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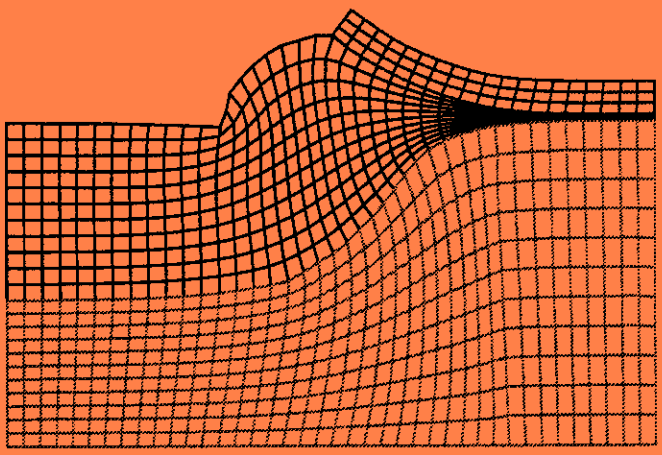

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INSTITUTE FOR MICROELECTRONICS

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Preface

Siegfried Selberherr

This brochure is the fourth research review of our institute. Provision has been made this year by the Austrian Ministry of Science and Research for one additional technical assistant. Thus the staff supported by the Ministry consists now of eight full time employees: the head of institute, four scientists, a secretary and two technical assistants. Fourteen (!) additional scientists are presently funded through scientific projects with industrial institutions. This is perhaps the upper bound of "additional" scientists which we can integrate into our institute.

We are glad to report that all our partners from the last review year have continued to support the institute.

The projects of the institute are still focused on microelectronics modeling issues. We assume that integrated Technology Computer-Aided Design will play a major role for the development of next generations of devices for Ultra Large Scale Integrated (ULSI) circuits. Parts of the VISTA framework which was heavily worked on during the last two years, are now already made available to interested scientific institutions. We sincerely hope to keep pace with the requirements of industry.

We are pleased to report that our institute participated in the evaluation process of the physics departments of Austria and did extremely well. We all enter the fifth 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 'Mikroelektronik' and of the Springer-Verlag book series 'Computational Microelectronics'.

Marion Kaltenbrunner was born in Vienna, Austria, in 1972. She joined the 'Institut für Mikroelektronik' in November 1991. Since that time she has been in charge of organizational and administrative work of the institute.

Ewald Haslinger was born in Vienna, Austria, in 1959. He joined the 'Institut für Mikroelektronik' in December 1991. Since that time he has been in charge of organizational, administrative and technical work of the institute.

Andreas Steidl was born in Herzogenburg, Austria, in 1965. He joined the 'Institut für Mikroelektronik' in September 1991. Since that time he has been in charge of all technical hardware and software work of the institute.

Capacitance Calculation with the Method of Finite Elements

Robert Bauer

The realistic extraction of capacitances in nonplanar VLSI circuits requires numerical methods for the electrostatic field calculation. Today, three methods are commonly used to tackle this problem: the method of finite differences leads on a tensor product grid to a huge number of unnecessarily discretized nodes, while the reduction of volume discretization to surface discretization is the great advantage of the boundary integral method, although fast results can only be obtained for a small number of dielectric regions and conductors. The chosen finite element method can be extended to nonlinear capacitances. A large number of different materials can be handled easily. The disadvantage of this method is the complicated mesh generation in three dimensions.

We use a variational integral formulation, whose minimization condition is equivalent to the differential formulation. The integral holds exactly twice the electrostatic field energy. With the given contact potential we obtain the capacitance directly.

Currently, a commercial input processor is used to produce a boundary conforming hexahedron element mesh, based on a three-dimensional transfinite interpolation. To avoid numerical integration of the element stiffness matrices, all elements are split into tetrahedron elements.

Quadratic element shape functions for ten–node tetrahedron elements allow a precise potential calculation for the energy determination.

Each element with its shape functions builds a local stiffness matrix which will be assembled in a global stiffness matrix. This global stiffness matrix is sparsely occupied.

To achieve an efficient usage of computer memory, a compressed matrix format is used. A direct access with the original indices to an entry to the columnar packed matrix is not possible. An entry will be found with a binary search of the column index in an additional index matrix. Five searching steps are used on average.

Comparisons with simple examples to our two-dimensional simulator VLSICAP which is also based on finite elements for linear and nonlinear capacitances, show a mismatch in the range of a few percent. The calculated two–conductor problems needs only a few minutes for assembling and solving the linear system.

Robert Bauer was born in Vienna, Austria, in 1963. From 1983 to 1984 he worked in the support of medical analysis devices. In the course of his studies he has held various summer positions in the medical branch. He received the degree of 'Diplomingenieur' in electrical engineering from the Technical University of Vienna in 1990. After seven months of industrial development of Brain Mapping Systems – a medical brain diagnostic device, in spring 1991 he joined the 'Institut für Mikroelektronik', where he is currently working toward his doctoral degree in the field of three-dimensional interconnect simulation of multilevel wired VLSI circuits.

VLSI Interconnect Simulation and Technology CAD environments

Franz Fasching

Our two-dimensional interconnect simulator VLSICAP is able to calculate linear and nonlinear capacitances of arbitrary geometries with multiple contacts. VLSICAP is now integrated into our VISTA Technology CAD (TCAD) environment both from the data level (simulation data) and the task level (user interface) point of view.

The data level integration provides simulation data exchange with all other TCAD tools in the framework. This is achieved by accessing all relevant data in a PIF database using the PIF Application Interface which is now linked to VLSICAP. Therefore, not only can geometries created with the PIF Editor, or process simulation results stored in the PIF database, be fed as input into VLSICAP, but also all important VLSICAP results like scalar and vector attributes can be visualized using the powerful VISTA visualization tools which range from simple User Interface Agent vector graphics to advanced visualization tools coupled through the VISTA Visualization Format.

