NUMERICAL TECHNIQUE TO SOLVE NONLINEAR ELLIPTIC PDE's ARISING FROM SEMICONDUCTOR DEVICE MODELING.

Rakesh K. Sharma and John R. Rice

Abstract

Based on the partitioning principle and approximating the nonlinear terms with a linear system which is to be solved for the coefficient matrix, a new numerical technique is developed for the scaled model where it is assumed that mobilities are constant and Einstein relations are valid. We have also introduced new variables α, β and γ inside the nonlinear system, which help us control the discretization error and assure convergence of the sequence of approximate solutions.

Numerical method and experimental results

We use the scaled model given in [7], where it is assumed that mobilities are constant and Einstein relations are valid. It is common to introduce the "quasi-fermi levels" v and w defined through $n = e^{u-v}$ and $p = e^{w-u}$. The simulation problem is given by the following system of partial differential equations, now written in terms of the (x, y) coordinate system.

$$\begin{aligned} \lambda^2(u_{xx} + u_{yy}) - e^{u-v} + e^{w-u} + k_1 &= 0 \\ e^{u-v}[v_{xx} + v_{yy} + (u_x - v_x)v_x + (u_y - v_y)v_y] &= 0 \\ e^{w-u}[w_{xx} + w_{yy} + (w_x - u_x)w_x + (w_y - u_y)w_y] &= 0 \end{aligned} \tag{1.1}$$

The solutions are subject to an appropriate mixed boundary conditions described in [7].

A typical domain for a semiconductor is shown in Figure 1, which describes the domain for two-dimensional model of an n-channel MOSFET. The electric potentials are applied at the *source, gate, drain* and *backgate* contacts.

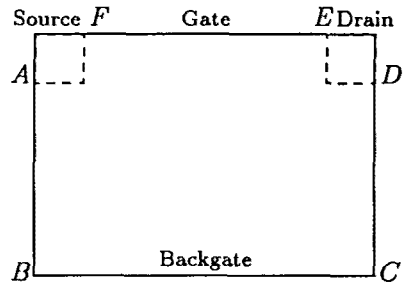

Figure 1. Two dimensional domain for a typical semiconductor model.

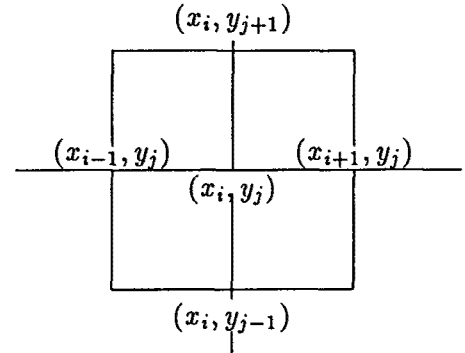

Figure 2. The simple uniform discretization mesh with $x_{i+1} - x_i = y_{i+1} - y_i = h$.

We transform the system (1.1) into another system with the following exponential substitutions:

$$\bar{R} = e^{\frac{u}{\alpha}}, \quad \bar{S} = e^{-\frac{v}{\beta}}, \quad \bar{T} = e^{\frac{w}{\gamma}} \tag{1.2}$$

and so obtain

$$u = \alpha \ln \bar{R}, \quad v = -\beta \ln \bar{S}, \quad w = \gamma \ln T. \tag{1.3}$$

Equations (1.1) become

$$\begin{aligned}
\lambda^2(\bar{R}^{\alpha-1}(\bar{R}_{xx}+\bar{R}_{yy}) &- \bar{R}^{\alpha-2}(\bar{R}_{x^2}+\bar{R}_{y^2})) \\
&- \frac{1}{\alpha}(\bar{R}^{\alpha}\bar{S}^{\beta}-\frac{\bar{T}^{\gamma}}{\bar{R}^{\alpha}})\bar{R}^{\alpha} = -\frac{1}{\alpha}\,\bar{R}^{\alpha}k_1 \\
\bar{S}^{\beta-1}(\bar{S}_{xx}+\bar{S}_{yy}) &- \bar{S}^{\beta-2}(\bar{S}_{x^2}+\bar{S}_{y^2}) + \alpha\frac{\bar{S}^{\beta-1}}{\bar{R}}(\bar{R}_x\bar{S}_x+\bar{R}_y\bar{S}_y) \\
&+ \beta\bar{S}^{\beta-2}(\bar{S}_{x^2}+\bar{S}_{y^2}) = 0 \qquad (1.4) \\
\bar{T}^{\gamma-1}(\bar{T}_{xx}+\bar{T}_{yy}) &- \bar{T}^{\gamma-2}(\bar{T}_{x^2}+\bar{T}_{y^2}) + \gamma\bar{T}^{\gamma-2}(\bar{T}_{x^2}+\bar{T}_{y^2}) \\
&- \alpha\frac{\bar{T}^{\gamma-1}}{\bar{R}}(\bar{T}_x\bar{R}_x-\bar{T}_y\bar{R}_y) = 0
\end{aligned}$$

