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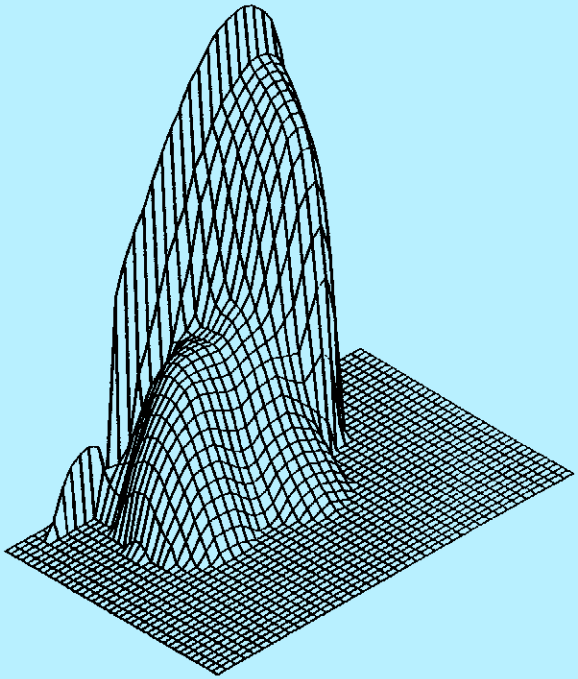

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Preface

Siegfried Selberherr

This brochure is the very first research review of our institute which was founded at the end of June 1988 by the Austrian Ministry of Science and Research. Provision has been made by the Ministry for four full time employees: the head of institute, two scientists and a secretary. Due to intensive collaboration with industrial institutions it has become possible within the first year to also fund six additional full time scientists. However, we suffer considerably from the total lack of skilled technicians.

The allocation of floor space is under the autonomy of the Technical University. This constitutes a source of major problems for our institute. Only about 70 square meters for a student computer laboratory have been permanently dedicated to our institute. 160 square meters of office space and 60 square meters of air-conditioned computer room have been loaned for at most three years from other institutes of the University in exchange for some of our computer resources. In view of this situation any significant further expansion of our institute is unlikely, although we have received more queries regarding positions from both students and industry.

Concerning the equipment infrastructure our institute has been considerably supported by our industrial partners. The institute runs a DIGITAL VAX 8800 mainframe computer, eight DIGITAL VAX 3200 high resolution color graphics workstations and numerous small workstations and personal computers. Regarding research our situation has to be judged as internationally competitive. However, for educational purposes on an undergraduate level we have a serious lack of appropriate input/output peripherals.

All projects of the institute are presently focused on microelectronics modeling issues. Almost exclusive emphasis is put on analysis and simulation of the fabrication steps and the electrical behaviour of miniaturized semiconductor devices. This is accomplished by means of specially developed computer programs which are disclosed freely to the scientific community in order to increase interaction and collaboration. Scientific output has been quite satisfactory with, for instance, sixteen contributions at international conferences.

Austrian scientists have a remarkable potential for significant technical achievements. Thus we enter the second year of our institute with high expectations.

Siegfried Selberherr was born in Klosterneuburg, Austria, in 1955. He received the degree of 'Diplomingenieur' in electrical engineering from the Technical University of Vienna in 1978. Since that time he has joined the 'Institut für Allgemeine Elektrotechnik und Elektronik' – previously called the 'Institut für Physikalische Elektronik' – at the Technical University of Vienna. He received his doctoral degree in 1981. Dr. Selberherr has held the 'venia docendi' on 'Computer-Aided Design' since 1984. He has been the head of the 'Institut für Mikroelektronik' since 1988. His current topics are modeling and simulation of problems for microelectronics engineering. Dr. Selberherr is editor of 'The Transactions of the Society for Computer Simulation', of 'Electrosoft', of 'Mikroelektronik' and of the Springer-Verlag book series 'Computational Microelectronics'.

Sylvia Zentner was born in Tulln, Austria, in 1965. She joined the institute in October 1988. Since that time she has been in charge of all the organizational and administrative work of the institute.