On the task level, an easy to use point-and-click user interface has been developed for VLSICAP during a research stay with SONY Atsugi/Japan. The automatic menu generation facility of the VISTA User Interface Agent was used to create popup menus for all VLSICAP components, thus enabling the user to run VLSICAP ses-

sions just using a pointing device and minimum keyboard input.

As the VISTA project at our institute evolves, several new modules aiding the integration and development of TCAD tools have been implemented on the task level, two of which are described below.

The VISTA Operating System (VOS) was designed to provide operating system features in an operating system-independent way to TCAD task level tools. The most important part is a filename representation based on LISP expressions, which can be converted to and from an operating system-dependent file specification.

To access named resources in the TCAD environment, the VISTA Resource Resolver has been developed. The resources are internally represented as hierarchically built name-value pairs (association lists), but resources can also be derived from PIF binary and ASCII files, the process environment or the process command line. Future extensions will allow resources to be fetched over the network, enabling the implementation of a network-wide resource server holding, e.g., material constants, tool abstractions etc.

Franz Fasching was born in Steyr, Austria, in 1965. He received the degree of 'Diplomingenieur' from the Technical University Vienna in electrical engineering in 1989. In February 1990 he joined the 'Institut für Mikroelektronik', where he is currently working towards his doctoral degree. In 1992 he held a Visiting Research position at SONY, Atsugi, Japan. His work is focused on the VISTA Technology CAD environment and improvement and extension of the capacitance simulator VLSICAP.

Towards MINIMOS 6

Claus Fischer

The progress of the PIF integration of MINIMOS allows one to examine certain aspects of this task more closely. The general tendency shows that the FORTRAN interface of the PIF application layer is at a fairly developed stage and satisfies all fundamental requirements of the simulation program MINIMOS. Several extensions of the PIF application interface, which have been made in the meantime, make the programmer's life easier by offering comfortable and useful extensions. The future cooperation of the PAI developers with programmers of many different applications will very likely lead to a further enrichment of the PIF application interface's capabilities; the present form, nevertheless, meets the basic demands of the programmers quite well.

A first performance evaluation is one of the most interesting points, since MINIMOS uses the PIF as a temporary storage of information during the simulation. This is rather exceptional, because most of the simulation programs will use the PIF just for input and output at the beginning and end of the simulation run; however, by total integration MINIMOS provides valuable statistical information as to the performance and the amount of data transported. As could be expected from the careful design of the PAI, the overhead compared to a simple memory-copy operation is negligible when using large arrays of data; for discrete pieces of data, naturally, the relative overhead is larger, but the effect on the overall performance remains negligible. For tools which use the PAI just for input/output before and after the simula-

tion, no remarkable delays can be expected. Especially the caching and future compressing features of the PIF application interface will help application programmers concentrate on their main interests.

During the last year, MINIMOS has been split into some fairly independent modules which only share the geometry data, and whose execution is controlled by the stack sequencer. Several controlling schemes, for transient simulation as well as for different physical models, can be applied to perform a problem specific simulation, and the schemes are interpreted at run-time. As a future goal, cooperation of the simulator and the TCAD shell will also include detailed commands given to the simulator, thus allowing the individual modules to be treated like independent tools acting on the MINIMOS working PIF.

Future work will also be necessary on the correct representation of transient boundary conditions (such as contact voltages and currents) in the PIF, which is required by the transient simulation capabilities of MINIMOS. The discretized representation of deep trap distributions will also be taken from the PIF file in future, thus allowing the coupling to future process simulation programs which are capable of describing interface states.

Claus Fischer was born in Vienna, Austria, in 1967. Having received the degree of 'Diplomingenieur' in electrical engineering from the Technical University Vienna in 1989, he joined the 'Institut für Mikroelektronik' in January 1990. He is currently working towards his doctoral degree, and his research interests include the new structure of MINIMOS, in particular the integration of MINIMOS into the Viennese TCAD environment.

Simulation of SiGe-MODFETs

Peter Grubmair

In conventional MOSFETs, surface scattering at the Si/SiO_2 interfaces and impurity scattering at low temperatures have deleterious effects on the carrier velocity. In order to alleviate this problem, devices consisting of several Si_xGe_{1-x} layers with different germanium mole fractions and thicknesses, such as SiGe MODFETs and quantum well MOSFETs, are currently under experimental and theoretical investigation. For design engineers it is desirable to have powerful simulation tools. Therefore, the capabilities of our device simulator MINIMOS, which is currently being integrated in the VISTA-TCAD environment, are being enlarged to deal which such devices.

The first physical models which are under implementation handle the above mentioned devices in a classical manner. The different layers are assigned to PIF-segments, and inside each segment the drift diffusion approximation is assumed to hold, while the continuity equations of the different layers are coupled by a thermionic emission term which includes tunneling. In a strict sense, these models are only valid for thick layers, but the solution will be used as a starting point for future models. As all layers are matched with their in-plane lattice constants to a thick buffer layer, they are subject to heavy mechanical tensions. This has a significant influence on the electronic properties: different band alignments and splitting of the conduction band in two-fold and four-fold X-valleys, while the three-fold degenerated hole band is split in a light-hole, heavy-hole and a spin-off band. This band structure has its equiv-

alent in a band description within MINIMOS. Since in a MODFET's graded layer the germanium mole fraction varies continuously, the above mentioned band description as well as other parameters (e.g. permittivity, low field mobility) must be definable at every point in the grid.

