PROCESS AND DEVICE SIMULATION WITH ONE AND THE SAME PROGRAM

P.Pichler, W.Jüngling, S.Selberherr, E.Guerrero, H.Pötzl

Institut für Allgemeine Elektrotechnik und Elektronik
Abteilung für Physikalische Elektronik
Gusshausstrasse 27-29, 1040-Wien, AUSTRIA

The increasing complexity of the demands in device- and particularly process simulation calls for simulation programs which support the easy exchange of models and model parameters. To master these needs we have developed general purpose solvers which are able to treat fairly arbitrary systems of non-linear coupled partial differential equations in one and two space dimensions. The adopted structure of the differential equations will be explained and an example will be shown outlining the simulation of a standard MOS-process followed by the simulation of the electrical behaviour of the device with the program PROMIS (PROcess Modeling In Silicon semiconductors).

1. INTRODUCTION

Numerical simulation of processes and devices has shown to be an important tool for development in the field of VLSI devices. With increasing miniaturization second order effects become more and more important in process modeling. The implementation of models, taking those effects into account, or even the exchange of parameters in existing programs is usually extremely laborious or even impossible. Thus it was our intent to make general purpose solvers which are capable to solve an arbitrary number of non-linear coupled differential equations (PDEs) in two space dimensions. The simulation program PROMIS (PROcess Modeling In Silicon semiconductors) has been developed primarly to satisfy the needs of process simulation. However, due to the general structure of the PDEs which can be treated, it can equally be applied to solve the basic semiconductor equations and similar problems. In Section 2 we will outline the features of the program and the structure of the differential equations which can be solved. In Section 3 the simulation of a simple MOS-process is demonstrated and in Section 4 the simulation of the electrical behaviour of the device is shown.

2. FEATURES OF PROMIS

The main goal of PROMIS is the two-dimensional simulation of PDEs describing the redistribution of dopants and other physical quantities, e.g. vacancies, interstitials... The program can handle systems of N coupled equations of the form

$$\sum_{j=1}^{N} a_{ij} \cdot \frac{\partial c_j}{\partial t} + \operatorname{div} J_i + G_i - R_i = 0 \qquad (1)$$

$$J_i = \sum_{j=1}^{N} \left(d_{ij} \cdot \operatorname{grad} C_j + \mu_{ij} \cdot C_j \cdot \operatorname{grad} \Psi \right) \qquad (2)$$

The coefficients a_{ij}, d_{ij}, μ_{ij}, G_i and R_i can be functions of the simulation time, the simulation temperature, the space variables and any of the dependent variables C_i.

This system of PDEs allows to simulate coupled and uncoupled diffusions, dynamic and static cluster models, the basic semiconductor equations or systems of PDEs corresponding to problems in other fields of science.

The formulation of the boundary conditions (3) allows the usually found Dirichlet and Neumann boundary conditions but also mixed boundary conditions with sums of currents defined by (2):

$$\sum_{j=1}^{N} \xi_{ij} \cdot (J_j \cdot \bar{n}) + F_i = 0 \qquad (3)$$

The coefficients ξ_{ij} can be functions of the simulation time and the space variables, F_i can be function of the quantities C_j, time and the space variables. The quantity $\bar{n}$ denotes the unit vector normal to the boundary.

The present level of PROMIS restricts itself to rigid boundaries. This means that the simulation of oxidations with moving boundaries is excluded. However, some effects of oxidation (e.g. interstitial and vacancy generation) can be taken into account by the boundary conditions, cf. /2/.

A detailed description of the adopted structure of the PDEs and the boundary condtions as well as the detailed description of the subroutines which have to be supported by the user can be found in /3/.

