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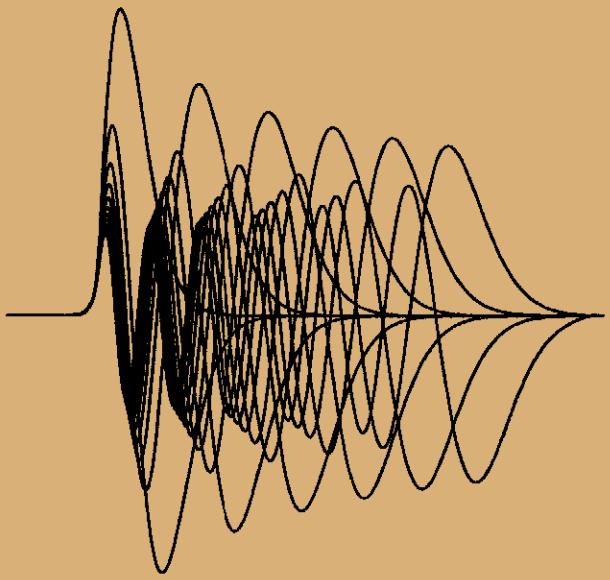

Annual Review
June 1990

INSTITUTE FOR MICROELECTRONICS

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Preface

Siegfried Selberherr

This brochure is the second research review of our institute. Provision has been made this year by the Austrian Ministry of Science and Research for a full time technician. Thus the staff supported by the Ministry consists now of five full time employees: the head of institute, two scientists, a secretary and a technician. Eleven (!) additional scientists are presently funded through scientific projects with industrial institutions. This might be the upper bound of "additional" scientists which we can integrate into our institute due to the small number of core staff. Nevertheless, we have received many more queries regarding positions from both students and industry.

There are two new partners in our colaborative research activities, namely "Austrian Industries" and "Sony". Furthermore, the institute has been granted financial support by the "Wiener Handelskammer" for the project "Automatic Translation from Fortran to C".

All projects of the institute are focused on microelectronics modeling issues. We put almost exclusive emphasis on analysis and simulation of the fabrication steps and the electrical behaviour of miniaturized semiconductor devices for integrated circuits. The computer programs which are developed in our research work are disclosed freely to the scientific community.

Regarding academic and scientific output we are quite satisfied. We are particularly pleased with the number of students who finished this year their master's theses at

our institute.

We all enter the third year of our institute with considerable motivation!

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.

Peter Nebenführ was born in Vienna, Austria, in 1965. He joined the institute in January 1990. Since that time he has been in charge of all technical hardware and software work of the institute.

Simulation of High Voltage Double Diffused MOS-Transistors

Peter Dickinger

High voltage DMOS devices are mostly used in telecommunication systems and automobile electronics. The main properties are the high breakdown voltage, up to 120V, low R_{ON} and high reliability. To find new concepts for increasing the breakdown voltage and optimizing the other capabilities, simulations with the two dimensional device simulator BAMBI have been performed. Thus variations of device geometry and doping profiles can easily be investigated without expensive experiments. One of the main constraints for the long term stability of n-channel DMOS transistors is hot electron degradation. As electrons have enough energy to transgress the energy barrier between semiconductor and oxide, these carriers are often trapped by oxide defects. These degradation effects cause changes of the I-V curves over time and reduce reliability. With experience it is possible to interpret the simulation results to determine the regions where these effects take place. Low on resistance and high voltage breakdown must be traded off, and the optimized behavior can only be determined with device simulation.

The SPICE built-in analytical MOS models can not be applied to high voltage DMOS devices, since these devices behave different electrically than standard MOS devices. Separate models for n- and for p-channel devices have been developed. It was also necessary to create a new model for the capacitances of these transistors. Some comparisons of measured data taken from amplifier cir-

cuits with simulated curves show good agreement.

Knowledge about heat generation and temperature distribution is of special interest in simulation of bipolar devices. The introduction of a new model into BAMBI makes it possible to perform selfconsistent simulations of these physical quantities. Although the initial results look promising, there are still problem areas to be investigated.

