NUMERICAL ANALYSIS OF FUNCTIONALLY INTEGRATED VLSIC ELEMENTS TAKING INTO ACCOUNT THERMAL EFFECTS. I. MODEL

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A discrete physical-topological model intended for calculating the elements of VLSIC taking thermal effects into account is studied.

An important problem in the physics of semiconductor devices is multidimensional numerical analysis of functionally integrated elements (FIE) of very large scale integrated circuits (VLSIC) taking into account thermal effects, which impose a fundamental (principal) limit on the increase in the degree of integration of VLSIC [1]. In this connection, in this work, which consists of three parts, we describe a model (part I), a method, and a program (part II), and the results (part III) of two-dimensional modeling of FIE of VLSIC with injected power in the stationary case taking into account the mutual effect of self-heating and the temperature of the environment.

Starting Model. The continuous model is based on the fundamental system of equations for the physics of semiconductors, supplemented by the equation of heat conduction, namely [2]:

$$\varepsilon\nabla^2\psi = -q(p - n + N_d - N_a), \tag{1}$$

$$\nabla\mathbf{J}_p = -qR, \tag{2}$$

$$\nabla\mathbf{J}_n = qR, \tag{3}$$

$$\mathbf{J}_p = -q\mu_p p\nabla\psi - kT\mu_p\nabla p, \tag{4}$$

$$\mathbf{J}_n = -q\mu_n n\nabla\psi + kT\mu_n\nabla n, \tag{5}$$

$$\nabla K\nabla T = -Q_T \tag{6}$$

with the auxiliary relations

$$Q_T = (\mathbf{J}_T\cdot\mathbf{E}), \tag{7}$$

$$n = n_i\exp[q(\psi - \Phi_n)/kT],\quad p = n_i\exp[q(\Phi_p - \psi)/kT]. \tag{8}$$

The recombination-generation processes are described by the traditional Shcokley–Read–Hall model, while the well-known formula from [3] is employed for the mobility at T_0 = 300 K. In addition, in this work, like in [2], the field dependence of the mobility in forward-biased p-n junctions is neglected. The temperature dependence of the mobility was described with the help of a formula from [4], and the model described in [2] was employed for the intrinsic density. The coefficient of thermal conductivity of silicon is described by the formula presented in [2].

The boundary conditions are given directly for the four basic unknowns n, p, ψ, and T. For the surfaces of an element, not covered with ohmic contacts, the following relations are employed:

$$\nabla n\cdot\mathbf{N}_S = \nabla p\cdot\mathbf{N}_S = \nabla\psi\cdot\mathbf{N}_S = 0, \tag{9}$$

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TABLE 1. Normalizing Coefficients

Normalized quantity	Notation	Formula	Value
Temperature	T	T_0	300 K
Potentials	ψ, Φ_n, Φ_p, V_{app}	$\varphi_{T_0} = kT_0/q$	0,0258 V
Coordinates	x, y	$L_D = \sqrt{\frac{\varepsilon\varphi_{T_0}}{qn_i(T_0)}}$	$3{,}31\cdot10^{-3}$ cm
Charge density	n_i, p, n, N_d, N_a	$n_i(T_0)$	$1{,}5\cdot10^{10}$ cm^{-3}
Diffusion coefficients	$\frac{kT}{q}\mu_n$, $\frac{kT}{q}\mu_p$	D_0	1 cm^2/sec
Mobility	μ_n, μ_p	D_0/φ_{T_0}	38,7 cm^2/(V·sec)
Current density	$\mathbf{J}_T$, $\mathbf{J}_p$, $\mathbf{J}_n$	$qD_0n_i(T_0)/L_D$	$0{,}725\cdot10^{-6}$ A/cm^2
Recombination-generation rate	R	$D_0n_i(T_0)/L_D^2$	$1{,}37\cdot10^{15}$ cm^{-3}·sec^{-1}
Lifetime	τ_n, τ_p	L_D^2/D_0	$1{,}1\cdot10^{-5}$ sec
Coefficient of thermal conductivity	K	$K(T_0)$	1,5486 W/(cm·K)

where N_S is the normal to the surface. The electrostatic potential and the mobile carrier density on the ohmic contacts are calculated with the hlep of the following relations:

$$\psi|_{o.c} = V_{app} + (kT/q)\,\mathrm{sign}\,(N_d - N_a)\ln\left[\sqrt{\left(\frac{N_d - N_a}{2n_i}\right)^2 + 1} + \left|\frac{N_d - N_a}{2n_i}\right|\right], \tag{10}$$

$$n|_{o.c} = n_i\left[\sqrt{\left(\frac{N_d - N_a}{2n_i}\right)^2 + 1} + \left(\frac{N_d - N_a}{2n_i}\right)\right], \tag{11}$$

$$p|_{o.c} = n_i\left[\sqrt{\left(\frac{N_d - N_a}{2n_i}\right)^2 + 1} - \left(\frac{N_d - N_a}{2n_i}\right)\right]. \tag{12}$$