Simulation of High Voltage Double Diffused MOS-Transistors

Peter Dickinger

For the further development and optimization of high voltage DMOS devices it is necessary to use network analysis programs and device simulation programs. Our two dimensional transient device simulation program BAMBI is used to determine physical quantities, especially the electric field, to find improved concepts for high voltage devices. Small changes in geometry and doping profiles can easily be carried out by simulation to investigate the effects of field plates, field rings and different oxide thicknesses. Oxide charges provide a problem for these so-called RESURF (REduced SURface Fields) devices. These charges are caused by hot electrons which are injected into the oxide in high field regions (Fig. 1). They significantly influence the I-V curve. The high voltage breakdown of these devices strongly depends on the epitaxial doping and the length of the drift region.

The standard MOS models in SPICE (level 1,2,3) are not applicable for high voltage DMOS devices. Therefore two new models (one for p- and one for n-channel devices, as they behave differently) have been developed. In addition to these two models a new approximation for the DMOS transistor capacitances has been developed. The improvements in technology make it necessary that the simulation models must be adapted for these new demands.

Another way to get better agreement of simulated and measured curves is the integration of the device simulator

MINIMOS into SPICE. This is possible since MINIMOS5 is able to perform AC analysis. Network simulation with this new feature takes a lot of computing time so that it is practicable only for investigation of standard cells and new technologies.

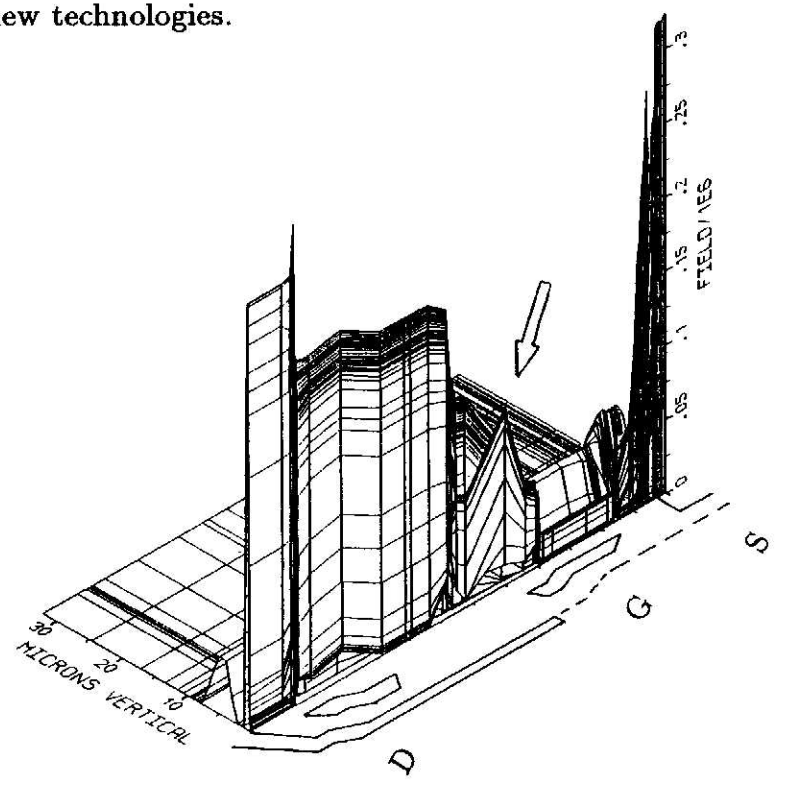


Fig.1: Field Distribution in a Lateral DMOS Device

Peter Dickinger was born in Gmunden, Austria in 1961. He received the degree of 'Diplomingenieur' from the Technical University of Vienna in 1987 in electrical engineering. He joined the simulation group of Prof. Selberherr in August 1987. He currently works towards his doctoral degree focusing on network and device simulation of high voltage DMOS transistors.

Physical Parameters for Analysis and Simulation of Carrier Transport in Semiconductor Devices

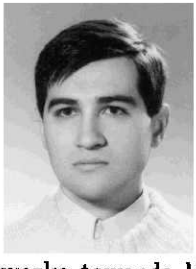
Predrag Habaš

The proper numerical simulation of MOS-devices in submicron regions necessitates a refinement of the present approaches to the modeling of transport processes in the inversion layer. Improved physically based models for the surface mobilities, current densities, carrier energies and avalanche generation are the basic prerequisite to the self-consistent simulation of degradation due to hot carrier injection into the oxide. The starting point in our work is a proper modeling of the above mentioned physical quantities.