To achieve accurate results in analog MOS circuits, it is necessary to determine the exact static and dynamic behavior of all transistors. This is usually done by the analytical models in e.g., SPICE. On the other hand, the fully two-dimensional device simulator MINIMOS makes it possible to get exact results based on fundamental physical principles for the specific structure of each transistor. The implementation of a fully two-dimensional AC-analysis in MINIMOS enables the accurate calculation of capacitances and conductances. Therefore we combined network and device simulation. This new approach gives the highest possible accuracy regarding device models for circuit simulation.

Peter Dickinger was born in Gmunden, Austria, in 1961. He received the degree of 'Diplomingineur' 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 devices

Simulator Coupling with PIF
and
VLSI Capacitance Simulation

Franz Fasching

The growing demand of simulation in the device design process requires the use of various process and device simulators for a particular device. It is a tedious task to bring several complex simulators to work together, since every simulator uses its own convenient input and output format. Coupling can be done by developing translation programs from one simulator's output to another simulator's input format. As the number of involved simulators grow, the number of translators will grow with the square of the simulators - the need for a standardized data exchange format becomes obvious.

Some time ago S. Duvall at Intel Corp. proposed a Profile Interchange Format (PIF) for simulation data such as geometries, grids, attributes and snapshots, which uses LISP-like syntax. Based upon this format we tried to clarify the syntax of this proposal to make it directly usable for application programmers. Since this is an ASCII format, it is only useful for data exchange between sites (intersite form of PIF). For effective data exchange between tools, a binary format will be needed (intertool form of PIF), which is based upon an object oriented database called PDB (PIF DataBase). To make this database accessible by the simulators, a standardized PIF application interface (PAI) is needed. Additionally, PIF tools, such as a PIF editor (PED), which enables graphical editing of device structures and display of simulation results, and the PIF database manager (PDBM), will be

developed based on the PAI and the LISP Technology CAD shell.

The miniaturization of devices increases interconnection capacitances between conductors. Additionally, the simulation of semiconductor junction capacitances is an important factor for a rigid device design. Thus the LAPLACE equation has to be solved for the linear case (i.e. structures consisting only of conductors and ideal insulators), and the POISSON equation for the nonlinear case of semiconductor structures. The capacitance simulator VLSICAP, developed at our institute by F. Straker, is capable of simulating both interconnection and semiconductor junction capacitances in 2D space. Automatic interconnection capacitance calculation of multi-conductor geometries is available too. In order to compute C-V characteristics of semiconductor junction capacitances a loop mode will be provided. Further work on VLSICAP will involve a complete PIF adaption for geometry input with PED, grid generation and solver improvement, and a 3D capability for conductor-insulator structures (linear case).

Franz Fasching was born in Steyr, Austria, in 1965. He received the degree of 'Diplomingenieur' in 1989 in electrical engineering. In February 1990 he joined the 'Institut für Mikroelektronik', where he is currently working towards his doctoral degree. His work is focused on improvement and extension of the capacitance simulator VLSICAP and on a Profile Interchange Format environment for a Technology CAD shell .

Grid Generation and Modeling of MODFET Transistors with MINIMOS

Claus Fischer

The investigation of the generation of finite difference grids in arbitrarily shaped two-dimensional structures led to a new algorithm for the initial grid generation in BAMBI (**B**asic **A**nalyzer of MOS and **B**ipolar Devices). The geometry information is converted into a special format of so-called "Interval Relations", which contain all aspects of the geometrical structure that are important to the grid. The number of generated grid lines is kept small, according to the user's requirements. This work has been finished in 1989.

The current research work deals with the connection of classical drift-diffusion approaches with the special features of heterojunctions. In equilibrium the carrier concentration near the heterojunction can be obtained by calculation of a self-consistent solution to the Schrödinger equation

$$-\frac{\hbar^2}{2m^*}\Delta\psi_n + V\psi_n = E_n\psi_n$$

and Poisson's equation

$$\Delta V = \frac{q\rho}{\epsilon},$$

where V is the electrostatic energy of the carriers (electrons). The space charge concentration ρ and the wave functions ψ_n are related by the Fermi-Dirac statistics,

which determine the occupation of the energy levels E_n. Far away from the heterojunction, the carrier densities obtained by this calculation approach the concentrations resulting from the classical semiconductor equations. At the junction, however, there are some basic differences between the two approaches. While the classical equations deliver a maximum concentration of carriers in the potential well, the wave functions reduce to very small values.