In order to study the charge control behaviour and the size quantization effects in SiGe MODFETs, an existing one-dimensional Schrödinger-Poisson solver which relies on a wave-envelope function description and the effective mass approximation, was improved to deal with such structures. The solver also takes into account exchange-correlation potential and Fermi-Dirac statistics for dopants. As momentum mixing at the interfaces is considered an important effect for Si_xGe_{1-x} layers by some researchers, an attempt to account for it by using a matrix interface condition for the wave envelope function and its derivative on both sides of the interface, similar to that found in the literature for tunneling currents in AlGaAs/GaAs, was used; however, the results did not show significant differences from the normally used interface condition, which relies on the continuity of the wave envelope function and of the probability flux density.

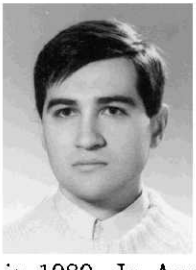
Peter Grubmair was born in Scheibbs, Austria, in 1961. While studying Control Engineering and Industrial Electronics at the Technical University of Vienna, he held various vacation jobs at local firms. He also worked as a student assistant at the 'Institut für Nachrichtentechnik und Hochfrequenztechnik', where he was concerned with multicarrier data transmission. After having received the degree of 'Diplomingenieur' in March 1991, he joined the 'Institut für Mikroelektronik' in May 1991, where he is currently working towards his doctoral degree. His interests lie in the fields of MODFETs and semiconductor physics in general.

Charge Pumping and Tunneling Effects

Predrag Habaš

In our activity in modeling physical effects in small, thin oxide, MOSFETs, special attention has been paid to the analysis of interband tunneling and to the investigation of the charge-pumping experiment.
We have developed and implemented in MINIMOS a two-dimensional numerical model for the interband tunneling, taking account of the direct and phonon-assisted processes. By analyzing the location and the amount of the generated electron-hole pairs for several graded and abrupt drain junctions at different terminal biases, it is found that the tunneling leakage is strongly dependent on the two-dimensional potential and field distribution in the critical area. Significant variations of the electric field along the tunneling path are observed. An expression for the number of the generated pairs by internal field emission in a linearly variable field assuming direct tunneling is derived. The expression is based on the two-band $\mathbf{k}\cdot\mathbf{p}$ model and the WKBJ approximation, and reduces to the Kane expression for a constant field. An accurate expression for the interband tunneling rate in a constant field has been derived by improved integration in the parallel and normal impulse space, assuming the two-band $\mathbf{k}\cdot\mathbf{p}$ band model. Small differences between the derived and the Kane expressions have been observed, showing that the latter is a satisfactory solution to the problem.
The self-consistent two-dimensional transient model for the charge-pumping experiment, which has been developed and implemented in MINIMOS, has been applied to study several effects. The stretch-out of the charge-

pumping curve $I_{cp}(U_G)$ due to the junctions and the trapped-charge–potential feedback effect has been investigated. Moreover, the change in $I_{cp}(U_G)$ after nonuniform stress, when a damaged region is produced near and within the junctions, have been analyzed. We have examined the accuracy of some analytical models for I_{cp} and for the interface-state density extraction. The definition and the location on I_{cp} of the charge-pumping threshold and flat-band voltage have also been investigated. The geometric components of I_{cp} in Si MOSFETs for the 2D case have been explained after intensive study. Extraction of the spatial distribution of interface traps by the charge-pumping experiment has been studied in detail. The charge-pumping characteristics of virgin and stressed LDD MOSFET's have been studied. We noticed that, in order to calculate the contribution of the LDD regions to I_{cp} due to the gate-edge fringing effect, a 2D-transient approach becomes indispensable. The coupling between the front and the back interface and the dimensional/geometric parasitic components of I_{cp} in thin-film SOI devices have been studied by the numerical simulation to improve the present understanding of these effects.



Predrag Habaš was born in Vrbas, Yugoslavia, in 1962. He received the degree of 'Diplomingenieur' from the Faculty of Technical Sciences of Novi Sad in electrical engineering in 1985 and the mr degree from the Faculty of Electrical Engineering of Belgrade in physical electronics in 1989. From 1985 he worked at the Institute for Power and Electronics University of Novi Sad as Research Assistant and Instructor, where he became a full assistant in 1989. In April 1989 he joined the 'Institut für Mikroelektronik', where he currently works towards his doctoral degree. He held a Visiting Research position at the ASD Department at Digital Equipment Corporation, Hudson, Massachusetts in 1990. His research area includes physical electronics in general, and physics and modeling of MOSFETSs in particular.

New Physical Aspects of Device Modeling

Michael Hackel

The problem of electron transport in semiconductors and insulators is commonly tackled by the Boltzmann Transport Equation (BTE). Since a numerical application of quantum transport theory in a consistent formulation is still lacking, the BTE as a semiclassical approach is an important tool for calculating physical observables of interest. As we go to smaller and smaller electronic devices, quantum effects cannot be neglected any longer. The particle-wave dualism and the discrete energy spectrum represented by the wave function may play an eminent role in simulating submicron devices. Aspects of solid state physics such as scattering phenomena and band-structure effects must also be considered.

The first numerical approach to solve the BTE was the drift-diffusion model. With the rapid increase of computer resources during the last ten years, less approximate solutions could be sought by the Monte Carlo method. The Monte Carlo method, as applied to charge transport in semiconductors, is based on the simulation of one or more electrons inside the crystal of the semiconductor, subject to the action of external forces due to the applied electric field and the given scattering mechanisms. The duration of the carrier free flight (the time between two successive collisions) and the scattering events involved in the simulation are selected stochastically in accordance with some given probabilities describing the microscopic processes. As a consequence, any Monte Carlo method relies on the generation of a sequence of random numbers

evenly distributed between 0 and 1 at a sufficient fast rate.

