THE USE OF FACTORIZATION METHODS FOR SOLVING THE CHARGE TRANSFER EQUATIONS IN SEMICONDUCTOR DEVICES

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The paper presents the results of the application of the known factorization method for continuity equations for electrons and holes. It is shown that the Buleev-Stone method traditionally employed in the given situation yields considerably to another version of the factorization method. The explicit expressions for iterative formulae in both cases are represented.

Introduction

At present there is published a considerable number of papers [1-6] devoted to the application of the factorization methods for solving the equations of mathematical physics. The substantiation of the factorization algorithms convergence is carried out mainly for the cases when a system of difference equations approximating the initial differential equations satisfies the diagonal predominance condition. In practice in a number of cases such a predominance is absent as, f.e., for equations of electron and hole transfer in semiconductor. In this situation up to now the Buleev factorization method has been traditionally used which enables one to find the solution also in the absence of the diagonal predominance. In the present paper there is suggested for the mentioned case to make use of the known modification of the Buleev method which allows to reduce essentially the computational efforts for deriving the solution.

I. The governing equation and the difference scheme

An equation describing the electrons transfer in a semiconductor in the diffusion-drift approximation after the passage to the dimensionless variables has the following form

$$\nabla(\nabla n - \mu n \nabla\varphi) = \frac{np-1}{\tau_p(1+n)+\tau_n(1+p)} \qquad (I)$$

Here , and , are the density and the life time of electrons and holes, respectively, is the electron mobility, is the electrostatic potential. Making use of the integral-interpolation Samarsky's formula 7 or of the Marchuk's integral identity 8 , one can derive the difference scheme 9 approximating the equation (I)

$$-a_{ij}n_{i-1j} - b_{ij}n_{ij-1} + e_{ij}n_{ij} - c_{ij}n_{i+1j} - d_{ij}n_{ij+1} = f_{ij} \qquad (2)$$

where $a_{ij} = \mu B(\varphi_{i-1j} - \varphi_{ij})/h_{i-1}$; $b_{ij} = \mu B(\varphi_{ij-1} - \varphi_{ij})/r_{j-1}$;

$c_{ij} = \mu B(\varphi_{i+1j} - \varphi_{ij})/h_i$; $d_{ij} = \mu B(\varphi_{ij+1} - \varphi_{ij})/r_j$;

$f_{ij} = 1/(\tau_p(1+n^0_{ij}) + \tau_n(1+p^0_{ij}))$;

$e_{ij} = \mu(B(\varphi_{ij} - \varphi_{i-1j})/h_{i-1} + B(\varphi_{ij} - \varphi_{ij-1})/r_{i-1} +$

$+ B(\varphi_{ij} - \varphi_{i+1j})/h_i + B(\varphi_{ij} - \varphi_{ij+1})/r_j) + f_{ij}\,p^0_{ij}$

The Bernoulli function $B(u) = u/(\exp(u)+1)$ steps in the coordinates $h_i = x_{i+1} - x_i$; $r_j = y_{j+1} - y_j$. The upper index 0 designates the values from the foregoing Gummel iteration. It is obvious from the form of coefficients of Eq.(2) that the diagonal predominance does not hold in this case. For solving the Eq.(I) there exist two alternatives: either pass on to the variables $\Phi_n = n\exp(-\varphi)$ and $\Phi_p \exp(\varphi)$, then write down the difference scheme which will satisfy the diagonal predominance condition or find an efficient method of solving the system (2). The first means is undesirable because a computer cannot operate at too large and too small numbers and the variables values Φ_n and Φ_p can change by many orders in virtue of the exponential character of the dependence on the applied voltage. So for the MOSFET's with the voltage on the substrate -5 and on the drain +5 the values of the mentioned variables chane more than by 150 orders, that it is inadmissible for most computers. In real schemes the MOSFET's function at the voltages up to a few tens of volts.