To satisfy the particular needs of process simulation all commonly used numerical models for ion-implantation have been implemented to serve as initial guesses for transient simulations. Alternatively, initial solutions for transient simulation can also be defined by reading data from external files or by specification via user-defined subroutines. Thus, data from SIMS, NAA or other measurement methods as well as results from Monte-Carlo programs can be used. The adaption of the spatial and the time grid is performed automatically in order to

relieve the user from unreasonable efforts as well as to minimize the computational errors. Time integration is done using backward difference formulae with a predictor/corrector system. The PDEs are linearized by using Newtons method and then discretized by applying finite difference schemes. The spatial discretization formalism used for the discretization of the continuity equations in (1) has been adopted from device modeling programs /4/. The resulting linear system of equations is solved by using the point successive overrelaxation method (SOR) with automatic paramter adaption, cf. /1/.

3. SIMULATION OF A SIMPLE MOS-PROCESS

The first step is the implantation and the annealing of the drain and source regions. As an initial doping distribution ion implantation of arsenic (80KeV, $1.5 \cdot 10^{15}$ cm^{-3}) is taken through an oxide mask with a step from 16nm to an infinite oxide thickness at the origin of the coordinate system and vice versa at 1.5μm in lateral direction.

Annealing of the profiles is assumed at 1000°C for 3600s. The differential equations to be solved are given by (4) and (5).

$$\text{div grad } \Psi = \frac{q}{\varepsilon} \cdot (2 \cdot n_i \cdot \sinh(\frac{\Psi}{U_t}) - C_{As}) \qquad (4)$$

$$\frac{\partial C_{As}}{\partial t} = \text{div} \left(D_{As}(\text{grad } C_{As} + \frac{C_{As}}{U_t} \cdot \text{grad } \Psi) \right) \qquad (5)$$

For the sake of simplicity clustering and degeneration effects have been neglected. Fig.1 shows the resulting arsenic profile after the heat treatment. The p-j-junction is at an assumed bulk concentration of $10^{15} cm^{-3}$ in a depth of approximately .35μm. The second simulation step describes the implantation and annealing of the channel implantation. Two implantations have been assumed with doses of $3.5 \cdot 10^{11} cm^{-3}$ and $1.4 \cdot 10^{11} cm^{-3}$ at energies of 25KeV and 100KeV, respectively, through an oxide mask of 16nm.

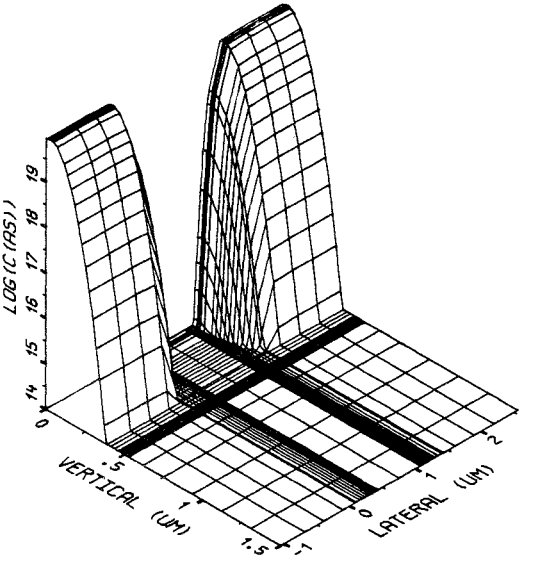

Fig.1: As-profile after 1. anneal

The annealing has been assumed at 925°C for 900s. The coupled diffusion is described by (6)-(8) under the above mentioned restrictions.

$$\text{div grad } \Psi = \frac{q}{\varepsilon}\cdot(2\cdot n_i\cdot\sinh(\frac{\Psi}{U_t}) + C_B - C_{As}) \tag{6}$$

$$\frac{\partial C_B}{\partial t} = \text{div } (D_B \text{ (grad } C_B - \frac{C_B}{U_t}\cdot\text{grad } \Psi)) \tag{7}$$

$$\frac{\partial C_{As}}{\partial t} = \text{div } (D_{As}(\text{grad } C_{As} + \frac{C_{As}}{U_t}\cdot\text{grad } \Psi)) \tag{8}$$

Fig.2 shows the boron concentration after annealing. The slight changes to the now two-dimensional structure have been caused by the field induced flux of boron.