Due to non-uniform scaling of the supply voltage and physical dimensions (channel length and oxide thickness) potential and carrier density gradients are very large and significantly affect the inversion layer mobilities. Because of quantum effects in strong inversion and/or at low ambient temperature the carrier gas forms a 2D system with the appropriate scattering processes. At room temperature and in the subthreshold region, due to population of the higher quantum levels, the classic description (3D gas) is a good approximation. It is necessary for future simulation of hot carrier injection to account in the mobility models for the contributions of: phonons, surface roughness, charges in surface states and oxide (for a given distribution) and ionized bulk impurities. At low ambient temperature and in the subthreshold region, carrier density fluctuations and localized states are also impor-

tant. The aim of this project is to develop a mobility model which reasonably takes into account all significant physical effects and which agrees with experimental data for mobility in both weak and strong inversion at 77K and at room temperature.

As the device dimension becomes less than $0.5\mu m$ the length of the region in which the very high field occurs is comparable to the mean free path for optical phonons and the field varies remarkably within a few free paths. So, the classic model for impact ionization rate in the local field strength concept is inappropriate and leads to inaccurate prediction of the substrate current and carrier energy distribution. The development of an accurate non-local model of an energy dependent impact ionization rate is one primary goal of our work. It will be an important starting point towards the time-dependent self-consistent simulation of hot carrier degradation phenomena in ULSI MOS-devices.



Predrag Habaš was born in Vrbas, Yugoslavia in 1962. He received the B.S. degree from the Faculty of Technical Sciences Novi Sad in 1985 and the M.S degree from the Faculty of Electrical Engineering Beograd in 1989, both in electrical engineering. From 1985 he worked at the Institute for Power and Electronics University of Novi Sad as Research Assistant and Instructor. In April 1989 he joined the 'Institut für Mikroelektronik', where he currently works towards his doctoral degree. His research area includes carrier transport in semiconductors, physics of small MOS-devices and analytical and numerical modeling and simulation of MOSFETs.

Transient Simulation with MINIMOS

Otto Heinreichsberger

Our two and three dimensional MOS device simulation program MINIMOS has recently undergone significant extensions. The original two-dimensional simulator, the latest version of which (MINIMOS 4) is publicly available, has been modified to simulate nonplanar Si - MOSFETS as well GaAs-MESFETS in three space dimensions. Our present attempt to perform additional transient simulation has to be preceded by a careful review of the underlying algebraic concepts, unless substantial reductions in performance are admitted. The bottlenecks of multi-dimensional simulations are obviously the solvers, i.e. the subprograms to solve the large systems of linear equations, which arise from the discretized semiconductor partial differential equations. Thus, a well designed and effective linear solver concept is an indispensable prerequisite.

Appropriate data structures have been defined and a uniform interface standard is proposed. The solving methods focus mainly on iterative methods, which are the subject of intensive current research. Iterative solver design proceeds as follows: First a so-called *stationary* iterative method such as the Jacobi method or the Gauss-Seidel method is applied, the convergence of which can later on be "accelerated" by conjugate gradients or a similar acceleration technique. A combination of such a method with definite block elimination schemes can lead to very fast convergence.

The convergence speed of iterative solvers is closely connected with the "condition number" of the linear sys-

tem of equations. Various quantities, such as doping profile, geometry and bias can sometimes yield almost rank deficient matrices. Therefore a conditioning analysis on MINIMOS matrices is attempted. The solvers provided are required to guarantee the necessary numerical stability to solve even badly conditioned systems with sufficient accuracy.

Iterative solvers are not only able to exploit specific matrix structures such as sparseness but are also ideally suited for implementation on vector and/or concurrent computers. Thus, an appropriately structured solver system, will enable MINIMOS to take full advantage of modern computer architectures.

The successive implementation of transient behaviour in MINIMOS is guided by similar implementations in related simulation tools. The time dependent carrier continuity equations will be solved with Gummel's algorithm in connection with an effective time step control. Attention is paid to the convergence properties of the transient Gummel algorithm in high current regions, because of expected numerical instabilities.