Presently a one-dimensional solver for the coupled system is developed to study the deviations from the classical approach. The crucial point is to evaluate characteristic lengths of the relevant device dimensions or doping profiles that restrict the usage of the classical formulas.

For the nonequilibrium case, a simple method has to be found to take into account the effects of the heterojunctions within the system of classical semiconductor equations. The various models for the determination of current flow across the heterojunction existing in the literature have to be considered to get a suitable model which can be integrated in MINIMOS.

Claus Fischer was born in Vienna, Austria, in 1967. He received the degree of "Diplomingenieur" in electrical engineering from the Technical University of Vienna in 1989. At that time he joined the "Institut für Mikroelektronik". Presently he is working towards his doctoral degree. His main interests are heterostructures in general and MODFET's in particular.

Physical Parameters for the Analysis and Simulation of Submicron MOS-Devices

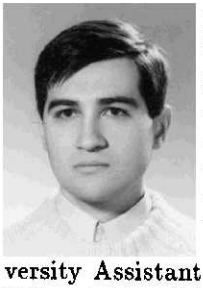
Predrag Habaš

The analytical MOSFET model, with an accurate physics based field-dependent mobility model, presented in my M.S. thesis, has been extended to include an accurate model of the inversion layer charge.

The effect of non-degenerate doping of the polysilicon gate in thin oxide MOS-devices has been investigated. An analytical one-dimensional model of the poly-gate–oxide–bulk structure has been developed in order to examine the relevant physical parameters in the effect. Using this model the influence of the activated impurity concentration in the poly-gate near the oxide and the charge at the polysilicon–oxide interface on the flat-band voltage, threshold voltage, inversion layer charge and the quasi-static C-V characteristic is quantitatively studied. Our simulator MINIMOS has been extended to solve also the basic semiconductor equations in the poly-gate area self-consistently (in fully non-planar geometry). Poisson's equation is solved usually in the whole area. For the continuity equations two equivalent approaches have been implemented: 1) the solution of both discretized continuity equations in the poly-gate simultaneously with the bulk area, or 2) using the carrier concentrations in the poly-gate calculated analytically assuming constant Fermi level in the poly-gate. The second approach performs the calculation in a significantly shorter computer-time. Fermi-Dirac statistics as well as band gap narrowing have been taken into account. A fixed oxide charge and interface trapped charge at the polysilicon–oxide in-

terface have been incorporated. An appropriate grid generation and adaption in the poly-gate has also been implemented.

The proper numerical simulation of a MOSFET in the deep submicron region necessitates a refinement of the present approaches to the modeling of transport processes. We restrict ourselves to the semi-classic approach in the form of balance equations. The performed comparisons between the present local solution for the mobility and carrier energy and the Monte Carlo simulation have shown remarkable discrepancies. Our starting point is an extension of the present local solution in order to include non-local effects. As the device dimensions become less than a half-μm the length of the region in which the field peak occurs is comparable to a few mean free paths for optical phonons and the field varies remarkably within the free path. The classic model for the impact ionization rate in the local field strength concept is therefore inappropriate. The development of an improved non-local model of the carrier energy and impact ionization rate is one important goal of our current work.



Predrag Habaš was born in Vrbas, Yugoslavia in 1962. He received the Graduate Electrical Engineer degree from the Faculty of Technical Sciences Novi Sad in 1985 and the Master of Electrical Engineering degree from the Faculty of Electrical Engineering Beograd in 1989 in physical electronics. From 1985 he worked at the Institute for Power and Electronics University of Novi Sad as Research Assistant and Instructor, where he became a University Assistant in 1989. 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.