The boundary conditions for the heat-conduction equation (6) are as follows: 1) at the housing–crystal boundary the temperature $T_{h.c}$ is constant and equals the temperature of the environment T_{env}:

$$T_{h.c} = T_{env}; \tag{13}$$

2) there is no heat flux through the remaining surfaces surrounding the element:

$$\nabla T \cdot \mathbf{N}_S = 0. \tag{14}$$

To decrease the volume of computer calculations, in the starting model under study the variables are normalized. The values of the coefficients are given in Table 1. After the variables are normalized and a number of simple transformations are performed, the basic equations (1)-(8) reduce to the following:

$$\nabla^2\psi = n - p - N_d + N_a, \tag{15}$$

$$\nabla\left[\mu_p(p\nabla\psi + T\nabla p)\right] = R, \tag{16}$$

$$\nabla\left[\mu_n(n\nabla\psi - T\nabla n)\right] = -R, \tag{17}$$

$$\nabla^2 U = \varkappa(\mathbf{J}_T \cdot \mathbf{E})/3, \tag{18}$$

$$n = n_i\exp\left[(\psi - \Phi_n)/T\right],\quad p = n_i\exp\left[(\Phi_p - \psi)/T\right], \tag{19}$$

where $U = T^{-1/3}$. The corresponding normalized form of the relations (9)-(14) can be easily derived, and is thus omitted here.

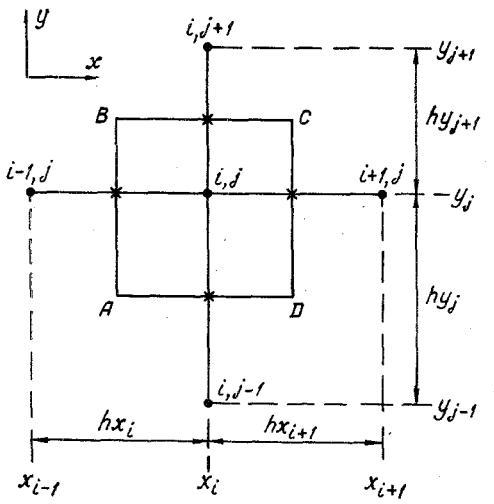

Fig. 1. Grid template.

Discrete Physical-Topological Model. The system of equations studied above and the auxiliary relations, comprising the continuous model, cannot be solved for n, p, ψ, T(U). Because of this, with the help of the method of finite differences we transfer from the starting continuous model to the discrete model. To this end, on a grid covering the apparatus we apply to Eqs. (15)-(19) the integrointerpolation approach of A. N. Tikhonov and A. A. Samarskii and, in particular, the method of G. I. Marchuk [5] together with the hierarchy of physical assumptions for approximating the integrals.

The single physical assumption that the charge density ρ in the cell ABCD remains constant is employed for Poisson's equation in the approximate problem on a fragment of the grid (Fig. 1). This leads to the following finite-difference approximation of Poisson's equation for the internal nodes of the grid (i, j):

$$A^{\psi}_{i,j}\psi_{i-1,j} + B^{\psi}_{i,j}\psi_{i+1,j} + D^{\psi}_{i,j}\psi_{i,j-1} + E^{\psi}_{i,j}\psi_{i,j+1} + C^{\psi}_{i,j}\psi_{i,j} = F^{\psi}_{i,j}, \tag{20}$$

where

$$A^{\psi}_{i,j} = 0{,}5\,(hy_{j+1} + hy_j)/hx_i;\ B^{\psi}_{i,j} = A^{\psi}_{i+1,j};$$

$$D^{\psi}_{i,j} = 0{,}5\,(hx_{i+1} + hx_i)/hy_j;\ E^{\psi}_{i,j} = D^{\psi}_{i,j+1};$$

$$C^{\psi}_{i,j} = -(A^{\psi}_{i,j} + B^{\psi}_{i,j} + D^{\psi}_{i,j} + E^{\psi}_{i,j});$$

$$F^{\psi}_{i,j} = \rho_{i,j}\,(hx_i + hx_{i+1})(hy_{j+1} + hy_j)/4;$$

$$\rho_{i,j} = (n_i)_{i,j}\exp\left[(\psi_{i,j} - \Phi_{ni,j})/T_{i,j}\right] - (n_i)_{i,j}\ \exp\left[(\Phi_{pi,j} - \psi_{i,j})/T_{i,j}\right] - N_{\mathrm{d}i,j} + N_{ai,j}.$$