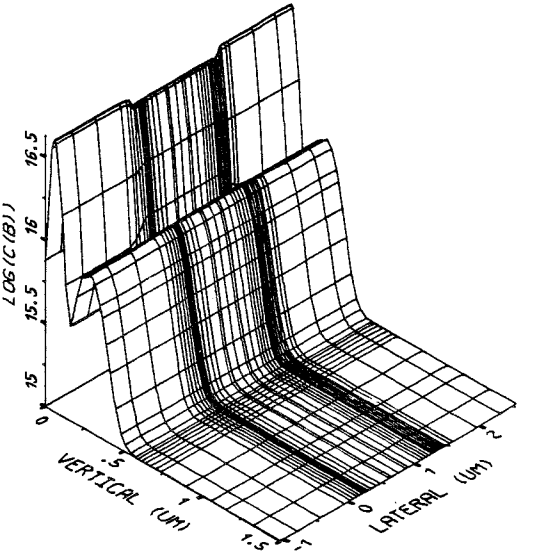

Fig.2: B-profile after 2. anneal

4. SIMULATION OF THE ELECTRICAL BEHAVIOUR OF THE DEVICE

In the following the electrical behaviour of the device the fabrication of which has been simulated in Section 3 will be consicered. The basic semiconductor equations (9)-(11) have been solved in order to obtain the quantities Ψ, n and p, denoting the potential and the electron and hole concentrations.

$$\text{div } \varepsilon \text{ grad } \Psi = -q\cdot(p-n+ND^+-NA^-) \tag{9}$$

$$\text{div } \mu_n\cdot(U_T\cdot\text{grad } n - n\cdot\text{grad } \Psi) - R = 0 \tag{10}$$

$$\text{div } \mu_p\cdot(U_T\cdot\text{grad } p + p\cdot\text{grad } \Psi) + R = 0 \tag{11}$$

Due to the generality of PROMIS only the solution is directly available. All consecutive results (e.g. currents, mobilities,...) can be computed by post processors. The simulation of the semiconductor equations with PROMIS has been performed as test for the code since the semiconductor equations are well known for their numerical malignity.

Fig.3 and 4 show the potential and the electron concentrations for a drain voltage of 3V and a gate voltage of 0V, Fig.5 and 6 show the profiles for drain and gate voltages of 3V. It can be seen from the pictures that the transistor is totally turned of at 0V gate voltage and that punch through has been avoided due to the deeper channel implantation. At 3V gate voltage the transistor is turned on and current flows mainly in the inversion layer directly under the surface.