Recently, great efforts have been made to include a correct band-structure for electrons in Monte Carlo models. In order to shed more light on "hot" electrons (electrons with high energy) we have to improve on our first principle assumptions. Although they are few in number, high-energy electrons have great influence on submicron devices, due to trapping/detrapping effects, degradation, leakage effects on drain currents due to crystal defects, tunneling and others. Thus, only a correct treatment of the background physics will lead to reliable quantitative results. Extending our Monte Carlo model to carrier transport in oxides we have to introduce polar optical, energy-absorbing phonons and, additionally, momentum-absorbing, nonpolar acoustic phonons to prevent "polar runaway" of the electrons at sufficient high electric fields.

Nevertheless, numerical aspects have to be faced, too. To save CPU time, it is possible to add an arbitrary constant to the physical scattering rate. We have developed and implemented a novel self-scattering algorithm. Instead of a sequence of step-shaped linear functions we introduce three linear enveloping functions which model the derivative of the physical scattering rates in order to minimize the self-scattering rate.

Michael Hackel was born in Vienna, Austria, in 1965. He studied technical physics at the Technical University of Vienna, where he received the degree of 'Diplomingenieur' in 1991. During his study he worked on projects of solid state physics and quantum field theory. He joined the 'Institut für Mikroelektronik' in January 1992. He is currently working towards his doctoral degree. His scientific interests include solid state device technology, device modeling and physical aspects in general.

A Generic X11 Based User Interface for Tool Integration

Stefan Halama

The importance of the user interface for advanced process and device simulation is often underestimated. The rapid development of software tools which use increasingly complex physical models and numerical methods calls for a generic user interface that meets the following requirements: it must fit into a TCAD system, typically consisting of a database interface simulator, and execution control; it must be flexible enough to accommodate easily the changing demands of new tools without necessarily changing the behavior of the user interface itself, and it should allow one to tailor the user interface to the specific needs of the user and to comply with existing environments, regardless of the underlying simulation tools.

The VISTA User Interface Agent (UIA) is built from a set of widgets which consists of the standard *Athena* widget set, additional specialized widgets which include advanced vector graphics capabilities, comfortable specification of integer and real values, and a visual programming interface. This extended widget set is accessible from within the TCAD shell. Using LISP as the implementation language, a layer of functions is provided which makes the programming interface fairly independent of the underlying widget set. The next layer is responsible for the creation of more complex user interface objects such as a periodic table menu, a symbolic PIF browser, a PIF attribute calculator or generic tool control panels.

Events coming from the user interface are passed on to

the interpreter by using the X11 callback method. In response to any user action (e.g., pressing a button), a LISP expression is evaluated. This expression is a property of the widget which issued the callback and can be used to change parameter values, trigger other events like the execution of a simulator, or start the evaluation of any LISP program.

The same callback concept is also used for the control of simulator execution. If a simulation tool terminates, it signals the termination to the parent process, which again causes the callback expression to be evaluated. Callbacks may be triggered by the user interface, error handler, network layer, timer, or by termination of child processes.

Our experience shows that the decoupling of the user interface from the actual simulators and the very generic functionality due to the bottom–up design and the interpretative LISP environment is very well suited for both, integrating existing simulation tools as well as implementing new ones.

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 collaborated 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. In winter 1991 he held a Visiting Research position at Digital Equipment Corporation, Hudson, Massachusetts. His research interests include process simulation, automatic grid generation, TCAD frameworks aspects, tool integration, visualization and software technology.

Monte Carlo Simulation of Si MOSFETs

Hans Kosina

A two-dimensional, steady state Monte Carlo device simulator which is especially suited for the simulation of submicron MOSFETs has been developed and implemented in the MINIMOS program. The semiconductor model takes into account the non-parabolic, anisotropic nature of the band-structure, and includes three-dimensional optical and acoustic phonon scattering, as well as ionized impurity and surface roughness scattering.

To perform the free-flight time calculation, a new self-scattering algorithm has been developed. The use of a piecewise linear total scattering rate allows for an efficient reduction of self-scattering events. Charge assignment to non-uniform grids is accomplished by a convolution method using non-trivial weighting functions. A trajectory multiplication algorithm is required to deal with the widely varying carrier concentration magnitudes occurring in a real device. A unique Monte Carlo–Poisson coupling scheme has been adopted, which converges faster than presently known schemes do. This technique is based on the so called Monte Carlo–drift-diffusion coupling, a method which proves to be correct within the semiclassical Boltzmann transport theory.

The coupling coefficients between the Monte Carlo and the drift-diffusion model are the carrier energy tensor and the mobility, which depend on the first three moments of the distribution function. An extended drift-diffusion-like current relation, which is motivated by the first momentum equation, in conjunction with these coupling coeffi-

cients exactly reproduces the Monte Carlo-transport behaviour. Approaching thermal equilibrium, the extended current relation simplifies to the conventional drift-diffusion relation.

The Monte Carlo–Poisson coupling is done by including the continuity equation and the extended current relation in the iteration loop. Each Monte Carlo step performs an update of the coupling coefficients. The expectation of a high convergence rate, which is based on theoretical considerations, has been confirmed empirically. Simulation of MOSFETs with gate lengths in the range of $0.15\mu m$ to $0.75\mu m$ clearly shows velocity overshoot in the pinch-off region. In that area a reduction of the carrier concentration is observed, thus compensating the influence of the velocity overshoot on the drain current. Therefore, self-consistency is mandatory for such small devices, otherwise the overshoot phenomena will be overestimated. The self-consistent treatment yields a potential distribution, which is smoother than that of a drift-diffusion simulation, thus predicting a lower field peak at the drain edge.

Hans Kosina was born in Haidershofen, Austria, in 1961. He received the 'Diplomingenieur' degree from the Technical University in 1987 in electrical engineering. He was for a year with the 'Institut für flexible Automation' and joined then in 1988 the 'Institut für Mikroelektronik', where he is currently employed as an assistant professor. Recently he received the doctoral degree from the Technical University of Vienna. His scientific interests include solid state device technology and behavior in general, and the physical and numerical methods applied to device modeling in particular.

