.

Let us consider certain results obtained by using the program "TREADE." Thus, it was used to realize the numerical modeling of two fundamental kinds of bipolar structures: a bipolar transistor with vertical structure (Fig. 1) and a single-collector I²L element (Fig. 2). The geometric dimensions of the structures (Figs. 1 and 2) are given in microns. The doping level of the transistor in Fig. 1 is: emitter $\sim 10^{20}$ cm⁻³, base $\sim 10^{18}$ cm⁻³, collector 10^{16} cm⁻³. For the element in Fig. 2: injector and base $\sim 1.4 \cdot 10^{18}$ cm⁻³, epitaxial film $n^- \sim 1.2 \cdot 10^{16}$ cm⁻³, latent emitter layer $\sim 2 \cdot 10^{18}$ cm⁻³, collector $\sim 1.2 \cdot 10^{20}$ cm⁻³.

The computation time needed for numerical modeling of the transistor (see Fig. 1) was approximately 11 min for the ES-1060 electronic computer for an emitter-base bias $V_{e,b} = -0.7$ V and a collector-base bias $V_{c,b} = 0$ V. Analogous results were also obtained for the biases $V_{e,b} = -0.7$ V, $V_{c,b} = 1$ V. The solution was carried out on a quasiuniform mesh in the device domains with $25 \times 24 \times 10$ nodes. Therefore, the total number of unknowns is around 18,000. According to the data of [8], approximately 1500 min is required for the electronic computer CYBER-175 to model such a structure for biases $V_{e,b} = -0.65$ V, $V_{c,b} = 1$ V by using

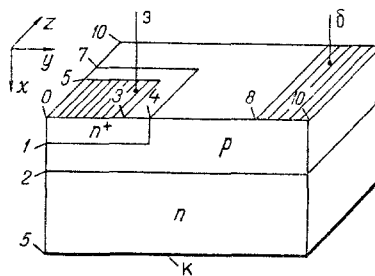


Fig. 1. Shape of the bipolar transistor being analyzed.

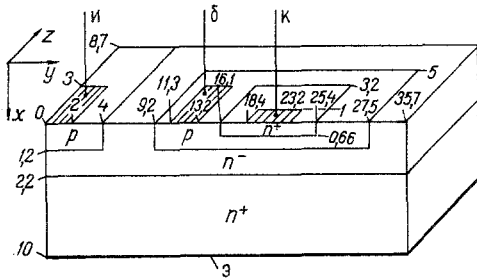


Fig. 2. Structure of the I²L element being analyzed.

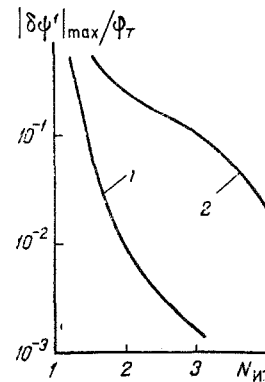


Fig. 3. Convergence of the iteration process of the method.

the algorithm STEPSOLVING, which indicates the sufficiently high efficiency of the program "TREADE," and therefore, of its underlying methodology.

Additional necessary information illustrating the high efficiency of the method utilized is the results on the convergence of the iteration process of the method. These data are presented in Fig. 3 for $V_{e.b} = -0.7$ V, $V_{c.b} = 0$ V (curve 1) and $V_{e.b} = -0.8$ V, $V_{c.b} = 0$ V (curve 2). The traditional criterion was used to terminate the iteration: $|\delta\psi^1|_{\max}/T \leq \epsilon^*$. For curve 1 we have $\epsilon^* = 0.002$, and $\epsilon^* = 0.02$ for curve 2, which is sufficient for the biases under consideration [16]. As the results of three-dimensional modeling show, taking account of high doping level effects (for empirical models) exerts negligible influence on the rate of convergence of the method.

It must be emphasized that the time expenditures required for the numerical modeling of the two kinds of structures are reasonable, which also indicates high efficiency of the program "TREADE." Thus the time expenditures for the electronic computer ES-1060 to compute the I²L element (see Fig. 2) for the typical biases $V_i = 0.65$ V, $V_b = V_c = V_e = 0$ V were approximately 122 min ($\epsilon^* = 0.002$). The solution was obtained on a quasiuniform mesh in the device domains, with $25 \times 58 \times 10$ nodes in the x, y, z measurements, respectively. Therefore, the total number of unknowns (nonlinear algebraic equations) was around 43,000 in this case; consequently, the distributions of the fundamental variables n, p, ψ and others are indeed not presented in this paper. It is pertinent to note here that the development of special machine methods of processing the output information about these unknowns for three-dimensional modeling with reliance on different technical facilities is still more urgent as compared with the two-dimensional case [17]. The prospect for these purposes can turn out to be the utilization of the method of automatic synthesis of equivalent circuits [12] as well as different physical principles and assumptions [17].

Therefore, the data presented indicate the sufficiently high efficiency of the developed general-purpose program for three-dimensional numerical modeling of the VLIC elements "TREADE" and its underlying methodology for a multidimensional analysis of transport phenomena in semiconductor devices and structures.