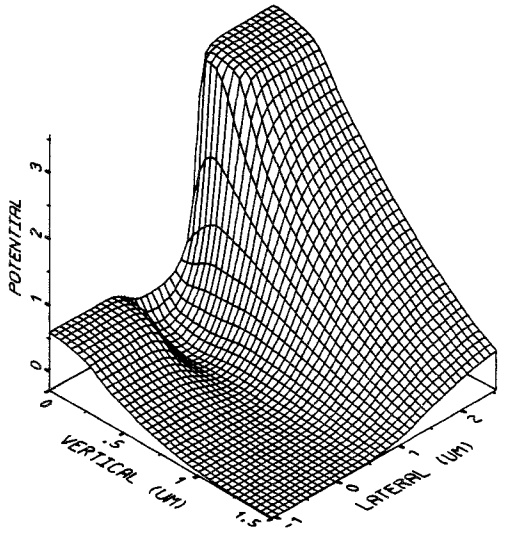

Fig.3: potential for U_D=3V, U_G=0V

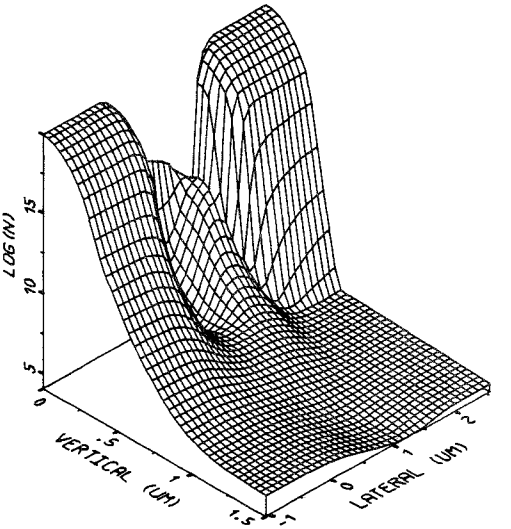

Fig.4: electron concentration for U_D=3V, U_G=0V

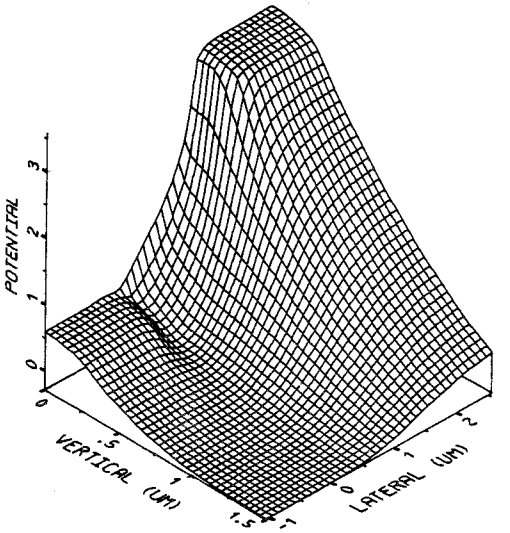

Fig.5: potential for U_D=3V, U_G=3V

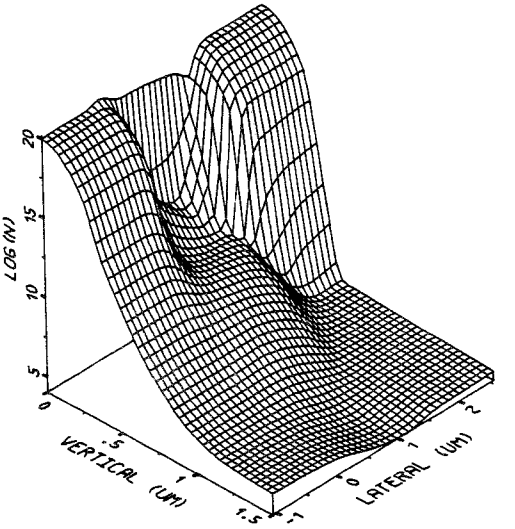

Fig.6: electron concentration for U_D=3V, U_G=3V

CONCLUSION

In this paper we have presented a general purpose program for the simulation of all common elliptic or parabolic PDEs. The program supports the easy implementation of advanced physical models and relieves the user from nonphysical tasks. An example treating the simulation of the fabrication and the electrical behaviour of the device has shown typical applications of the program.

Acknowledgements

This work has been sponsored by the Siemens Research Laboratories, Munich, BRD, and the 'Fonds zur Förderung der wissenschaftlichen Forschung', project S 43/10. The authors would like to thank Dr. Llanda Richardson, Digital Equipment Corporation, USA, who suggested the name for our program.

REFERENCES

/1/ Grimes R.G., Kincaid D.R., Young D.M., "ITPACK 2A A Fortran Implementation of Adaptive Accelerated Iterative Methods for Solving Large Sparse Linear Systems", University of Texas at Austin, 1980.

/2/ Jüngling W., Pichler P., Selberherr S., Guerrero E., Pötzl H., "Simulation of Critical IC Fabrication Processes Using Advanced Physical and Numerical Methods", IEEE Trans.Electron Devices, Vol.ED-32, No.2, pp.156-167, 1985.

/3/ Pichler P., Jüngling W., Selberherr S., Guerrero E., Pötzl H., "Simulation of Critical IC-Fabrication Steps", Accepted for publication in IEEE Trans.Electron Devices, October 1985.

/4/ Selberherr S., Ringhofer C., "Implications of Analytical Investigations about the Semiconductor Equations on Device Modeling programs", IEEE Trans.Computer-Aided Design of Integrated Circuits, Vol.CAD-3, No.1, pp.52-64, 1984.