Technical Programming in FORTRAN

Erasmus Langer

The aim of this project is the publication of a book in German with the translated title "Technical Programming in FORTRAN" which describes the programming language according to the new ANSI standard 90 which has been published May, 1991. As from experience it will last some time until the first compilers according to the new standard will be available. In the book, all new features are emphasized as well as the old ones. Therefore, it can also be used as manual for the actually spread standard 77. Furthermore, it serves as a basis for the solution of technical–mathematical problems in engineering as the topics "operating system specific applications" and "numerical mathematics" are included.

Most of the worldwide existing scientific programs are written in the programming language FORTRAN which has been developed during the early sixties especially for numerical applications. This is due to the efficiency of the executable program code most of the FORTRAN compilers can achieve and the strict standardization of FORTRAN which makes the software easily transferable from one computer and/or operating system to another.

During the last years the programming language C gained importance as a result of the increasing use of the operating system UNIX (with all its variations). Nevertheless, it is doubtful that the importance of FORTRAN as the dominant programming language in the scientific and technical fields using numerical methods will be diminished essentially within the immediate future. The reason for this assumption lies in the widespread use of FORTRAN program libraries and in the continuous de-

velopment of the language standard.
FORTRAN has been standardized the first time in 1966 and the second standard followed eleven years later. The most important progress between these two standards was the introduction of variables and constants of character type associated with the corresponding functions for string handling. Furthermore, the standard 77 included new language elements which allow more "structured programming". The new standard 90 certainly doubles the number of language elements — thus, a program written in the new standard and using all new features (e.g. neither depreciated nor obsolete language elements) hardly has any similarity to a FORTRAN 77 program. Nevertheless, the new standard is fully upward compatible and, therefore, a standard 77 program (without operating system dependent extensions) must be translatable with a standard 90 compiler without any changes.
The probably most important new features of FORTRAN 90 are: parameterization of intrinsic data types, array operations, dynamic memory allocation, user-defined data types and operators, pointers, variable attributes, internal subroutines, modules, free source format, partial line input/output, new control constructs, and many new intrinsic functions.

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 in the field of technical programming in FORTRAN and parameter extraction for the improvement and miniaturization of integrated semiconductor devices.

Advanced MOS Device Engineering Utilizing a Technology CAD Framework

Hubert Pimingstorfer

For the development of advanced devices the demands on technology CAD (TCAD) range from simple simulator coupling over process and device characterization to technology optimization. The TCAD framework VISTA has been developed and is undergoing further extension, integrating the required simulation tools, a simulation database, a TCAD shell and a graphical user interface into a homogeneous environment. The TCAD shell provides easy combination of all the different functional units with a powerful shell language for defining and solving high-level engineering tasks.

The utilization of this framework and the impact on computer-aided MOS device engineering have been demonstrated on concrete tasks carried out within our cooperation with Austria Mikrosysteme International GmbH (AMS). This industry partnership has been invaluable for gaining feedback and suggestions for the further development of VISTA.

The identification of the effect of variations in the fabrication process on device performance is a typical application field of a TCAD framework. The effect of varying the spacer width on the device behavior in the strong inversion regime has been investigated for a high-voltage CMOS technology.

Short shell programs couple process simulation with several runs of a MOS device simulator and postprocessing

tools to automate the computation of I-V characteristics and to display them immediately. Taking advantage of the inherent parallelism, the device simulator is run simultaneously on different remote machines of a workstation cluster.

For technology optimization, process and device simulation for extensive profile characterization are coupled within an optimization loop. A well-known example is the bulk-current minimization obtained by varying the LDD implant dose of an n-channel MOS transistor. The change in device characteristics for different tilt angles of the LDD implant has also been studied. Subject of other investigations, also carried out by utilizing our VISTA system, has been the improvement of the punch-through immunity of a p-channel device by raising the well doping concentration and simultaneously adjusting the threshold adjust implant dose under the constraint of an unchanged threshold voltage.

The capabilities of our TCAD framework ease and automate complex development tasks in process and device engineering. As a result, the user is supported efficiently in the design of tomorrow's MOS devices.

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.

The Profile Interchange Format Editor

Gerhard Rieger

The VISTA project provides a general data exchange format for simulation tools, named PIF. Its concept provides two major advantages. The first is the elimination of the so-called 'n(n-1)/2'-problem in simulator-coupling: instead of programming a data translation tool for every possible combination of two simulators (in practice every required combination), we only need an input and an output interface for each simulator.

The second advantage is that tools need not be programmed for every simulator data format, but are developed only once for PIF. One of the most important of these tools is a graphical editor for the interactive manipulation of PIF files, called PED.

A set of prerequisites that PED's architecture needs to satisfy are typical of the VISTA environment, i.e. the programming language (C), the extension language (XLISP), the X11 window system as user interface, and a callback philosophy.

Some other requirements are a generic and flexible undo-concept, and widget orientation. The latter is implemented by a two-stage widget tree. The lower stage makes it possible to display and edit one logical PIF file in several related windows. The upper stage allows editing of many logical PIF files by only one process instance of PED. This allows combination of various PIF files via a 'cut and paste' mechanism.

Although visualization is an intrinsic requirement of an

interactive graphical editor, it is not PED's main task. The most important features are comfortable and comprehensive input capabilities. Obviously these imply clear displaying of recently built or previously existing data.

The basis of an existing general data format makes it worthwhile putting some more effort into this editor to make it as comprehensive as possible. So PED is designed as an overall editing tool that may handle one-, two-, and three-dimensional geometries, n-dimensional attributes, orthogrids, and all kinds of attributes with their specific data types.