NOTATION

ψ , electrostatic potential; n, p, electron and hole concentrations; N_d , N_a , donor and acceptor concentrations; μ_n , μ_p , electron and hole mobilities; q, electron charge; j_n , j_p ,

electron and hole current density vectors; A , coefficient of asymmetry in narrowing; ΔV_g , total narrowing of the forbidden bandwidth; γ_n , γ_p , degree of electron and hole degeneration; φ_T , temperature potential; ϕ_n , ϕ_p , electron and hole Fermi quasilevels; n_{in} , n_{ip} , effective proper electron and hole concentrations equal to $n_i \gamma_n \exp(A \Delta V_g / \varphi_T)$ and $n_i \gamma_p \exp[(1 - A) \Delta V_g / \varphi_T]$, respectively; R , excess of the recombination velocity above the generation velocity; ϵ , dielectric permittivity of the material; $B_{i,j}$, value of the variable B at the node of the spatial discretization mesh with the subscripts i, j ; $|\delta \psi^1|_{\max}$, maximal value of $\{|\delta \psi_{i,j}^1|\}$ in the first Newton iteration; V_i , V_e , V_b , V_c , ohmic contact potentials of the injector, emitter, base, and collector, respectively; and N_{it} , number of complete iterations of the method.

LITERATURE CITED

1. G. G. Kazennov, V. Ya. Kremlev, and M. L. Khachaturov, *Electronic Engineering [in Russian]*, Ser. 3, Microelectronics, No. 6, 41-48 (1981).
2. B. V. Batalov and I. P. Norenkov, *Mikroelektronika*, 9, No. 5, 401-412 (1980).
3. I. I. Abramov and V. V. Kharitonov, *Inzh.-Fiz. Zh.*, 44, No. 2, 294-293 (1983).
4. I. I. Abramov and V. V. Kharitonov, *Inzh. Fiz. Zh.*, 44, No. 3, 474-480 (1983).
5. I. I. Abramov and V. V. Kharitonov, *Inzh.-Fiz. Zh.*, 50, No. 5, 845-852 (1986).
6. I. I. Abramov and V. V. Kharitonov, *Inzh.-Fiz. Zh.*, 51, No. 1, 136-143 (1986).
7. I. I. Abramov, *Izv. Vyssh. Uchebn. Zaved., Radioelektron.*, 27, No. 8, 16-22 (1984).
8. W. L. Engl, H. K. Dirks, and B. Meinerzhagen, *PIEEE*, 71, 10-23 (1983).
9. A. A. Samarskii, *Theory of Difference Schemes [in Russian]*, Moscow (1983).
10. G. I. Marchuk, *Methods of Computational Mathematics [in Russian]*, Moscow (1977).
11. T. W. Slotboom, *IEEE Trans.*, ED-20, No. 8, 669-679 (1973).
12. I. I. Abramov, *Izv. Vyssh. Uchebn. Zaved., Radioelektron.*, 28, No. 11, 63-69 (1985).
13. I. I. Abramov, *Izv. Vyssh. Uchebn. Zaved., Radioelektron.*, 27, No. 6, 107-109 (1984).
14. I. I. Abramov and V. V. Kharitonov, *Izv. Vyssh. Uchebn. Zaved., Radioelektron.*, 28, No. 12, 82-85 (1985).
15. E. V. Avdeev, A. P. Kotko, Yu. N. Mirgorodskii, et al., *Microelectronics and Semiconductor Devices [in Russian]*, No. 9, 99-111 (1984).
16. I. I. Abramov and S. G. Mulyarchik, *Izv. Vyssh. Uchebn. Zaved., Radioelektron.*, 24, No. 6, 59-67 (1981).
17. I. I. Abramov, "Modeling of bipolar IC elements on the basis of a discrete physicotopological model," *Candidate's Dissertation*, Minsk (1982).

HEAT AND MASS TRANSFER IN SKIN FORMATION

N. I. Nikitenko and Yu. N. Kol'chik

UDC 536.24

A mathematical model of the heat conduction and diffusion on heating an oxidizing metal is presented, together with a numerical method of calculation.

On heating ingots and semifinished articles in furnaces, their outer surface is oxidized, which leads to significant loss of material. The skin layer formed on oxidation has relatively low heat conduction and a high specific volume, and consequently this layer appears as a heat-insulating coating [1-3], which must be taken into account in optimizing the heating of metallic bodies.

It has been established that, in the skin layer, diffusion of metal to the outer surface occurs, and it is mainly oxidized at this surface [4]. The concentration distribution of the components in the oxide has apparently not previously been considered. Skin formation on heating a body of arbitrary form may be described mathematically as follows. Suppose that W_1 and W_2 are regions of space (x, y, z) occupied by the metal and its skin; Γ_1 is the boundary between the metal and the skin; Γ_2 is the external boundary of the skin; t_1 and t_2 are temperature functions for the metal and the skin; C is the concentration of unoxidized metal in

Institute of Engineering Thermophysics, Academy of Sciences of the Ukrainian SSR, Kiev. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 53, No. 1, pp. 141-148, July, 1987. Original article submitted March 12, 1986.