Otto Heinreichsberger was born in Amstetten, Austria, in 1963. He received the degree of 'Diplomingenieur' from the Technical University Vienna in 1987 in electronic engineering. After one year at the 'Institut für Geodesie', where he worked with automatic ranging and survey measurements, he joined the 'Institut für Mikroelektronik' in October 1988. He is currently working toward his doctoral degree. His work is focused on mathematical models and algorithms in multi-dimensional process and device simulation.

Monte Carlo Simulation of Si-MOSFETs

Hans Kosina

In the present project a device simulator based on a microscopic particle model will be developed. The simulator is planned to be two-dimensional and should provide steady state solutions. Since it will be especially suited for Si- MOSFET Simulation, it is planned to be an extension of MINIMOS.

Monte Carlo models are statistical models which provide a solution for the Boltzmann transport equation. In more physical terms, Monte Carlo models are particle models, thus allowing in many cases a deeper insight into the simulated device than traditional device simulators allow. Non-local, off-equilibrium transport conditions caused by high electric fields are treated in a rigorous way.

The physical model used is semi-classical and makes use of a state space representation. The three-dimensional band structure of silicon shows six minima along the $\langle 100 \rangle$ directions. These minima are approximated by six anisotropic, non-parabolic valleys. The interaction of carriers with the non-ideal crystal is modelled by different scattering mechanisms. Coulomb interaction with ionized impurities and deformation potential interaction causes intravalley transitions. Furthermore, intervalley scattering due to optical and acoustic phonons is included.

A trade off must be found between the use of improved physical models which have naturally rapidly increasing complexity and the overall complexity of the simulator itself. An improved physical model of the inversion layer could include quantization effects leading to subband en-

ergy levels. Degeneracy due to the Pauli exclusion principle can affect the energy distribution function at low temperatures; carrier – carrier interaction can be important in highly doped areas. At high carrier energies impact ionization becomes the predominant scattering mechanism.

Numerical difficulties are expected to arise from the widely varying carrier concentration over the device. Furthermore, the self consistent solution of carrier transport with the electric field, that can be obtained by a Gummel like iteration cycle, is very CPU – time intensive. Thus, highly optimized algorithms must be used. Recently different optimization techniques to reduce the amount of selfscattering events have been published. Techniques conveniently dealing with both rare events in real space and scarcely populated energy regions are available.

The boundary conditions of the Monte Carlo region have to be treated very carefully, since they have a large influence on the correctness of the solution.

Hans Kosina was born in Haidershofen, Austria, in 1961. After having received his degree of 'Diplomingenieur' from the Technical University of Vienna in 1985 in electrical engineering, he was with the 'Institut für flexible Automation' for one year. Since September 1988 he has been an assistant at the 'Institut für Mikroelektronik', where he is working towards the doctoral degree. His current scientific interests include solid state device technology and –behavior in general, and Monte Carlo simulation of MOSFETs in particular.

Electroacoustic Wave Propagation
and
Miniaturization of Integrated Devices

Erasmus Langer

The program package SABAWA (Surface And Bulk Acoustic Waves Analyzer) developed in recent years has been proved to be an important tool for the investigation and improvement of crystal cuts used for surface acoustic wave devices. This program allows the analysis of all undamped diffusible surface and bulk modes in arbitrary piezoelectric crystals and propagation directions. The implemented algorithm is based on the calculation of the so-called effective permittivity as a function of the phase velocity. A sensitivity analysis performed with SABAWA has shown that the influence of uncertainties in the material data on the calculated behavior of the acoustic modes (e.g. the phase velocity, the decay constant with respect to the depth, and the electro-acoustic coupling factor) is too large to be neglected. For this reason, investigations into the improvement of the coefficients of the material tensors using measured phase velocities as input for a balancing algorithm have been performed. The procedure we have developed also provides an error estimate for each constant derived from its sensitivity to a change in the velocity data and from the accuracy of this data.

The new project "Miniaturization of Integrated Semiconductor Devices" consists of the following research fields: Investigation of the influence of the variation of technological processes on the fundamental behavior of microminiaturized semiconductor devices, extraction of critical

parameters for a reduction in size of integrated devices, extraction of critical parameters for the long time stability of integrated devices, and the synthesis of engineering rules for the improvement and/or miniaturization of existing integrated devices. The aim of the investigations performed by way of these crucial points should be the development of general rules which must still be tested by an industrial partner according to his applications and requirements.