Currently, PED is able to display and edit two-dimensional and display three-dimensional graphical PIF objects.

VISTA includes another important part, the VV visualization tool. In it, a generic and rigorous axis generation and drawing technique provides easily readable, high-level diagrams. This implementation is a good example of PIF's power: All information, including the captions on the axes, can automatically be extracted from the PIF file without the need for additional information.

Gerhard Rieger was born in Vienna, Austria, in 1963. He studied electrical engineering at the Technical University of Vienna, where he received the degree of 'Diplomingenieur' in 1991. He joined the 'Institut für Mikroelektronik' in December 1991, where he currently works towards his doctoral degree. His research interests include programming languages and compilers, software technology, geometry, and visualization.

MINIMOS for AlGaAs/GaAs HEMTs

Cristiano Sala

The computer-aided simulation of the electrical behavior of ultrasmall, high-speed electronic devices manufactured from compound semiconductors such as gallium arsenide (GaAs) is an extremely active, global research domain. A case in point is provided by the current generation of AlGaAs/GaAs High Electron Mobility Transistors (HEMTs), which rank among the fastest solid state devices ever constructed, and are characterized by typical dimensions of one micron or less. In this size regime the response to an applied electric field can be highly non-linear, and an exhaustive physical theory for these phenomena is still lacking. Moreover, the perpendicular confinement of the active region to a surface layer only a few hundred Angstrom thick leads to significant size quantization effects.

In order to characterize the static behavior of this system, an existing one-dimensional Poisson-Schrödinger solver has been reviewed and improved upon, to allow it to calculate the capacitance of the HEMT as a function of the applied gate voltage. A number of technologically relevant features, amongst which the possibility of including partial ionization of the dopants in the AlGaAs layer, or a sophisticated initial guess for the inversion region, have been added. Comparisons with experimental data supplied by Siemens have shown satisfactory agreement, and have highlighted the importance of simulating the entire structure in a self-consistent manner. A further useful side-effect of this effort is the in-house availability of code which will gauge future MINIMOS prototypes.

For MINIMOS to be able to simulate HEMTs, and more generally any device whose operation relies on bandgap engineering, profound structural and conceptual changes are necessary. The devices often consist of layers having different material compositions, and hence different physical properties. Moreover, the band structure of these materials allows for the existence of carriers in separate energetic configurations. Compatibility with the PIF syntax is also an issue. A set of flexible geometrical constructs has been developed for this purpose. Up to three hole and three electron bands can be accounted for in each layer, and a rudimentary *material server* automatically supplies default values for the carrier's physical properties. At the time of writing, work is underway to upgrade relevant parts in MINIMOS and enable it to simulate these structures. As well as material-specific quantities such as mobilities and doping distributions, a generalized initial guess for the electrostatic potential is being developed, and carrier transport across heterojunctions is being critically reviewed.

Cristiano Sala was born in Milan, Italy, in 1964. He received the B.A. Oxon. degree in Physics from the University of Oxford, Great Britain, in 1983, the M.Sc. degree in Applied Physics from the California Institute of Technology, USA, in 1985, the 'Diploma di Laurea' in Physics from the University of Milan, Italy, in 1986, and the Ph.D. degree in Physics from the University of Leuven, Belgium, in 1991. His past interests have included investigating the thermal and structural stability of thin-film diffusion barriers and modelling the high-field transport of electrons in systems of low dimensionality. Since September 1991 he is with the 'Institut für Mikroelektronik', where he is in charge of extending MINIMOS' simulation capabilities to AlGaAs/GaAs HEMTs.

BiCMOS-Modeling

Gerhard Schrom

The combination of bipolar and MOS devices on one chip offers great advantages for their circuit performance and design flexibility over pure bipolar or CMOS processes. Special requirements such as low-voltage, low-noise, high-speed, high-precision, and mixed analog-digital applications are best met with a BiCMOS (Bipolar-CMOS) technology.

BiCMOS can be applied on two levels: the mere combination of pure bipolar and MOS devices (circuit level) and the combination of bipolar and MOS structures in one device (device level, merged-BiCMOS). In either case, issues such as process complexity, area consumption, yield, downscaling, device performance, and sensitivity to process parameters must be dealt with. Furthermore, circuit design technique as a new 'parameter' greatly influences all of the above quantities. The research activities in the BiCMOS field will include studies of the aforementioned questions as well as the solution of concrete problems with devices and processes. The cooperation with the Austrian semiconductor manufacturer AMS also provides access to experimental data which helps to improve both the simulations and the manufacturing processes.

The numerical investigation of BiCMOS structures is not a specialized, singular task but comprises process simulation, device simulation of bipolar, MOS, and merged-BiCMOS structures, parameter extraction, circuit simulation, and statistical analysis (to mention only the most important). Thus, several specialized numerical tools

must work together consistently and efficiently. This can only be achieved with a TCAD framework such as the VISTA system which is being developed at our institute. In this connection, a so-called PIF-browser was implemented. This new tool eases the use of PIF-files, especially when integrating or developing a new simulator.

Although CMOS is likely to predominate in the VLSI and ULSI domain, there will be a significant market for BiCMOS, e.g., in the fields of semi-custom ICs and telecommunications. Whether BiCMOS or CMOS will be the technology of the future, is not clear yet. However, research in both fields continually encounters new problems whose solutions are beneficial to either technology.

Gerhard Schrom was born in Mödling, Austria, in 1963. He studied electrical engineering at the Technical University of Vienna, where he received the degree of 'Diplomingenieur' in March 1992. During his study he worked on software development projects in the CAD field. He joined the 'Institut für Mikroelektronik' in April 1992, where he currently works towards his doctoral degree. His research interests include device and circuit simulation, circuit design and synthesis, signal and image processing, and TCAD framework aspects.