The difficulties of the work with a system of equations not satisfying the diagonal predominance condition are associated with the fact that a number of efficient methods ceases to converge at such conditions (as, f.e., the method of incomplete factorization and parabolic sweeps [1,6]). Many methods converge extremely slowly because a system of equations (2) is ill-conditioned (so, f.e., the

Zeidel method and the over relaxation method converge in thousand and more iterations). The Buleev-Stone method [3,4] without application of "canceling" (the iterative parameter in the method [4] is equal to zero) has proved to be sufficiently efficient method for solving the problem (2) which up to now is used in the applied computational programs of the semiconductor devices. In paper 5 there has been suggested the Stone method modification which is tested when solving the heat conduction equation and has proved to be more efficient as compared with the Stone method. In the given work there is carried out the comparison of the methods [4] and [5] when applied to the system (2).

II. Two means of constructing the factorization schemes

Write down a system of equations (2) in the matrix form

$$\Omega_{\ell_k} n_k = f_\ell \qquad (2a)$$

Here Ω_{ℓ_k} is the pentadiagonal matrix of the dimension $(N\,M) \times (N\,M)$, n_k is the vector of the solution, f_ℓ is the right-hand side vector. The correspondence of the indices i, j and k is set by the formula $k=(j-1)\cdot M+i$. The correspondence of the matrix coefficients Ω_{ℓ_k} to those of the system (2) is represented in Fig.I. Attempt to approximate as much as possible the matrix Ω_{ℓ_k} by the product of the lower triangular matrix L_{ℓ_m} and the upper triangular U_{m_k} matrix having the four-diagonal structure (see Fig.2). Performing the multiplication of the matrices L and U and equating $\Omega_{\ell_k}=(LU)_{\ell_k}$, we arrive at a system of equations relating the coefficients μ, ν, λ of the matrix L and those $\gamma, \delta, \varkappa, \rho$ of the matrix U with the coefficients of the governing system (2).

$$\begin{cases} e_\ell = \gamma_\ell + \lambda_\ell \delta_{\ell-1} + \mu_\ell \varkappa_{\ell-M+1} + \nu_\ell \rho_{\ell-M} \\ -a_\ell = \lambda_\ell \gamma_{\ell-1} + \nu_\ell \varkappa_{\ell-M} \\ -b_\ell = \nu_\ell \gamma_{\ell-M} \\ -c_\ell = \delta_\ell + \mu_\ell \rho_{\ell-M+1} \end{cases} \qquad (3)$$

$$\begin{cases} \alpha_\ell = \lambda_\ell \varkappa_{\ell-1} \\ \beta_\ell = \mu_\ell \delta_{\ell-M+1} \end{cases} \qquad (4)$$

For certainty we shall speak about electrons though all the said is referred to an equal extent to the holes also.

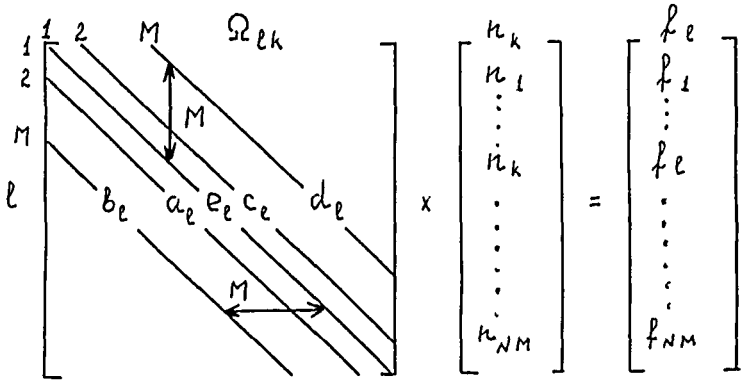
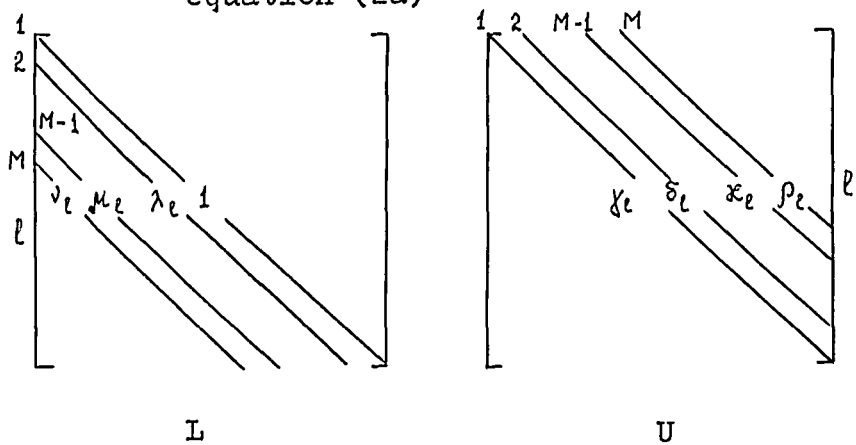