Process Simulation in Arbitrary Shaped and Multilayer Structures

Stefan Halama

Process simulation in 2D nonplanar multi-layer structures is a major requirement for thermal processing. Diffusion equations describing the evolution of doping profiles have to be solved for a structure composed of several domains with different material parameters.

Therefore, a major part of the work is dedicated to the extension of the class of simulation geometries which can be treated with PROMIS. Coordinate transformation methods are restricted to problems where the physical structure does not differ considerably from the coordinate domain in geometrical shape. To overcome this restriction, a solution method for diffusion equations using a finite difference / box discretization on a triangular grid is currently investigated. This triangular discretization method provides the greatest flexibility in terms of simulation geometry and device structure, additionally the triangular grid has the advantage of effectiveness of local refinement. First tests on the triangular grid generator have shown quite satisfying results.

The simulation of anomalous diffusion during rapid thermal annealing in two space dimensions calls for well-suited and efficient numerical methods to reduce the computational effort. Depending on the physical model, one has to solve 3 or 5 coupled diffusion equations.

Two major requirements must be satisfied for an adaptive grid: good resolution of gradients and good dose conser-

vation. This leads to two different grid criteria, which control the adaption of the grid according to the evolving dopant profiles.

First, the gradient criterion keeps grid lines in the area of large gradients in the doping profile. Second, the dose conservation criterion of PROMIS has been improved and now minimizes the local dose error $E_{LD} = -\frac{1}{12} f''(x_i) \cdot (x_{i+1} - x_i)^3$ which is consistent with the discretization of the diffusion equation.

The actual grid adaption is achieved by inserting and deleting grid lines. In the case of RTA simulations (which use Monte Carlo implantation results as initial conditions) special care must be taken to preserve grid quality and simultaneously avoid 'grid oscillations' (which is a periodic insertion and deletion of grid lines). To avoid this effect and to preserve a high sensitivity of the grid adaption, the 'relative grid accuracy' adaptivity damping mechanism of PROMIS has been redesigned.

Besides this improvement of the adaptive grid, a static clustering model (which assumes instantaneous clustering of dopants) and two RTA models (for arsenic and boron) have been investigated for PROMIS.

Stefan Halama was born in Vienna, Austria, in 1964. He studied electrical engineering at the Technical University of Vienna, where he received the degree of 'Diplomingenieur' in 1989. During his study he was with several austrian companies where he worked on software development projects in the CAD and computer graphics field. He joined the 'Institut für Mikroelektronik' in September 1989, where he currently works towards his doctoral degree. His research interests are focused on process simulation using triangular grids, grid generation and simulator tool integration.

4D–MOS-Device Simulation

Otto Heinreichsberger

Three-dimensional transient ("4D") simulation has significant importance for a full understanding of the physical effects in submicron MOS devices. Extending the capabilities of the three-dimensional stationary MOS device simulator MINIMOS to a transient simulation tool means solving the time-dependent semiconductor equations, a nonlinear parabolic system of partial differential equations. The solution of the transient problem involves two different time scales. It is thus an extremely stiff problem and makes the use of explicit timestepping schemes inapplicable. In the literature various alternatives to this problem are provided; three approaches are presently in consideration.

The most obvious alternative is an (implicit) one–step backward time differentiation method, which is unconditionally stable, and has successfully been implemented in the device simulator BAMBI already. The local truncation error (LTE) is known to be proportional to the timestep. The timestep control is based on some norm of the space charge increment between two adjacent timesteps.

The approach due to Bank uses a composite method. Starting from t_n the trapezoidal integration scheme is used to compute the solution at an intermediate timestep $t_n + \gamma h = t_{n+1}$, $\gamma < 1$. The two available solutions are now used to compute the solution at the timestep $t_n + h$ by a two-step backward differentiation formula. This procedure is unconditionally stable, too.

The third approach under consideration is due to Ringhofer. Since the transients can be separated into a 'fast' and a 'slow' component a composite method can be applied, namely the trapezoidal rule for the 'slow' component and backward differences for the 'fast' component. This avoids any restrictions on the time steps and is of second order accuracy.

