T_0, $\Theta_2(r, z, \tau) = T_2(r, z, \tau) - T_0$, excess temperatures; T_0, initial temperature; erf (x), probability integral; $C_{2n}^m = \frac{(2n)!}{m!\,(2n-m)!}$, binomial coefficients; $(3/2)_n = 2^{-2n} \cdot \frac{(2n+1)!}{n!}$, Pokhgammer symbol; $D_\nu(x)$, parabolic cylinder function; $A_{n,m}$, $B_{n,m}$, thermal amplitudes (from the text); $H_k(x)$, orthogonal Hermite polynomials; w_0, content (in time) density of radiation (W/m^2); $\gamma(n+2, r^2/r_0^2)$, incomplete gamma function; $W_{k,\mu}(x)$, Whittaker function; $Ki = w_0 r_0/(\lambda T_0)$, $Fo = a\tau/r_0^2$, Kirpichev and Fourier numbers; $\Theta_1^*(0, 0, \tau)$, $\Theta_2^*(r, 0, \tau)$, dimensionless relative temperatures; $L_k^\alpha(x)$, Laguerre polynomial.

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NUMERICAL ANALYSIS OF FUNCTIONALLY INTEGRATED VLSIC ELEMENTS TAKING INTO ACCOUNT HEAT EFFECTS.

II. METHOD AND PROGRAM

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The program and method of implementation of a discrete, multidimensional physical-topological model, taking into account heat effects, are described.

After analyzing construction of a discrete physical-topological model of functionally integrated VLSIC elements taking into account heat effects [1] we shall now present a method for implementing it and we shall describe a universal program.

Method for Selecting the Starting Approximation. The method is based on the solution of a truncated system of equations derived from the starting system (Eqs. (1)-(8) from [1]) with the help of a number of physical assumptions. The key assumption is the assumption that the temperature is constant over the structure of an element. This means that self-heating of the element is neglected in the starting approximation. As a result, Eq. (6) or [1] need not be solved.

The effect of the temperature of the surrounding medium must, however, be taken into account. Because of the adopted physical assumptions the equations for the current densities can be written in a different form:

$$\mathbf{j}_p = -q\mu_p(T_{oc})\, p \nabla \Phi_p, \tag{1}$$

$$\mathbf{j}_n = -q\mu_n(T_{oc})\, n \nabla \Phi_n. \tag{2}$$

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For the majority charge carriers we shall employ the assumption of quasiequilibrium. Taking into account the form of Eqs. (1) and (2) we obtain

$$\nabla\Phi_p \approx 0, \tag{3}$$

$$\nabla\Phi_n \approx 0. \tag{4}$$

We shall find the Fermi quasilevels of the nonequilibrium charge carriers with the help of the equation of continuity. A series of simple transformations gives for the electrons

$$\nabla^2\Phi_n + \nabla \ln [\mu_n (T_{0c})\, n]\, \nabla\Phi_n = -R(T_{0c})/\mu_n (T_{0c})\, n. \tag{5}$$

In Eq. (5) we assume that

$$|\nabla^2\Phi_n| \gg |\nabla \ln [\mu_n (T_{0c})\, n]\, \nabla\Phi_n|. \tag{6}$$

The approximation (6) is more general than (4), since it can be satisfied for small $\nabla\ln[\mu_n(T_{0c})n]$. Thus the simplified equation of continuity for electrons assumes the form

$$\nabla^2\Phi_n \approx -R(T_{0c})/\mu_n (T_{0c})\, n. \tag{7}$$

An analogous approach for holes gives

$$\nabla^2\Phi_p \approx R(T_{0c})/\mu_p (T_{0c})\, p. \tag{8}$$

With the use of the Shockley–Reed–Hall model the analysis of two limiting cases in (7) and (8), namely, 1) $pn >> n_i^2 (T_{0c})$ and $n >> p$; 2) $pn \to n_i^2 (T_{0c})$ and $p \to 0$, gives

$$\nabla^2\Phi_n \approx -1/\tau_n \mu_{n0} (T_{0c}), \tag{9}$$

$$\nabla^2\Phi_p \approx 1/\tau_p \mu_{p0} (T_{0c}). \tag{10}$$

In the calculation of Φ_n, Φ_p the regions of the majority and minority charge carriers are identified by the sign of the known function $N_d - N_a$.