Fig. 1 Schematic representation of the matrix equation (2a)



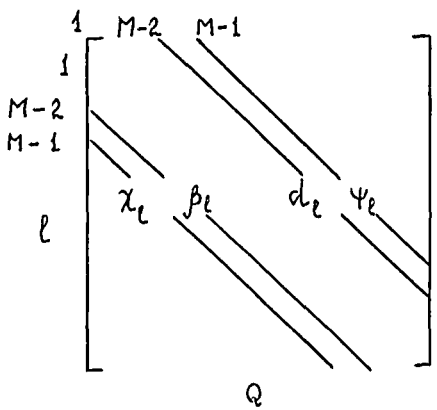


Fig. 2 Schematic representation of the matrices L, U, Q

$$\begin{cases} \Psi_\ell = \varkappa_\ell + \lambda_\ell \delta_{\ell-1} \\ \chi_\ell = \mu_\ell \gamma_{\ell-M+1} + \nu_\ell \delta_{\ell-M} \end{cases} \qquad (5)$$

As it can be easily seen, we have a system of nine equations with seven unknown quantities for each value of $\ell = 1,2,\ldots, M \cdot N$, i.e. it is impossible to represent the matrix $\Omega_{\ell k}$ exactly in the form of the product of two triangular matrices. As a result there remain either the "superfluous" diagonals α, β or Ψ, χ. The version $\alpha_\ell = \beta_\ell = 0$ corresponds to the Buleev-Stone method [3,4], and the version $\Psi_\ell = \chi_\ell = 0$ corresponds to the method stated in 5 (with the zero value of the iterative parameter). To complete a picture, we represent the expressions for computing the coefficients of the triangular matrices:

For the case (4):

$$\mu_\ell = 0;\ \varkappa_\ell = 0;\ \delta_\ell = -c_\ell;\ \rho_\ell = -d_\ell;$$
$$\gamma_\ell = e_\ell - \lambda_\ell \delta_{\ell-1} - \nu_\ell \rho_{\ell-M} = e_\ell + c_{\ell-1}\lambda_\ell + d_{\ell-M}\nu_\ell \qquad (6)$$
$$\lambda_\ell = -a_\ell/\gamma_{\ell-1};\ \nu_\ell = -b_\ell/\gamma_{\ell-M};\ \Psi_\ell = \varkappa_\ell + \lambda_\ell \rho_{\ell-1};\ \chi_\ell = \mu_\ell \gamma_{\ell-M+1} + \nu_\ell \delta_{\ell-M};$$

at that $\lambda_\ell = 0$; $\nu_\ell = 0$ at $\ell \le M$ in virtue of the coefficients a_ℓ and b_ℓ determination (at greater length see [4,5]);

for the case (5):

$$\rho_\ell = -d_\ell;\ \nu_\ell = -b_\ell/\gamma_{\ell-M};\ \gamma_\ell = e_\ell - \lambda_\ell \delta_{\ell-1} - \mu_\ell \varkappa_{\ell-M+1} + \nu_\ell d_{\ell-M};$$
$$\mu_\ell = -\nu_\ell \delta_{\ell-M}/\gamma_{\ell-M+1};\ \lambda_\ell = -(\nu_\ell \varkappa_{\ell-M} + a_\ell)/\gamma_{\ell-1}; \qquad (7)$$
$$\varkappa_\ell = \lambda_\ell d_{\ell-1};\ \delta_\ell = -c_\ell + \mu_\ell d_{\ell-M+1};\ d_\ell = \mu_\ell \delta_{\ell-M+1};\ \beta_\ell = \lambda_\ell \varkappa_{\ell-1};$$

as in the case (6) $\lambda_\ell = 0$ for $\ell = 1$; $\nu_\ell = 0$ for $\ell \le M$.