We discretize the system (1.4) on a uniform mesh by using five point star finite difference method. At the point (x_i, y_j) we have the following replacements.

$$\bar{R}_{xx}+\bar{R}_{yy}\,|_{(x_i,y_j)} = \frac{\bar{R}_{ij-1}+\bar{R}_{i-1j}-4\bar{R}_{ij}+\bar{R}_{i+1j}+\bar{R}_{ij+1}}{h^2} + \varepsilon_{ij}^{\bar{R}^1}(h,\alpha) \qquad (1.5)$$

and

$$\bar{R}_x^2+\bar{R}_y^2 = \frac{\bar{R}_{i+1j}^2+\bar{R}_{i-1j}^2-2\bar{R}_{i+1j}\bar{R}_{i-1j}+\bar{R}_{ij+1}^2+\bar{R}_{ij-1}^2-2\bar{R}_{ij+1}\bar{R}_{ij-1}}{4h^2} + \varepsilon_{ij}^{\bar{R}^2}(h,\alpha) \qquad (1.6)$$

where

$$\varepsilon_{ij}^{\bar{R}^1}(h,\alpha) = \frac{h^2}{4!\alpha}(u_{xxxx}+u_{yyyy})\bar{R}_{ij} + \frac{h^2}{4!\alpha^2}(\ldots) \qquad (1.7)$$

and

$$\varepsilon_{ij}^{\bar{R}^2}(h,\alpha) = \frac{h^2}{6\alpha}(u_{xxx}\Delta\bar{R}_{ij}+u_{yyy}\Delta\bar{R}_{ij})\bar{R}_{ij} + \frac{h^2}{4!\alpha^2}(\ldots) \qquad (1.8)$$

As usual, $\bar{R}_{ij}$ denotes the approximate value of $\bar{R}(x_i, y_j)$. Similar replacements are made for

$$S_{xx}+S_{yy}, \qquad S_x^2+S_y^2 \text{ and } T_{xx}+T_{yy}, \qquad T_x^2+T_y^2. \qquad (1.9)$$

The second transformation is made to make solutions independent of α, β and γ:

$$R = \bar{R}^{\alpha} = e^u, \quad S = \bar{S}^{\beta} = e^{-v}, \quad \bar{T} = \bar{T}^{\gamma} = e^w \qquad (1.10)$$

After some manipulation we obtain a discretized system of equations in the unknowns R_{ij}, S_{ij}, and T_{ij}, described in [7] with discretization errors described below.

$$\varepsilon_R = \frac{h^4}{4!\alpha}(u_{xxxx}+u_{yyyy}+4u_{xxx}\Delta\bar{R}_{ij}+4u_{yyy}\Delta\bar{R}_{ij})R_{ij} + \frac{h^4}{4!\alpha^2}(\cdots)+\cdots \qquad (1.11)$$

$$\varepsilon_S = \frac{h^4}{4!\beta}(v_{xxxx}+v_{yyyy}+4v_{xxx}\Delta\bar{R}_{ij}+4v_{yyy}\Delta\bar{R}_{ij})R_{ij} + \frac{h^4}{4!\beta^2}(\cdots)+\cdots \qquad (1.12)$$

$$\varepsilon_T = \frac{h^4}{4!\gamma}(w_{xxxx}+w_{yyyy}+4w_{xxx}\Delta\bar{R}_{ij}+4w_{yyy}\Delta\bar{R}_{ij})R_{ij} + \frac{h^4}{4!\gamma^2}(\cdots)+\cdots \qquad (1.13)$$

The magnitude of $\varepsilon_R, \varepsilon_S$ and ε_T can be made small by choosing large values for α, β and γ. Furthermore, we are solving our linear systems for R, S and T which are independent of α, β and γ. In other words, the one at α, β and γ is made to control the discretization error.

We compute a sequence of iterates $R^0, R^1, \ldots, R^N, \ldots$ for R and similar sequences for S and T. The systems are linearized by evaluating everything in the bracket from one iterate and then solving for the next iteration values. The generic term in these iterations is of the form

$$\ldots + \left[\frac{1}{2}T_{ij}^{N-1} - \frac{3}{4}T_{ij+1}^{N-1}\right] T_{ij}^{N} + \ldots$$

which creates a linear system to be solved for each iteration.

This solution is then used as the initial guess for a second stage of the numerical algorithm. We return to the system (1.4) and apply the method in [6]; this method is a parametrized variant of Newton's method. The method of [6] is used in conjunction with a partitioning of the domain. A typical example is shown in Figure 3.