Simulation and Analytical Modeling of High Voltage DMOS Transistors

Martin Stiftinger

As a first approach for an analytical model for vertical DMOS transistors a "subcircuit" description consisting of standard models (e.g. the SPICE device models) has been developed. In comparison to a new analytical model which describes the whole device, a subcircuit model can be built and varied rather easily. In this way, different subcircuit approaches can be compared in a straightforward manner. Device simulation gives insight into the important physical processes occurring in the device and helps to design a subcircuit model.

The DC behavior of a vertical DMOS transistor can be described rather satisfactorily by a subcircuit in which the channel is represented by a MOSFET model and the influence of the drift region is approximated by a standard JFET model. The static behavior at reverse bias conditions is described by bipolar transistors. Comparisons with measured data and device simulation show that there is an important influence on the device behavior, especially in the AC case, from the strongly non-uniform channel doping in the lateral direction. The channel doping profile of the n-channel device is defined by the different lateral diffusions of p-base and n^+-source.

The first approach, found in the literature, was to integrate the expression for the drain current in the strong inversion regime without taking into account the non-uniform doping. One factor of the result can be identified as the derivative of the bulk depletion charge with

respect to the channel potential. This factor is calculated separately by taking into account the non-uniform doping on the assumption of a linear distribution of the electrostatic potential along the channel. The results of this method can not be easily interpreted physically, and there is no straightforward way to extend this approach for a charge-based capacity model.

Thus, an alternative approach has been chosen. The drain current in the strong inversion regime is integrated for a non-uniform channel doping also under the assumption of a linear channel potential distribution. For a constant channel profile the "classical" result is obtained (as in the first approach), and the result seems to be more physically sound as in the first approach. Another benefit of the new approach is its extendability to state-of-the-art, charge-based capacitance models to account for the non-uniform channel doping.

Device simulations using BAMBI also give physical insight in the drift region. Therefore, the standard JFET model from the first subcircuit model has been replaced by a model for the drift region which also accounts for the device-specific geometry of the DMOS transistor.

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 non-symmetric linear systems and the vectorization of those algorithms. He is currently working towards the doctoral degree, focusing his work on device and network simulation of DMOS and high voltage CMOS transistors. His research area also includes parameter extraction and fitting strategies.

Monte Carlo Simulation of Ion Implantation

Hannes Stippel

Starting from an already existing two-dimensional code for amorphous targets, which contains some extensions for special three-dimensional structures, a more general module for the three-dimensional case has been developed. This module can handle arbitrary trench structures. A polygonal cross-section in the x/z-plane together with the length specifies the geometry of the trench. In the y-direction, the structure is either limited by planes or semicircles. For the round trench, the walls are specified by arcs in planes parallel to the surface. Additionally, the trench is assumed to be symmetric relative to the x/z-plane. As most of the simulation time is usually consumed in detecting whether the particles cross a boundary between different materials, a special focus was put on the efficiency of these geometric checks.

Furthermore, a general module for amorphous targets has been developed. It is not restricted to trenches, but it can handle any structure which is defined by planar polygones. Special attention was paid to the representation of the geometry and to the optimization of the geometry checks, since these checks are critical in terms of simulation time for three-dimensional structures. Moreover, the chosen data representation allows for an easy coupling of this module with three-dimensional topography simulators.

In this general module, a so-called **"octree"** is used for the representation of the geometric data. By use of the

octree the geometry is discretized using cubes. Every cube is recursively subdivided into eight subcubes, until either the desired accuracy of the discretization is reached – this is defined by the sidelength of the cube –, or no intersection of the cube under scrutiny with the polygones defining the geometry exists. During the simulation of ion trajectories, simple comparisons can be used instead of very complicated and numerically sensitive computations of intersections. To determine the location of an ion, only a test of the coordinate to the related coordinates of the sidewalls of the cube is required, because a cube is a simple and convex geometrical object. By use of the octree, in contrary to common assumptions, the computation time per ion could be decreased.

Besides this, the integration of PROMIS, especially the ion implantation modules, into the VISTA system has been nearly completed. Some minor final changes were necessary to allow the coupling of the Monte Carlo ion implantation module with other simulation tools. To verify the capabilities of this module and of the whole VISTA system, it has been coupled with the topography simulator SAMPLE.

Hannes Stippel was born in Vienna, Austria, in 1966. During his study at the Technical University of Vienna he held various vacation jobs at local companies. He also worked as a teaching assistant at the 'Institut für Hochbau für Architekten'. He received the degree of 'Diplomingenieur' in electrical engineering from the Technical University of Vienna in 1990. In July 1990 he joined the 'Institut für Mikroelektronik'. He is working towards his doctoral degree, and he is currently holding a Visiting Research position at National Semiconductor Corporation, Santa Clara, California. His work is focused on ion implantation in three-dimensional structures.

Three-Dimensional Simulation of Etching and Deposition Processes

Ernst Strasser

Etching and deposition are important process steps in modern semiconductor technology. The increasing complexity of integrated circuits requires a better understanding of the fundamental chemistry and physics concerning these fabrication steps.

Previous research has applied different physical models to specific algorithms for topography evolution.

The string method uses a string of connected points to approximate the wafer surface. Points on the surface are moved according to the local etch rate. A segment control is necessary to avoid loops or excessively long line segments. The extension to three dimensions is possible, but rather difficult.

The cell-removal algorithm divides the material being etched into a large array of rectangular prismatic cells. The surface or etching boundary consists of unetched or partially etched cells that are in contact with fully etched cells. The cells are removed one by one according to the local etch rate and the number of cell faces exposed to the developer.