The iterative process of finding the solution is constructed in the following way: at first a value of the auxiliary variable shouls be found

$$z_m = u_{mk} h_k^{t+1} = \sum_{\ell=1}^{NM} (L^{-1})_{m\ell} \left(f_\ell + \sum_{s=1}^{NM} Q_{\ell s} h_s^t \right) \qquad (8)$$

where $Q_{\ell s}$ is the matrix embodying the "superfluous" diagonals, the rest of its elements equals zero, t being the iteration number. Then we find the solution

$$h_k^{t+1} = (U^{-1})_{km} z_m \qquad (9)$$

For convenience we represent the explicit formula for (8,9) in the case of using the schemes (6) and (7).

For the scheme (6) we have a direct sweep

$$(m = 1,2,\ldots,NM)$$

$$Z_m = -\lambda_m Z_{m-1} - \nu Z_{m-M} + f_m + \nu_m \delta_{m-M} h^t_{m-M+1} + \lambda_m \rho_{m-1} h^t_{m+M-1} = \quad (10)$$

$$= f_m + \frac{a_m}{\gamma_{m-1}}(d_{m-1} h^t_{m+M-1} + Z_{m-1}) + \frac{\beta_m}{\gamma_{m-M}}(c_{m-M} h^t_{m-M+1} + Z_{m-M}),$$

and a reverse sweep ($m = NM, NM-1, \ldots, 1$

$$h^{t+1}_m = (Z_m - \delta_m h^{t+1}_{m+1} - \rho_m h^{t+1}_{m+M})/\gamma_m = (Z_m + c_m h^{t+1}_{m+1} + d_m h^{t+1}_{m+M}) \quad (11)$$

Similarly for the scheme (7) we have for

$m = 1,2,\ldots,NM$

$$Z_m = f_m + \mu_m(\delta_{m-M+1} h^t_{m-M+2} - Z_{m-M+1}) + \lambda_m(\varkappa_{m-1} h_{m+M-2} - Z_{m-1}) - \quad (12)$$
$$- \nu_m Z_{m-M}$$

and for $m = NM, NM-1, \ldots, 1$

$$h^{t+1}_m = (Z_m - \delta_m h^{t+1}_{m+1} - \varkappa_m h^{t+1}_{m+M-1} - \rho_m h^{t+1}_{m+M})/\gamma_m \quad (13)$$

The method [3,4] without "canceling" is given by expressions (2,6,10,11) and the method [5] by expressions (2,7,12,13).

III. Computational results

A comparison of the schemes (6) and (7) efficiency is carried out at the example of the solution of the continuity and Poisson equation for the MOSFET in the two-dimensional approximation.

The results are represented in Table I and in Figs. 3a,b. There is considered a case of the MOSFET with the impurity concentration: in regions of the source and the drain 10^{20} cm, in the substrate $10^{}$ cm , applied voltage to the source 0, to the substrate 0, to the drain +3 and to the gate +5 volts, the efficient channel length 3.5 μm. It is seen from the table that the scheme (7) is essentially more economical with respect to the number of iterations. So for the continuity equation for holes and for the Poisson equation it is required two timess less iterations for achieving the same accuracy and for solving the continuity equation for electrons it is required even 3-4 times less iterations. Since the number of operations needed for one iteration is close in both cases, the time of the central processor needed for solving the equation in the case of using the scheme (7) is less. For the first two equations it is less 1.5-1.7 times, for the latter - 2.5-3.5 times.