A particular problem is the interaction of the spatial grid with the time discretization. The transient currents are rather sensitive to interpolation errors introduced by the adapted grid on previous timesteps. Such effects can be reduced drastically by computing successive solutions on the adapted grid for very small timesteps in order to relax the interpolation error.

Careful attention is paid to the performance of Gummel's decoupling algorithm under the influence of transient currents. Awesome convergence properties of this iterative method are expected when employing a straightforward extension to the transient case. Remedies for this problem are either nonlinear vector extrapolation techniques applied to the decoupling scheme or the use of inexact Newton methods with block-iterative solvers for the inner linear systems.

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 Geodäsie', 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

For more accurate modeling and better understanding of the effects in sub-micron MOSFETs, we are developing a Monte Carlo (MC) device simulator. The MC model is more rigorous than the widely used Drift-diffusion model. It supplies information about carrier heating, non local effects such as velocity overshoot and ballistic transport, and properties of the carrier energy distribution. The latter is important for the description of degradation effects due to hot carrier injection into the oxide and impact ionization.

The physical model we implemented consists of six anisotropic, nonparabolic valleys for the conduction band, different phonon modes for inter- and intravalley scattering, the Brooks-Herring formulation for impurity scattering and surface roughness scattering. For simulation of MOSFETs we coupled the MC-program with our device simulator MINIMOS. Firstly, MINIMOS is run to supply input data required by the MC-routine, which are potential distribution, doping profile and grid. Around each node of the grid a mesh cell with constant electric field is established. The electron trajectory in real space to be calculated is made up of parabolic segments corresponding to the paths within each mesh cell. In the practical simulation of an n-channel MOSFET electrons are injected in source, where they fully thermalize before entering the channel. In the region of interest, usually near the drain, a sufficiently large number of particles is supplied by a particle split algorithm, thus reducing the statistical uncertainty of the resulting profiles. The

steady state averages are calculated from the so called 'before scattering' distribution function and are assigned to the nodes of the nonuniform grid by employing an extended 'cloud in cell' (CIC) method.

Up to this point our MC simulation can be seen as post-processing step after a conventional simulator run. We plan to obtain a selfconsistent solution of carrier transport and electric field by iterating between the conventional- and the MC-simulator. Therefore a novel coupling scheme will be implemented and tested for the first time. The conventional Drift-Diffusion equation for electrons implemented in MINIMOS has to be slightly extended toward the exact form of the first momentum equation of the Boltzmann transport equation (BTE). The parameters occuring in this equation, namely space dependent mobility $\mu(\mathbf{x})$ and thermal voltage tensor $U_{ij}(\mathbf{x})$, are functionals of the local distribution function in k-space, which is calculated by means of the MC-procedure. The extended current relation using these parameters is capable of recovering the MC results for $n(\mathbf{x})$ and $\mathbf{J}_n(\mathbf{x})$. The solution of the Poisson equation and continuity equation applied to the new current relation is performed with MINIMOS using the Gummel algorithm. This coupling method of MC and conventional simulation can be justified rigorously from the BTE.

Hans Kosina was born in Haidershofen, Austria, in 1961. After having received his degree of 'Diplomingenieur' from the Technical University of Vienna in 1987 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 problems related to MOS transistors in the sub-micron regime in particular.

Miniaturization of Integrated Devices

Erasmus Langer

This project consists of research within the "CHRISTIAN DOPPLER LABORATORY FOR INTEGRATED DEVICES" which represents a bridge between the Institute for Microelectronics and the company Austria Mikrosysteme International GmbH (AMS) in Unterpremstätten near Graz. The Christian Doppler Laboratories which are administrated by the Christian Doppler Society were founded by the Austrian Industries Company as institutions for basic research. As each Laboratory is established at a university, the company has direct access to work of a high scientific level. The individual laboratories conduct basic or fundamentally oriented research on topics of interest to group companies. These areas include primarily the science of materials and electrical engineering, process technology, plastics, fine chemicals and all areas related to microelectronics.