A third approach for topography simulation describes the material surface by solving a diffusion equation. At the etch front material is reduced in density. The material can be considered porous and the material surface can be described by a constant concentration area. The movement of the etch front corresponds to the movement of

the contour surface. This method relates the etch rate to the diffusion coefficient. The diffusion equation can be solved by numerical analysis using a finite difference method, periodically reinitializing the boundary conditions at the simulation area.

Etching and deposition phenomena can be characterized by connecting the etch or growth rate with various physical models.

The decision as to which specific algorithm should be used for our simulation tool has not yet been made. Some of the approaches offer certain advantages, but they suffer from either inaccuracy, applicability to a limited number of process models, implementation complexity, or computational inefficiency. There is still room for further investigations in that field.

Ernst Strasser was born in Salzburg, Austria, in 1966. He studied electrical engineering at the Technical University of Vienna, where he received the degree of 'Diplomingenieur' in 1991. In January 1992 he joined the 'Institut für Mikroelektronik', where he currently works towards his doctoral degree. His work is focused on process simulation, especially on algorithms and mathematical models for three-dimensional simulation of etching and deposition processes in integrated circuit fabrication.

The PIF 1.0 Release

Walter Tuppa

The PIF Application Interface was released in March 1992 as the first part of the VISTA (Viennese Integrated System for TCAD Applications). This release supported several different machine architectures and operating systems such as VAX/VMS, Ultrix, HP/UX, Apollo Domain (BSD emulation), SONY NEWS/OS and Interactive Unix (PC). Later on, this release was adapted to a SUN 4 (Sparc) workstation and an IBM RS6000 RISC computer without any problems.

The release supports `C` and `FORTRAN` as a multilingual feature, since most simulators are currently written in `FORTRAN`, whereas the PIF Application Interface was written in `C`. The link module between this two languages is automatically generated from an abstract description. This is mandatory because every operating system uses different methods for parameter passing (e.g. `C` strings versus CHARACTER variables in `FORTRAN`) and different representations for the logical values. The automatic code generator is currently not part of the release, but the bindings for all different systems are pregenerated.

The PIF Application Interface is organized in six different layers. The system layer allows the file layer which does the actual data transfers and implements file locking, to operate in a unique way for the required system functions. Above the file layer is the network layer, which will allow access to a database server in the future. For maximum speed, the caching layer stores the most recently used parts of the PIF file in memory. All these

layers have no information about the stored data. The basic layer implements simple data structures like arrays and linked lists. The interface layer is generated almost automatically from a syntax description of the PIF file. Thus, every PIF file generated by the interface layer is syntactically correct. This layer provides a wide support for searching for PIF objects in many different ways, e.g., by name, by type or by reference. This allows easy access to the database. The top layer is the Application Layer which implements some functions for accessing whole data structures with semantical meaning. It also has a `FORTRAN` binding for multilingual support.

The last part of the PIF release is the PBFM (PIF Binary File Manager) which allows a conversion between a binary representation and ASCII format of the PIF file for transfer between different architectures which are not binary-compatible. On conversion to binary, the syntax is checked automatically by the tables of the interface layer; however, no semantical checking is possible. This tool also allows to repair a PIF file which has not been closed correctly on program exit.

Walter Tuppa was born in Vienna, Austria, in 1966. He received the degree of 'Diplomingenieur' in computer science in 1991 and in electrical engineering in 1992 from the Technical University of Vienna. In July 1991 he joined the 'Institut für Mikroelektronik', where he is developing the PIF Application Interface of VISTA. At present, he is working towards his doctoral degree in electrical engineering.

Two-Dimensional Process-Simulation in Nonplanar Structures

Karl Wimmer

Governed by the potentiality of the Profile Interchange Format (PIF) and the VISTA framework, our two-dimensional process simulator PROMIS has been restructured, and now allows nonplanar geometries to be used for all process steps.

For each physical process step (ion implantation, thermal processes, etc.), a separate program module exists. Each module fetches all required input data from a standard PIF binary file, and output information is written exclusively to PIF binary files too. This simplifies the addition of new modules. A prerequisite for the partition of PROMIS into independent modules was the implementation of a one-pass capability. The feature of user-definable physical models is supported in a manner fully compatible with previous versions, in order to facilitate model development.

The new nonplanar modules for diffusion problems and steady state problems (e.g., oxidant flow) are based on a transformation method. Particular attention has been given to convective fluxes which appear in problems with time-dependent geometries (e.g., during oxidation), and on divergence-free time- and space-discretization methods to avoid spurious source terms.

The new module for the analytic simulation of ion implantation is able to calculate profiles implanted into arbitrary non-planar multilayered structures at arbitrary

implantation angles. During the calculation, "artificial" boundaries receive special consideration. In cooperation with industrial users, lookup tables for profiles in one-dimensional slices of the geometry have been implemented, improving the performance by more than one order of magnitude.

To provide a real "hierarchy" of diffusion models, the library of standard models has been extended towards both simple, but fast models, and physically sophisticated, but computational expensive models. A quick idea of the evolving dopant profiles can be achieved from an uncoupled model which assumes independent diffusion of the dopants and neglects high concentration effects. A pair-diffusion model is available for low thermal budget processes, where transient-enhanced diffusion effects occur.

In all new implemented modules, the parameters for physical models are placed apart from the source code in separate resource files to support future parameter optimizers within the VISTA framework, and to simplify the calibration process.

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 towards the doctoral degree. From 1977 to 1986 he held summer positions in Austria and Switzerland working on industrial automation and adaptive control. He was Visiting Scientist at the Advanced Semiconductor Development Department at Digital Equipment Corporation, Hudson, Massachusetts in winter 1990, and at the Advanced Product Research and Development Laboratory at Motorola Incorporated, Austin, Texas in summer 1991. His research interests include process simulation in nonplanar structures and numerical grid generation.

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