The basis of this project is the application — after having performed some improvements and modifications, if necessary — of all available software tools in the field of process and device modeling. During the last year, the most important models for the physical parameters within the basic semiconductor equations have been investigated, i.e. space charge, carrier mobility, carrier heating, and carrier generation/recombination.

Erasmus Langer was born in Vienna, Austria in 1951. After having received the degree of 'Diplomingenieur' from the Technical University of Vienna in 1980 he was employed at the 'Institut für Allgemeine Elektrotechnik und Elektronik' first as a research assistant (until 1984) and then as assistant professor. His research field was first the numerical simulation of semiconductor devices and later the generation and excitation of electro-acoustic waves in anisotropic piezoelectric materials where he also received his doctoral degree in 1986. Currently he works mainly in the field of critical parameter extraction for the improvement and miniaturization of integrated semiconductor devices.

Development of MINIMOS into a GaAs-MESFET Device Simulator

Philipp Lindorfer

During the last few years, MESFETs more and more have become a serious alternative to MOSFETs. The main advantages MESFETs offer, compared to MOSFETs, are: simpler fabrication processes, because of the low temperature process steps, reduced radiation sensitivity, because of the absence of a gate oxide, higher carrier mobilities, because of current transport occurs deeper in the bulk and no minority carrier storage effects, which results in faster speeds for high frequency applications. GaAs MESFETs especially have become increasingly popular for high speed analog and digital circuits since their introduction in 1970. GaAs FET amplifiers, oscillators, mixers, etc. are widely used in microwave applications, whereas very fast digital circuits have been developed based on GaAs MESFET logic.

Based on MINIMOS 5, which is our integrated two- and three-dimensional device simulator for silicon MOSFETs with small signal analysis capabilities, models allowing the simulation of MESFETs and models for III-V compound semiconductors, in particular GaAs, have been implemented.

The Schottky boundary condition that has been implemented is:

$$\psi = \psi_{app} - \psi_s$$

$$J_n = -q \cdot v_n \cdot (n - n_0)$$

$$J_p = q \cdot v_p \cdot (p - p_0)$$

with current dependent surface recombination velocities, which lead also to realistic results for a forward biased Schottky contact. The current dependency of the surface recombination velocities is modeled after our recent results. This Schottky contact model also accounts for the field dependent lowering of the Schottky barrier.

New process models had to be implemented. These include new implantation statistics for several dopants in GaAs and various diffusion parameters.

New models for the carrier mobilities, recombination, generation and some other physical parameters, which are necessary for accurate simulation, have yet to be developed. Enhancements to the 'silicon' transport equations also have to be made to obtain qualitatively and quantitatively appropriate results.

Because most of todays MESFETs have a nonplanar geometry, algorithms which allow the simulation of devices with nonplanarities in all three space dimensions have been implemented. The necessary concepts for this task were developed by M.Thurner for the first 3D Version of MINIMOS. Various enhancements have been made to allow simulation of different recessed gate and T-gate structures, which are used today for improved MESFET designs.

Philipp Lindorfer was born in Steyr, Austria, in 1962. He received the degree of 'Diplomingenieur' from the Technical University Vienna in 1987 in electrical engineering. In November 1987 he joined the 'Institut für Mikroelektronik', where he is currently working towards his doctoral degree. His work is focused on models for III-V compound semiconductors in multi-dimensional device simulation.

Grid Generation and Current Calculation in Device Simulation

Gerd Nanz

For the development of BAMBI (Basic Analyzer of MOS and **BI**polar devices) a new method for the initial grid design has been found. Since BAMBI is suitable for arbitrarily shaped devices a flexible strategy for grid design has been implemented which provides a good starting grid for the simulation of most working conditions. In the construction of the grid a common "measure" for all sub-regions of the device is chosen in order to avoid numerical problems during the automatic grid refinement. This also means that the condition of the resulting sparse equation system will be improved.

For boundaries and interfaces which are not parallel to the coordinate axes a new strategy based on the theory of graphs has been developed and implemented in the program. In order to minimize the number of points for these structures, an optimal geometry change within given limits will be allowed. This it is determined by quadratic optimization.