To complete the construction of the difference scheme a finite difference approximation of the boundary conditions must be constructed. The method of internal boundary conditions is employed on the free surfaces. This means that, for example, the approximation $\partial\psi/\partial x = 0$ is performed with the help of formulas of the form $(\psi_{1,j} - \psi_{2,j})/hx_2 = 0$, and in addition the point with the indices 1, j lies on the boundary of the element and the environment. It is not difficult to verify that the value of the potential $\psi_{1,j}$ sought in this case will be determined with second-order accuracy relative to the unknown value at the internal node $\psi_{2,j}$.

Let us examine the question of constructing difference schemes for the continuity equations. We note that Eqs. (4) and (5) were written under the assumption that the effect of the thermal currents of holes and electrons can be neglected [6]. In this connection, in approximating the continuity equations we employ the assumption that the temperature is constant over the structure of the element. We shall study the equation of continuity of holes (16). In approximating it with the help of the method of G. I. Marchuk we employ the following physical assumptions: 1) the electrostatic potential varies linearly; 2) the rate of recombination-generation R on the cell ABCD (see Fig. 1) is constant; and, some other assumptions. This leads to the following approximation at the internal node i,j:

$$[(a_{i+1/2,j}+a_{i-1/2,j})h_2+(a_{i,j+1/2}+a_{i,j-1/2})h_1]p_{i,j}-$$

$$-d_{i+1/2,j}h_2p_{i+1,j}-d_{i-1/2,j}h_2p_{i-1,j}-d_{i,j+1/2}h_1p_{i,j+1}-d_{i,j-1/2}h_1p_{i,j-1}=-R_{i,j}h_1h_2, \tag{21}$$

where $h_1=(hx_{i+1}+hx_i)/2$; $h_2=(hy_{j+1}+hy_j)/2$;

$$a_{i+s,j}=\mu_{pi+s,j}\frac{[(\psi_{i+2s,j}-\psi_{i,j})/hx_{i+1/2+s}]}{\exp[2(\psi_{i+2s,j}-\psi_{i,j})/(T_{i+2s,j}+T_{i,j})]-1}; \tag{22}$$

$$d_{i+s,j}=a_{i+s,j}\exp[2(\psi_{i+2s,j}-\psi_{i,j})/(T_{i+2s,j}+T_{i,j})], \tag{23}$$

and s assumes the values $-1/2$ and $1/2$.

The foregoing approximations for the coefficients $a_{i+s,j}$ and $d_{i+s,j}$ are employed when $\Delta\psi T\in[\varepsilon_1^p,\ \varepsilon_2^p]$, where $\Delta\psi T=|2(\psi_{i+2s,j}-\psi_{i,j})/(T_{i+2s,j}+T_{i,j})|$; ε_2^p is determined by the word length of the computer employed (for the ES computer $\varepsilon_2{}^p\leq 174$), while $\varepsilon_1^p\in[10^{-5},\ 10^{-2}]$. In the case when $\Delta\psi T<\varepsilon_1{}^p$, the following expressions are employed for $a_{i+s,j}$ and $d_{i+s,j}$:

$$a_{i+s,j}=-0{,}5\mu_{pi+s,j}[(\psi_{i+2s,j}-\psi_{i,j})-(T_{i+2s,j}+T_{i,j})]/hx_{i+1/2+s}; \tag{24}$$

$$d_{i+s,j}=0{,}5\mu_{pi+s,j}[(\psi_{i+2s,j}-\psi_{i,j})+(T_{i+2s,j}+T_{i,j})]/hx_{i+1/2+s}. \tag{25}$$