The first period of a Christian Doppler Laboratory is two years; two prolongations (each five years) are possible. The budget is about 3 million AS per year and the Christian Doppler Laboratory for Integrated Devices has spent the budget of the first year for two full time scientists and some hardware equipment (e.g., a superminicomputer with high floating point operation power).

The project "Miniaturization of Integrated Semiconductor Devices" consists of the following research fields: Investigations of influences with respect to the variation of technological processes on the fundamental behavior of microminiaturized semiconductor devices, extraction of

critical parameters for a reduction of integrated devices, extraction of critical parameters with respect to 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 the way of these crucial points should be the development of general rules which have to be tested by the industrial partner AMS according to their 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 on the field of process and device modeling. Since the beginning of the Christian Doppler Laboratory for Integrated Devices, investigations about the process identification of the 2μ–CMOS-technology of AMS have been performed. The present goal is the extraction of critical parameters for a scaled 1.2μ–technology.

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.

GaAs–MESFET Simulation with MINIMOS

Philipp Lindorfer

The rapid development of analog and digital circuits for microwave applications is tightly connected to the developments and improvements of the GaAs MESFET. The GaAs MESFET offers a numbers of advantages compared to the most commonly used silicon technologies. Due to the physical properties of GaAs and the MESFET structure, one can reach highest operating frequencies at low power and very low noise combined with a good radiation hardness using GaAs MMICs.

The framework of MINIMOS 5, which is our integrated two- and three-dimensional device simulator for silicon MOSFETs with small signal analysis capabilities, has been used to implement models allowing the simulation of the MESFET structure using GaAs as additional substrate material.

Therefore, a sophisticated Schottky boundary condition with current dependent surface recombination velocities, process models for the implantation of several dopants in GaAs, and the appropriate diffusion parameters and the material characteristics of GaAs have been implemented. Different models for the carrier mobilities, and generation and recombination have been tested.

An important point in this respect was the implementation of a deep trap model, which permits both deep donor and acceptor traps to be taken into account in the semi-insulating GaAs substrate, which is used in today's GaAs technologies. It has been experimentally found that these

deep traps (e.g., deep 'EL2' donors compensating shallow acceptors in LEC GaAs substrates) very strongly determine the entire device characteristics by influencing the junction properties at the active layer – semi-insulating substrate interface.

This enhanced version of MINIMOS was also successfully used to investigate the location and the nature of avalanche breakdown in power MESFETs, where the origin and the behaviour of both 'before' and 'after' – pinch-off breakdown could be simulated in a self-consistent way.

For the investigation of realistic device structures, enhancements to allow the simulation of fully nonplanar structures, such as recessed gate types or self-aligned 'T-gate' MESFETs using epilayers or implantation technology, have been developed.

The current work includes an investigation of extensions to the classical drift–diffusion approach for the accurate simulation of very small GaAs MESFETs.

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.

Technology CAD Shell based on LISP

Hubert Pimingstorfer

The typical procedure in the field of IC process and device CAD (Technology CAD or TCAD) involves going several times through a loop consisting of generating an input deck for a simulator, running this simulator, extracting data from the output files, making some calculations or postprocessing, producing another input deck and running the simulator again.

This is done on a command level by typing many commands involving various tools, each perhaps with a different command syntax, and most importantly, each may be highly system dependent. Furthermore, the command shells of the different operating systems lack sufficient capabilities for numerical calculations and data storage.

We are developing a shell for TCAD engineering in which all the work can be system independent and offer an interactive and a batch mode. These goals can be met by choosing LISP as the basis of a TCAD shell, and moreover, all the powerful features of this high level language can become available to TCAD.

The advantages of LISP in TCAD engineering are:

- LISP is system independent
- LISP is interactive, but if necessary a LISP interpreter in batch mode can be used or compilation done.
- LISP with its generality and powerful data storage concept fits the needs in an ideal manner
- LISP is the natural way to deal with the PIF intersite mode, because of its LISP-like syntax definition

- LISP is the interface to AI techniques in process and device engineering
- LISP leads to the application of the object-oriented programming paradigm

A LISP based shell can supervise a simulator by generating the input, reading the output, performing numerical calculations, changing the input file and restarting it again. In this form a LISP program can produce a controlled closed loop over simulators and so fit the basic needs of so called *inverted simulation* (which means in very general words: specifying *what* you want to achieve and computing *how* to reach it).