A new method for the calculation of terminal currents has been developed. This algorithm is based on the evaluation of a volume integral instead of a line integral as is commonly done. Through the choice of the weight functions for the contacts, current conservation is more easily observed than for the line integral. Furthermore, the results become independent of the space grid. The weight functions $w^{n,p}$ for the electron and the hole current are determined by the solution of the set of partial differential

equations

$$\text{div } (\frac{n,p}{n_i} \text{ grad } w^{n,p}) \;=\; 0$$

with Neumann and Dirichlet boundaries

$$\begin{aligned} w_i^{n,p} &= 1 && \text{at the } i\text{–th contact} \\ w_i^{n,p} &= 0 && \text{at all other contacts} \\ \frac{\partial w_i^{n,p}}{\partial \vec{n}} &= 0 && \text{otherwise} \end{aligned}$$

The weight function for the displacement current is determined by the solution of a set of Laplace equations with the same boundary conditions.

This choice of the weight functions guarantees that the method is applicable to arbitrary device geometries and provides current conservation on the order of the machine accuracy.

Gerd Nanz was born in Munich, West-Germany, in 1959. He received his M. S. degree from the Technical University of Munich in 1985 in mathematics and computer sciences. After 15 months at the 'Lehrstuhl für Baustatik' at the Technical University Munich, where he was involved in the development of a fully self-adaptive finite-element-code for plates and shells (h- and p-version), he joined the Simulation group of Prof. Selberherr in November 1986. At present he is working towards his doctoral degree. His thesis topic deals with numerical algorithms and with grid generation in device simulation.

Two-Dimensional Nonplanar Oxidation

Karl Wimmer

The numerical simulation of the local oxidation of silicon (LOCOS) is getting more and more important in MOS-technology in order to evaluate methods of reducing the lateral size of insulating areas between neighbouring transistors.

The oxidation of silicon is a thermal process by which the oxidizing species diffuse through an existing oxide layer and react with silicon atoms. The chemical reaction is accompanied by a 125% volume expansion so that the existing oxide is forced away by the newly formed oxide layer. As a consequence, oxidation is a problem involving oxidant diffusion, volume expansion and boundary motion.

The physical model of oxidation is based on a steady state oxidant diffusion and a slow incompressible viscous flow of the oxide. This model will be implemented in our 2D process simulator PROMIS, using finite differences and a quasi-conformal mapping method. The nonplanar physical domain is mapped onto a rectangular mathematical domain, where the moving boundary remains stationary. With this approach the solution domain is simplified at the expense of complicating the equations and boundary conditions.

Cross derivatives occur in the mapping equations (elliptic system of partial differential equations) but are also found in the transformed physical equations. For the discretization of cross derivatives it was necessary to implement 9-point discretization. Special solvers have been designed

for the linear equation systems which result from the 9-point discretization, in particular a direct (GAUSS) and an iterative (Block SOR) solver.

The main advantage of a quasi-conformal mapping is that the grid lines intersect (approximately) orthogonally. Orthogonal coordinate systems produce less additional terms in the transformed partial differential equations, and thus reduce the amount of computational work required. Furthermore severe departure from orthogonality will introduce truncation errors in the difference expressions. Coordinate systems that are orthogonal, or at least nearly orthogonal near the boundary, make the application of boundary conditions more straightforward.

In addition to this research, some other improvements to PROMIS have been made. New algorithms for the estimation of the initial time step and for time step control have been developed. Both are based on local computations. The time step control considers both the relative and the absolute error of the time discretization as well as the numerical accuracy. To make PROMIS more "user friendly" it has been provided with an automatic scaling technique and a uniform syntax for the user supplied parameters of the differential equations and boundary conditions.

Karl Wimmer was born in Ostermiething, Austria, in 1962. He received the degree of 'Diplomingenieur' in electrical engineering from the Technical University of Vienna in 1987. At that time he joined the 'Institut für Mikroelektronik', where he currently works toward his doctoral degree. From 1977 to 1986 he held several summer positions in Austria and Switzerland working on industrial automation and adaptive control systems. His research interests include process simulation in nonplanar structures and numerical grid generation.

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