Workshop on

Advances in Modeling and Simulation of Semiconductor Devices

July 14–16, 2004, Berlin, Germany

Weierstrass Institute Berlin

This workshop is supported by DFG WIAS

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20 44 975
Phone: +49 30 20 372 0
Web: http://www.wias-berlin.de

Contents

AMaSiS'04

The aim of this workshop is to bring together applied mathematicians and scientists from semiconductor physics and technology and to give them the opportunity to exchange experience in the field of modeling and simulation of micro-, nano-, and optoelectronic devices. The main topics of the workshop include:

- Physical modeling of micro-, nano-, and optoelectronic devices and their technology,
- Design of efficient simulation software,
- Presentation of simulation results of state-of-the-art devices,
- Analytical and numerical investigation of relevant model equations,
- Study of systems of nonlinear partial differential equations arising in related application areas (e.g. self-gravitating systems, plasma instabilities, phase separation models).

Organizing Committee:

Annegret Glitzky, Jens A. Griepentrog, Rolf Hünlich, Hans-Christoph Kaiser, Joachim Rehberg (all WIAS Berlin).

Programme

Wednesday, July 14, 2004

Time	Event
09.00 – 09.30	Registration
09.30 – 09.40	Opening
09.40 – 10.20	Ch. Schmeiser (Wien) *Transport in Semiconductors at Saturated Velocities*
10.20 – 10.40	Coffee Break
10.40 – 11.20	N. Ben Abdallah (Toulouse) *Kinetic and Diffusive Models for Partially Quantized Systems*
11.20 – 11.55	A. Arnold (Münster) *Transparent Boundary Conditions for Quantum-Waveguide Simulations*
11.55 – 12.10	Ch. Manzini (Pisa) *On the 3-d Wigner–Poisson–Fokker–Planck Problem*
12.10 – 14.00	Lunch Break
14.00 – 14.40	T. Nadzieja (Zielona Góra) *Global and Exploding Solutions in a Model of Self-Gravitating Systems*
14.40 – 15.20	P. Biler (Wrocław) *Mean Field Models for Self-Gravitating Particles*
15.20 – 15.40	Coffee Break
15.40 – 16.20	A. Jüngel (Mainz) *Analysis and Simulation of Quantum Diffusion Models* *for Semiconductor Devices*
16.20 – 16.40	E. Schöll (Berlin) *Nonlinear and Chaotic Spatio-Temporal Dynamics* *in Semiconductor Nanostructures*
16.40 – 17.00	Break
17.00 – 17.20	A. Zisowsky (Berlin) *Discrete Transparent Boundary Conditions* *for Time-Dependent Systems of Schrödinger Equations*
17.20 – 17.40	I. Lobanov (Berlin) *Impurity Center in the Quantum Dot:* *Analytical and Numerical Results*

Thursday, July 15, 2004

Time	Event
09.00 – 09.40	G. Dziuk (Freiburg) *Harmonic Maps as Tools for Grid Improvement* *on Boundaries and Interfaces for Flow and Transport*
09.40 – 10.20	P. Degond (Toulouse) *Plasma Instabilities in the Ionosphere*
10.20 – 10.40	Coffee Break
10.40 – 11.20	W. Jäger (Heidelberg) *Asymptotic Analysis and Effective Laws*
11.20 – 12.00	K. Gärtner (Berlin) *Dissipative Discretization Schemes for Drift-Diffusion* *and Phase Separation Models with Applications*
12.00 – 14.00	Lunch Break
14.00 – 14.40	K.H. Hoffmann (Bonn) *Mathematical Methods for Sensor-Design*
14.40 – 15.20	J. Frehse (Bonn) *L^p-Estimates for the Convective Terms of Compressible Fluids*
15.20 – 15.40	Coffee Break
15.40 – 16.20	L. Recke (Berlin) *Newton Iteration Procedure* *and Nonlinear Elliptic Boundary Value Problems with Non-Smooth Data*
16.20 – 16.40	V. Geyler (Berlin) *Numerical and Analytical Investigation of the Fermi Surfaces* *for the Periodic Schrödinger Equation with a Magnetic Field*
16.40 – 17.00	Break
17.00 – 17.20	P.N. Racec (Cottbus) *Application of R-Matrix Formalism in Modeling* *of Semiconductor Nanostructures*
17.20 – 17.40	R. Plato (Berlin) *Entropy Estimates for a Fully Discretized Fokker–Planck Equation*
18.30	Dinner Party