PIF (Profile Interchange Format) is the format for interchanging data between simulators, pre- and postprocessors and a database system. As the syntax definition is LISP-like, we use directly LISP to deal with it. Importing such a PIF-file means only that the built-in 'read' command be executed. There is no conflict between the TCAD shell and PIF, as these concepts complement each other.

Hubert Pimingstorfer was born in Linz, Austria, in 1964. He received his degree of 'Diplomingenieur' from the Technical University Vienna in 1989 in electrical engineering. In November 1989 he joined the 'Institut für Mikroelektronik', where he is currently working towards his doctoral degree in the field of integrating and applying simulators for the improvement and miniaturization of integrated semiconductor devices.

Iterative Solution of Large Nonsymmetric Systems of Linear Equations

Martin Stiftinger

A first (pre-release) three-dimensional version of our MOS/ MESFET simulator `MINIMOS` used Gaussian elimination for solving the large, sparse, and nonsymmetric systems of linear equations which arise from the discretization and linearization of the carrier continuity equations for electrons and holes. The three discretized semiconductor equations for the electrostatic potential ψ and the carrier densities n, p are decoupled by Gummel's algorithm and solved sequentially in the actual version of `MINIMOS`. From our concept of finite difference discretization the ranks, of the coefficient matrices easily reach 10^5.

Moreover, the computer resources required for a direct solution of those linear equations are inacceptably high (CPU–time as well as storage requirement), so that three-dimensional simulations can not economically be done. A very attractive alternative is the use of iterative methods for non-symmetric linear systems, which have increasingly been the subject of intensive research, especially for the past 10 years.

As a consequence of the bad condition number of our problems pre-conditioning is indispensable. The original linear system $\mathbf{A}\vec{x} = \vec{b}$ is transformed to $\mathbf{P}_L^{-1}\mathbf{A}\mathbf{P}_R^{-1}\mathbf{P}_R\vec{x} = \mathbf{P}_L^{-1}\vec{b}$, which can also be written as $\mathbf{B}\vec{\tilde{x}} = \vec{\tilde{b}}$ with $\vec{x} = \mathbf{P}_R^{-1}\vec{\tilde{x}}$. The pre-conditioning matrices have to be chosen such that the condition number of the transformed system is smaller than that of the original system. Various

accelerators such as CGNR, ORTHOMIN, BCG, BIOMIN^2 (CGS), BIORES^2, BIODIR^2, GMRES, and SOR in combination with Jacobi, ILU(k), modified ILU(k), block ILU, and modified block ILU preconditioners have been implemented and their applicability for our problems has been compared. With the ILU and modified ILU preconditioners the degree of fill-in ($k = 0, 1, 2$ in our implementation) can be chosen. A higher degree of fill-in causes a better numerical condition of the linear system and less iterations to solve the equation at the expense of more work per iteration.

Iterative solvers can be vectorized and parallelized to a very high extent. Problems concerning vectorization are caused by the ILU preconditioners. $\mathbf{P}_L$ and $\mathbf{P}_R$ involve backward substitutions for sparse upper and lower triangular matrices. The recurrence relations being introduced can be vectorized by reordering the matrix elements. All points in a computational wavefront (hyperplane) can be computed independently. So these algorithms can be run very efficiently on vector computers.

The implemented algorithms are summarized in a software package for nonsymmetric systems of linear equations arising from the 5– and 7–point finite difference discretization of partial differential equations.

Martin Stiftinger was born in Linz, Austria, in 1964. He received the degree of 'Diplomingenieur' from the Technical University Vienna in 1989 in electrical engineering. In February 1990 he joined the 'Institut für Mikroelektronik', where he first was concerned with the iterative solution of large, sparse, and nonsymmetric linear systems, which was also topic of his 'Diplomarbeit'. He is working towards the doctoral degree, now focusing his work on device and network simulation of DMOS and high voltage CMOS transistors.