The potential ψ is determined from the solution of the Poisson equation (1) of [1] under the assumption of quasineutrality and thermodynamic equilibrium over the regions with different conductivity in the device:

$$\rho(\Phi_p,\ \psi,\ T_{0c}) = 0, \quad \rho(\Phi_n,\ \psi,\ T_{0c}) = 0 \tag{11}$$

for regions of the p and n types, respectively.

Thus in choosing the starting approximation the truncated system of equations, consisting of (3), (4), (9), (10), and (11), is solved for the corresponding regions of the device. The boundary conditions (9) and (10) from [1] are employed for the potential ψ, and the following relations are employed for the Fermi quasilevels: 1) $\Phi_n = \Phi_p = V_{np}$ on ohmic contacts and 2) $\nabla\Phi_n \mathbf{N}_s = \nabla\Phi_p \mathbf{N}_s = 0$ on other boundaries.

The equations (11) can be solved analytically for the Φ_n and Φ_p found:

$$\psi = \Phi_p + \psi_0, \quad N_d - N_a < 0; \quad \psi = \Phi_n + \psi_0, \quad N_d - N_a \geqslant 0$$

for p and n type regions, respectively; in addition, ψ_0 is calculated from the formula

$$\psi_0 = (kT_{0c}/q)\ \mathrm{sign}(N_d - N_a) \ln \left[\sqrt{\left(\frac{N_d - N_a}{2n_i (T_{0c})}\right)^2 + 1} + \left| \frac{N_d - N_a}{2n_i (T_{0c})} \right| \right].$$

In the finite-difference approximation the physical assumptions that $\mu_n(T_{0c})$, $\mu_p(T_{0c})$, τ_n, τ_p are constant on the cell ABCD (see Fig. 1 of [1]) are employed at the anterior node i, j. After ψ, Φ_n, Φ_p are calculated (T equals T_{0c}) over the entire structure of the element the densities are determined from (8) [1], while the variable U is determined with the help of the equation relating it with T [1].

In the case when one contact is not brought directly up to the region of the p or n element, the approaches studied in [2] are employed.

Classification of Methods of Vector Relaxation of Systems. A systems approach to the solution of systems of partial differential equations, forming a continuous model, was formulated in [3]. This method can be used to classify the methods of vector relaxation of systems (VRS) for solving the equations of the discrete physical-topological mode. The main distinguishing properties of the VRS methods are 1) the basis and 2) the sequence of the solution of the systems of algebraic equations of the model. They can be classified precisely based on these two properties. Thus Hummel's method is a one-step VRS method in the basis R, n, p, $\delta\psi$, ψ of variables which are unknown grid vectors for the discrete model.* A number of other methods can be classified according to Table 1. In accordance with the table, in the short representation of the VRS method an opening brace { and a closing brace } are employed to distinguish the basis of each step. As a result the differences between the methods become obvious even in the short representation.

In accordance with the adopted approach to the classification the method studied below can be interpreted as a three-step VRS method.

Three-Step VRS Method. In solving the system (29)-(32) [1] we carried out a series of preliminary transformations. We shall quasilinearize the discrete analog of Poisson's equation with respect to the correction $\delta\psi$ taking into account (8) [1], more precisely, for fixed values of Q_n, Q_p, and T. This gives

$$A^{\psi}(n,\ p,\ T)\,\delta\psi = -E^{\psi}(\psi,\ n,\ p). \tag{12}$$

In transforming the discrete analogs of the continuity equations the linearization is performed by introducing three additional variables instead of R:

$$W = \tau_n [p + n_i(T)] + \tau_p [n + n_i(T)], \tag{13}$$

$$W_p = pW^{-1}, \tag{14}$$

$$W_n = nW^{-1}. \tag{15}$$

The transformation to the corrections δn and δp is performed next. This gives

$$A^{n}(\psi,\ T,\ W_p)\,\delta n = -E^{n}(\psi,\ n,\ T,\ W_p,\ W), \tag{16}$$

$$A^{p}(\psi,\ T,\ W_n)\,\delta p = -E^{p}(\psi,\ p,\ T,\ W_n,\ W). \tag{17}$$

A similar equation can also be derived for the correction δU:

$$B^{\psi}\delta U = -E^{u}(\psi,\ n,\ p,\ T,\ U). \tag{18}$$

The main point of the transformation to δn, δp, and δU lies in the fact that this transformation reduces the effect of the round-off errors, which is especially important in the analysis of functionally integrated elements. The specific form of A^{ψ}, E^{ψ}, A^{n}, E^{n}, etc., can be easily found from (29)-(32) [1] taking into account (20)-(28) of [1]; we omit it here because of its cumbersomeness. The boundary conditions are taken into account automatically just like in [7].

As a result the three-step VRS method can be represented as follows: 1) the starting approximation for ψ°, n°, p°, U° is given; 2) S1 = 0; 3) S1 = S1 + 1, S2 = 0; 4) S2 = S2 + 1, S3 = 0, and the discrete analogs of the Poisson equation and the continuity equations for holes and electrons with fixed T, i.e., T^{S1-1}, are solved simultaneously; 5) the discrete analog of Poisson's equation is solved by Newton's method for ψ with fixed Q_n and Q_p: a) m = 1, where m is the number of the Newton's iteration; b) (12) is solved for $\delta\psi^{m}$ for fixed A^{ψ} and E^{ψ}) $\psi^{S1,S2,m-1}$, $n^{S1,S2,S3,m-1}$, $p^{S1,S2,S3,m-1}$; c) the new values $\psi^{S1,S2,m} = \psi^{S1,S2,m-1} + \delta\psi^{m}$, and the concentrations $n^{S1,S2,S3,m} = n^{S1,S2,S3,m-1}\exp(\delta\psi^{m}/T^{S1-1})$, $p^{S1,S2,S3,m} = p^{S1,S2,S3,m-1}\exp(-\delta\psi^{m}/T^{S1-1})$, m = m + 1) are found; d) the substeps 5b and 5c are repeated a fixed number of times or in accordance with the criterion $|\delta\psi^{m}|_{max}/|\delta\psi^{m-1}|_{max} \geq K$, where $K \approx 10$ (after this the index m is dropped); 6) S3 = S3 + 1, the discrete analogs of the equa-

*In accordance with the notation of [1], n, p, ψ, etc., are grid vectors $\{n_{i,j}\}$, $\{p_{i,j}\}$, $\{\psi_{i,j}\}$, etc. In this part of the work i, j and the braces are omitted for simplicity.

tions of continuity are solved simultaneously by the VRS method with fixed ψ; 7) W^{S_3}, $W_p^{S_3}$, and $W_n^{S_3}$ are calculated according to (13)-(15) with fixed n^{S_1,S_2,S_3-1}, p^{S_1,S_2,S_3-1}; 8) (16) and (17) are solved for δn^{S_3}, δp^{S_3}, with fixed A^n, A^p, E^n, E^p) ψ^{S_1,S_2}, n^{S_1,S_2,S_3-1}, p^{S_1,S_2,S_3-1}, W^{S_3}, $W_n^{S_3}$, $W_p^{S_3}$; 9) the new values of $n^{S_1,S_2,S_3} = n^{S_1,S_2,S_3-1} + \delta n^{S_3}$, $p^{S_1,S_2,S_3} = p^{S_1,S_2,S_3-1} + \delta p^{S_3}$ are calculated; 10) the steps 6-9 are repeated either a fixed number of times NS3 or until the required convergence is achieved; 11) the steps 4-10 are repeated either a fixed number of times NS2 or until the required convergence is achieved (after this the indices S2 and S3 are dropped); 12) Eq. (18) is solved for δU^{S_1} with fixed E^u) ψ^{S_1}, n^{S_1}, p^{S_1}, U^{S_1-1}, T^{S_1-1}; 13) the new values of $U^{S_1} = U^{S_1-1} + \delta U^{S_1}$ and $T^{S_1} = (U^{S_1})^{-3}$ are found; 14) the steps 3-13 of the three-step VRS method are continued until the required accuracy is achieved. We note that when the upper right index is set to zero in any variable the last value of that variable is used automatically.