This situation appears often in quasineutral regions of the structure. A number of other approximations can also be employed instead of (24) and (25), but in so doing Ohm's law may not be obeyed when it should be obeyed. For $\Delta\psi T>\varepsilon_2{}^p$ two different situations arise. When $(\psi_{i+2s,j}-\psi_{i,j})>0$:

$$a_{i+s,j}=0;\ d_{i+s,j}=\mu_{pi+s,j}(\psi_{i+2s,j}-\psi_{i,j})/hx_{i+s+1/2}, \tag{26}$$

and when $(\psi_{i+2s,j}-\psi_{i,j})<0$:

$$a_{i+s,j}=-\mu_{pi+s,j}(\psi_{i+2s,j}-\psi_{i,j})/hx_{i+1/2+s};\ d_{i+s,j}=0. \tag{27}$$

It should be emphasized that the cases (26) and (27), studied above, do not necessarily arise for large reverse biases, but they are often encountered at low temperatures. As a result, they must be taken into account in constructing a discrete model taking into account thermal effects.

Expressions for the other coefficients $a_{i,j+s}$, $d_{i,j+s}$ $(s=\pm 1/2)$ can be easily derived by interchanging the indices and replacing hx by hy. We note that at T = 300 K, in the one-dimensional case, the foregoing finite-difference approximation to the continuity equation is identical to the formulation of the Sharfetter–Gummel type [7]. The boundary conditions can also be approximated by the method of internal boundary conditions. A difference scheme is also constructed by an analogous method for the equation of continuity for electrons (17).

The finite-difference approximation of Eq. (18) can be derived by the method of G. I. Marchuk using the physical assumption that the density of the power liberated in the cell ABCD remains constant. This leads to the following approximation at the internal node i, j:

$$A_{i,j}^{\psi}U_{i-1,j}+B_{i,j}^{\psi}U_{i+1,j}+D_{i,j}^{\psi}U_{i,j-1}+E_{i,j}^{\psi}U_{i,j+1}+C_{i,j}^{\psi}U_{i,j}=F_{i,j}^{U}, \tag{28}$$

where $F_{i,j}{}^U=\kappa(J_{Tx}E_x+J_{Ty}E_y)_{i,j}$. The boundary conditions can also be approximated by the method of internal boundary conditions.

As a result of the foregoing transformations we obtain a complete difference shceme, consisting of the difference schemes for the Poisson equation, the equations of continuity for electrons and holes, and the analog of the heat-conduction equation. Their matrix form is:

$$B^{\psi}\psi=F^{\psi}, \tag{29}$$

$$B^{n}n=F^{n}, \tag{30}$$

$$B^p p = F^p, \tag{31}$$

$$B^\psi U = F^U. \tag{32}$$

The complete form of the matrix of coefficients B^ψ, B^n, B^p and the column vectors F^ψ, F^n, F^p, F^U can be derived by the foregoing method (see (20)-(28)). This system of coupled nonlinear algebraic matrix equations (29)-(32), supplemented by a relation coupling U and T, comprises the discrete physical-topological model of FIE of VSLIC taking into account thermal effects. To implement the model, it must be solved for the unknown grid vectors, i.e., $\{\psi_{i,j}\}$, $\{n_{i,j}\}$, $\{p_{i,j}\}$, $\{T_{i,j}\}$, $\{U_{i,j}\}$, where the indices i, j run through all values for the grid covering the element. In conclusion, we note that after the grid vectors are found, the unnormalized values of the quantity sought can be easily calculated with the help of the coefficients given in the table.

NOTATION

ε, dielectric constant of the semiconductor; ψ, electrostatic potential; n and p, electron and hole densities; N_d and N_a, densities of ionized donors and acceptors; J_p and J_n, hole and electron current density vectors; q, electron charge; R, excess of the recombination rate over the generation rate; μ_p and μ_n, hole and electron mobilities; k, Boltzmann's constant; T, temperature; K, coefficient of thermal conductivity of silicon; Q_T, density of the power liberated in the elements; J_T, total current density vector ($J_T = J_p + J_n$); E, electric field intensity ($E = -\nabla\psi$); n_i, intrinsic density; Φ_n, Φ_p, quasi-Fermi levels of electrons and holes; τ_p, τ_n, lifetimes of holes and electrons; μ_0, mobility at $T = T_0$; V_{app}, voltage applied to the ohmic contact; $Z_{i,j}$, value of the variable Z at the node of the spatial grid with indices i, j; J_{Tx}, J_{Ty}, X and Y components of the total current density vector; E_x and E_y, components of the electric field intensity vector; and κ, dimensionless coefficient of the transformation from (6) to (18), equal to $1.3367 \cdot 10^{-13}$ for silicon.

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