Table I

N_G	1	2	3	4	5	6	7	8
n	61	47	42	38	36	34	32	31
	13	12	11	11	10	10	10	9
p	152	59	56	53	47	42	35	31
	80	33	32	26	23	19	13	11
φ	64	63	62	61	60	58	56	54
	30	29	29	29	28	28	27	26

N_G	9	10	11	12	13	14	15
n	30	29	28	27	27	26	25
	9	9	9	9	9	9	8
p	28	23	18	16	16	16	15
	10	8	6	7	8	7	7
φ	53	50	47	40	38	38	36
	25	25	23	19	19	18	16

The number of iterations necessary for achieving the preset residual by solving the continuity equations for electrons (n) and holes (p), and the Poisson equation (φ) for the given number of Gummel iteration N_G. The upper number is the number of iterations necessary for the method (2,6, 10,11); the lower one for the method (2,7,12,13).

The dependence of the residual on the iteration number is given in Figs. 3a,b for the continuity equation of electron and hole, respectively. It is seen that in all the cases the scheme (7) has proved to be

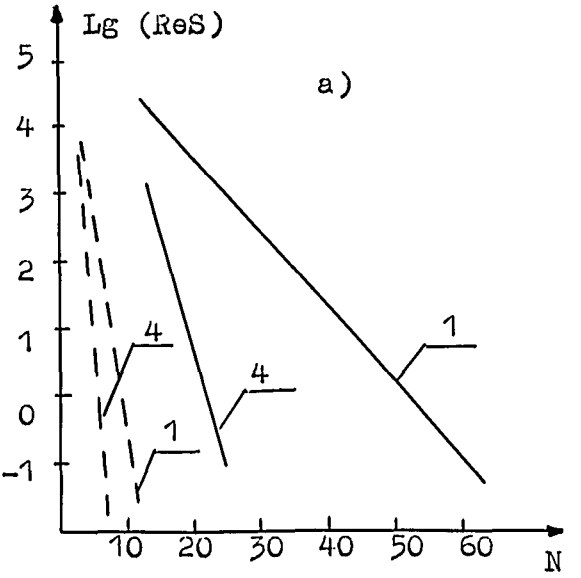
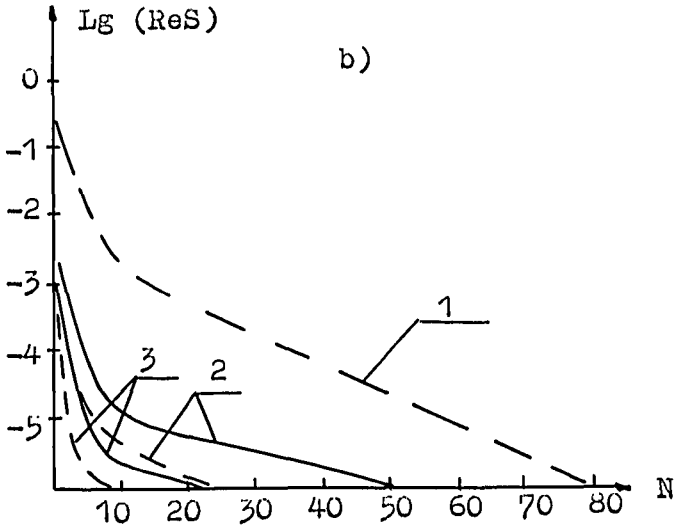


Fig 3



Figs. 3a,b Dependence of the decimal logarithm of residual of solving the continuity equation for electrons (a) and holes (b) on the iteration number.

——— - method (2,6,10,11)
- - - - - method (2,7,12,13)
1,2,3,4 - 1-st, 5-th, 10-th and 15-th Gummel iteration

more efficient. The residual was determined via the formula

$$R_e^t S = \max_{\ell=1,2,\dots,NM} | \Omega_{\ell k} n_k^t - f_\ell |$$

at that the coefficients of the governing system were normalized by a central one so that $\varrho_\ell \equiv 1$.

Conclusions

The method suggested in [5] without "canceling" (the iterative parameter is equal to zero) whose computational formulae are given in (2,7,12,13) is more efficient than the other methods employed nowadays for solving the charge transfer equation in semiconductor devices. The method is easily programmed, it can be applied to systems without diagonal predominance.

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