The foregoing method can be briefly written as follows: $\{\{\psi, \{Q_n, Q_p\}\}, \delta U, U, T\}$. In addition, the internal steps of the method (the steps 6-10) are implemented in practice, taking into account the linear relationship between n, p, and Q_n, Q_p for fixed ψ and T, in the basis n and p of the main variables. Therefore, they can be implemented as follows: $\{W, W_n, W_p, \delta n, \delta p, n, p\}$. The significance of this step lies in the fact that the total current density is conserved ($\nabla \mathbf{j}_T = 0$) at each iteration, denoted by index S2.*

The significance of the second set of steps (4-11) lies in the fact that the basic difficulty in implementing the model is the solution of the discrete analogs of the continuity and Poisson equations with fixed T. This is a reflection of the smaller contribution of self-heating compared with effect of the temperature of the surrounding medium on current transport in VLSIC elements. As a result of this, the changes in the temperature caused by self-heating are best taken into account after the discrete analogs of the continuity and Poisson equations have already been solved (for example, $|\delta\psi^1|_{max}$ is small and equals 0.1 in normalized units).

Universal Modeling Program. The method described above was used to develop a universal program for two-dimensional numerical simulation of semiconductor devices and structures UNTEMP. It is written in FORTRAN-IV for the ES series of computers (OS operating system) and its structure is similar to that of the PNAIIL program [2].

The main information output by UNTEMP is: 1) the distribution of the electrostatic potential ψ, the hole density p, the electron density n, the temperature T, and the current densities $\mathbf{j}_n$, $\mathbf{j}_p$, and $\mathbf{j}_T$ over the structure of the element; 2) the currents through the contacts.

The calculation of the latter quantities can be difficult in many cases (sometimes for very small values of expressions of the type $|(\psi_{i+2S,j} - \psi_{i,j})/(T_{i+2S,j} + T_{i,j})|$ at the contact [1]). It is not desirable to perform an enormous number of iterations, even with double-precision accuracy, in order to obtain superhigh accuracy in the calculation of the main variables for the purpose of subsequent calculation of the currents by integration of $\mathbf{j}_t$ over the contact, since tens and hundreds of iterations will be needed merely to suppress the roundoff errors. Different algorithms, realizable on a computer, for the construction and implementation of discrete models will behave differently in such situations. In addition, the following factors could have significant effect: 1) the parameters of the structure; 2) the applied voltages; 3) the spatial grid; 4) the methods employed to solve the systems of linear algebraic equations and their parameters; 4) the methods for calculating the coefficients of the difference scheme (for example, simply a transportation of the sequence of calculations†), leading to different propagation of roundoff errors in the computational process, and many others. In addition, the final results for the main variables will differ insignificantly (by less than 0.1%). In this connection, in calculating the currents in these situations the principle of conservation of the total current, i.e., the integral analog of $\nabla \mathbf{j}_T = 0$, can be employed successfully.

The main difficulty lies in the method used to select the integration contour ABC encompassing the contact (see Fig. 1). After this is done, the current through the contact I_c can

*This property should not be confused with the property of full conservativeness of the difference scheme [5], evaluated on the solution of the problem.

†The introduction of additional arithmetic operations can have a bad effect in this case.