Parameter Extraction Automation

Peter Verhás

A typical procedure in the field of IC process development involves the running of simulators to extract values of electrical parameters of the devices. This work is usually done on command level by typing many commands, and running various simulators many times.

When the parameter extraction is finished, the device engineer usually changes some values in the process and runs the parameter extraction again until the parameters satisfy prescribed requirements.

We simulate transistors with original and slightly modified parameters to check whether the optimal technology parameters were used for fabrication. To reach accurate simulation results we have to fit technology parameters which are difficult to measure. This means that by changing these parameters within a realistic window, we minimize the difference between measured and simulated characteristics.

The simulation can be formalized with a function

$$RESULT = f(INPUT).$$

Parameter extraction needs many simulations for several $INPUTs$ which are sometimes very close to each other. In many cases a new simulation can be replaced with interpolation from close inputs.

We are developing a program that runs MINIMOS autonomously and generates a "map" of simulation results. When this map is ready the investigation of the transistor

does not require additional simulations, only the map and an associated interpolation technique is required to extract the results which the simulator would produce. This greatly reduces the required computational resources.

The present version of the program builds up a table which can be used to interpolate the drain current of the simulated MOS transistor on the (U_D, U_G) domain. The structure of the interpolation table is a tree. Each node of the tree is assigned to a rectangular part of the simulated domain. The root of the tree is assigned to the whole domain. Each interior node has four sons as the assigned domain is split into four parts. The domains assigned to a leaf node are not split. When interpolating the value of the drain current for a given bias point the interpolation algorithm can go through the tree from the root to the leaf which contains the point. This search technique requires $O(log\ n)$ time where n is the number of the calculated points in the interpolation table.

Peter Verhás was born in Budapest, Hungary, in 1966. He received his degree of 'Diplomingenieur' from the Technical University Budapest in 1989 in electrical engineering. In November 1989 he joined the 'Institut für Mikroelektronik', where he is currently working towards his doctoral degree in the field of integrating and applying simulators for the improvement and miniaturization of integrated semiconductor devices.

Two-Dimensional Nonplanar Process-Simulation

Karl Wimmer

The treatment of nonplanar structures is an absolute necessity for the simulation of many fabrication steps in modern device technology, in particular for oxidation.

In our 2D process simulator PROMIS a transformation from physical space to computational space is used to deal with nonplanar domains. This transformation is accomplished by specifying a generalized boundary fitted coordinate system which maps the nonrectangular grid system in the physical space to a rectangular grid in the computational space. With this approach the solution domain is simplified at the expense of complicating the equations and boundary conditions.

Several grid generation techniques have been investigated for PROMIS. Algebraic methods, like the transfinite interpolation, afforded fast results, but could not guarantee a one–to–one mapping. Methods based on elliptic partial differential equations (quasi-conformal transformation), as well as variational methods yield high quality grids. Variational methods are favoured due to their flexibility and stability.

For the transformation of the governing equations a special integral attempt has been made. This lead to 'conservative formulations' of the discretized equations, and therefore global conservation properties are satisfied automatically without any additional computational expense.

The PROMIS model library has been upgraded. Several models for point defect assisted diffusion under local oxidizing conditions (OED/ORD) have been implemented. To keep the simulation area small, a three level second order boundary condition has been implemented for the fast diffusing point defects.

A redesign of the internal structure of PROMIS has been performed to improve cpu performance. Without any restriction of flexibility and compatibility, more than 30% speed improvement has been reached for typical annealing steps.

For the coupling to other simulation tools a file handling for PIF (Profile Interchange Format) files has been implemented in PROMIS. In addition to binary result files, the user can now save results in ASCII PIF standard format. In consideration of nonplanar geometries, the flexibility of PIF is an important prerequisite.

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, and a Visiting Research Position at the Advanced Semiconductor Development Department at Digital Equipment Corporation, Hudson, Massachusetts in winter 1990. His research interests include process simulation in nonplanar structures and numerical grid generation.

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