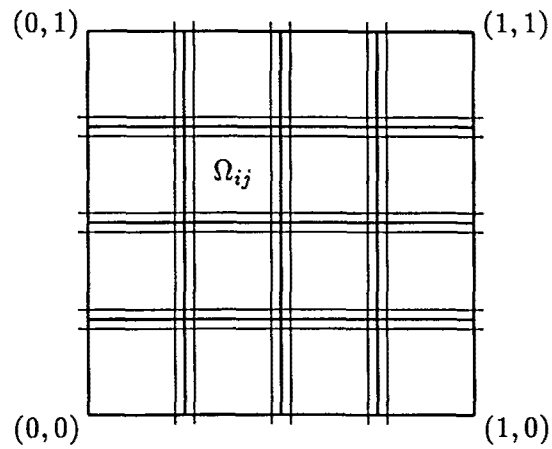

Figure 3. Subdomains of the semiconductor used for applying the method of [6].

In [6] Rice and Sharma have already established that if the sequence of approximate solutions generated by using the method in [6] converges, then it converges to a solution of the given problem on a fixed mesh.

The results of an experiment are shown in Figures 4-7.

Parameter	Value
Thermal voltage	.0259V
Radius doping profile	7×10^{-6} cm
Length device	10^{-4} cm
Depth device	10^{-4} cm
Width source	7×10^{-6} cm
Width drain	7×10^{-6} cm

Table 1: Device Parameters

Example
$\max(k_1) = 9.184 \times 10^{17}$
$U_{\text{source}} = .5$
$U_{\text{drain}} = .75$
$U_{\text{backgate}} = 0$
$\|u^N - u^{N-1}\|_2 = 10^{-4}$
$\|v^N - v^{N-1}\|_2 = 10^{-6}$
$\|w^N - w^{N-1}\|_2 = 10^{-6}$

Table 2: Applied Boundary Conditions

We have solved the system (1.1) on a 30×30 mesh. We also computed the residual of the potential equation and it is noticed that the residual goes to 0 when N gets large. The magnitude of the residual after 50 iterations was less than 10^{-7} at almost all the points of the mesh. The number of iterations needed for convergence was 50. Figures 4-7 show various quantities for the example.

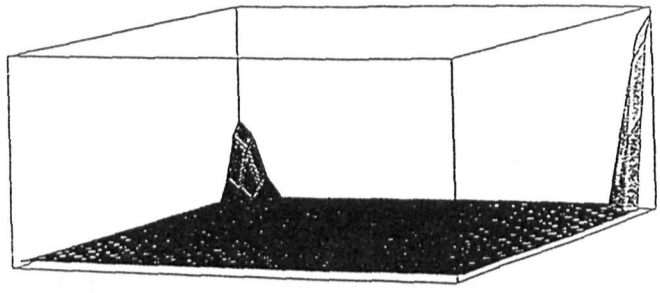

Figure 4
Natural log graph of the doping function k_1

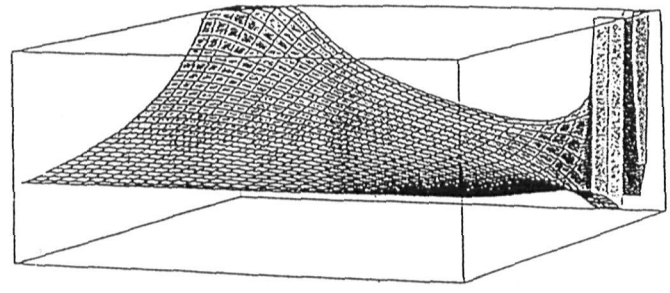

Figure 5
The electrostatic potential function u

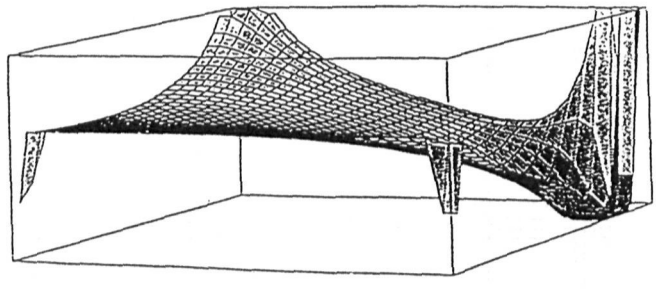

Figure 6
Natural log graph of the electron density function $n = e^{u-v}$

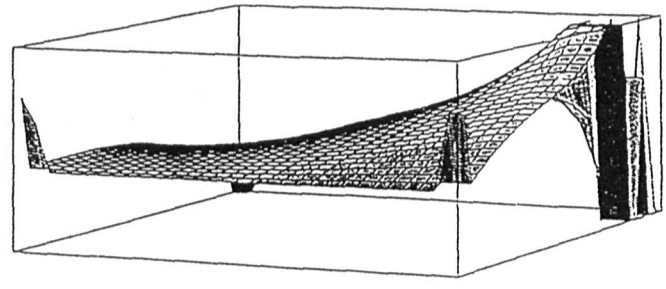

Figure 7
Natural log graph of the hole density function $p = e^{w-u}$

References

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