TABLE 1. Classification of VRS Methods

Class	Method	Basis, short notation*
One-step	Hummel [4]	$\{R, n, p, \delta\psi, \psi\}$
One-step	Seidman-Chu [4]	$\{W, W_n, W_p, n, p, \delta\psi, \psi\}$
One-step	Pol'skii-Pokhvalina [5]	$\{W, W_n, W_p, n, p, \bar{\psi}\}$
One-step	Batalov–D'yakonov–Kremlev [6]	$\{\delta\psi, \psi, n, p, W, R, \delta\Phi_n, \delta\Phi_p, n, p\}$
One-step	[4]	$\{W, W_{Qn}, W_{Qp}, Q_n, Q_p, F\}$
Two-step	[3]	First step $\{F, Q\}$, where $Q = \{Q_n, Q_p\}$ Second step $\{W, W_{Qn}, W_{Qp}, Q_n, Q_p\}$ or, briefly, $\{F, \{W, W_{Qn}, W_{Qp}, Q_n, Q_p\}\}$

*The representation of the VRS methods in the short form corresponds to that adopted in the works indicated in the "Method" column.

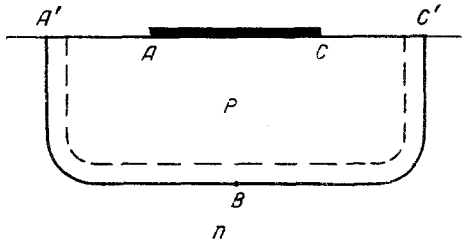

Fig. 1. Choice of the contour for the calculation of the current flowing through the contact.

be calculated from the formula

$$I_{\text{к}} = -\int\limits_{A'BC} \mathbf{j}_T \mathbf{N}_S dl.$$

Several concrete variants of methods for selecting the contour for a bipolar transistor are given in [8, 9]. We employed quite general variants, admitting automation of the process, namely, 1) the encompassing contour within the structure of the element is chosen to pass between neighboring nodes of the grid, for which relations of the type $k_2 \leq |(\psi_{i+2S,\,j} - \psi_{i,\,j})/(T_{i+2S,\,j} + T_{i,\,j})| \leqslant K_1$ hold in the perpendicular direction, while violations of this rule are allowed only on the surface (segments A'A and CC') through which current does not flow [1]; 2) the component of the total current density perpendicular to the contact is calculated on a coarser grid, obtained by eliminating nodes from the grid in the corresponding direction, and in addition for the new grid a condition of the type $|(\psi_{n+2S,\,r} - \psi_{n,\,r})/(T_{n+2S,\,r} + T_{n,\,r})| \geqslant K_2$, must hold, where n and r enumerate the nodes of the coarse grid, while $\psi_{n+2S,r}$, $\psi_{n,r}$, $T_{n,r}$, $T_{n+2S,r}$ are the values of the variables which have already been calculated at the nodes of the fine grid that coincide with the nodes of the coarse grid. Both methods give good results. Although the first method is more accurate, the second method is applicable in practically all cases.

The different electric parameters of the elements can be easily calculated based on the indicated output information (especially from the Current–voltage characteristics).

NOTATION

T, temperature; T_{env}, temperature of the environment; Q_T, density of the power released in the element; $\mathbf{j}_p$, $\mathbf{j}_n$, and $\mathbf{j}_T$, hole current, electron current, and total current density vectors; q, electron charge; μ_p and μ_n, mobilities of the holes and electrons; μ_{p0} and μ_{n0}, values of μ_p and μ_n in weak fields; p and n, hole and electron densities; Φ_p and Φ_n, Fermi quasilevels of holes and electrons; R, excess of the recombination rate above the generation rate; n_i, intrinsic density; τ_n and τ_p, electron and hole lifetimes; N_d and N_a, densities of ionized donors and acceptors; ρ, volume charge density; V_{app}, applied voltage; N_S, normal to the boundary; k, Boltzmann's constant; U, an auxiliary variable, equal to $T^{-1/3}$ [1]; S1, S2,

and S3, numbers of iterations at the first, second, and third steps of the VRS method; Z^{S_1}, value of the variable Z at the S1-th iteration; Q_n and Q_p, auxiliary variables, equal to $n_i \exp(-\Phi_n/T)$ and $n_i \exp(\Phi_p/T)$, respectively (normalized form); Z_{ij}, value of the variable Z at the node of the spatial grid with indices i and j; and K_1 and K_2, parameters.

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