Friday, July 16, 2004

Time	Event
09.00 – 09.40	G. Wachutka (München) *Macromodeling of Microdevices:* *Virtual Prototyping by Predictive Simulation*
09.40 – 10.20	N. Strecker (Mountain View) *Mesh Generation for Three Dimensional Process Simulation*
10.20 – 10.40	Coffee Break
10.40 – 11.20	R. Richter (München) *Silicon Radiation Detector Development* *Using Two-Dimensional Device Simulation*
11.20 – 12.00	R. Stephan (Dresden) *Advanced Microelectronic Front End Processes, Transistors,* *and Back End Processes Challenging the Modeling and Simulation* *of the Semiconductor Processes and Devices*
12.00 – 14.00	Lunch Break
14.00 – 14.40	B. Heinemann (Frankfurt (Oder)) *BiCMOS Integration of High Performance SiGe:C HBTs*
14.40 – 15.20	H. Wenzel (Berlin) *Simulation of High-Power Semiconductor Lasers with WIAS-TeSCA*
15.20 – 15.40	Coffee Break
15.40 – 16.20	M.F. Pereira (Cork) *Nonequilibrium Green's Functions Theory for Intersubband Optics*

Transparent Boundary Conditions for Quantum-Waveguide Simulations

Anton Arnold (Münster)

The electron transport through a quantum waveguide can be modeled in good approximation by a two-dimensional SCHRÖDINGER equation on an unbounded domain. For numerical simulations, however, it is necessary to restrict this problem to a finite domain. This is possible without changing the solution by introducing *transparent boundary conditions* (TBC), which are non-local in time (convolution type).

The numerical discretizations of these artificial boundary conditions is a main challenge, as it may easily render the initial-boundary value problem unstable. Based on a CRANK–NICHOLSON finite difference discretization of the SCHRÖDINGER equation, we shall discuss a dicrete TBC, which makes the overall scheme unconditionally stable. Further, we derive approximations of the involved discrete convolutions by exponential sums, and analyze the stability of theresulting numerical scheme.

The derived boundary conditions are illustrated by simulations of a wavequide with a resonating stab.

Kinetic and Diffusive Models for Partially Quantized Systems

Naoufel Ben Abdallah (Toulouse)

Classical motion of charged particles (say electrons) can be described by kinetic equations (Vlasov, Boltzmann) coupled to the Poisson equation for the electrostatic forces. For ultrasmall electron systems, like nanostructures, quantum effects are important and are well described by the Schrödinger–Poisson model. In partially confined electron systems like two-dimensional electron gases (2DEG), nanotubes or nanowires, both quantum and classical effects are present. Indeed, the width of a two-dimensional electron gas lying at a heterojunction is a few nanometers. As this length is comparable to the electron de Broglie length, the description of transport phenomena necessitates the use of the Schrödinger equation. In the direction parallel to the heterojunction, the length scale is usually several times higher, and a classical description for electron transport is suitable. This leads to a coupling between classical and quantum models in momentum space (which are obtained in the Born–Oppenheimer approximation).

The aim of this presentation is the study of a kinetic subband model coupled to the Poisson equation as well as a diffusion model in the same framework. In the sequel, the confined direction is denoted by $z \in (0,1)$ while the non-confined direction is called $x \in \omega \subset \mathbb{R}^d$. The problem consists in finding, for $t \in (0,T)$, $x \in \omega$, $z \in (0,1)$ and $v \in \mathbb{R}^d$, the unknowns $V(t,x,z)$, $(\epsilon_p(t,x), \chi_p(t,x,z), f_p(t,x,v))_{p\in\mathbb{N}^*}$ solving

$$\partial_t f_p + v \cdot \nabla_x f_p - \nabla_x \epsilon_p \cdot \nabla_v f_p = 0\,, \tag{1}$$

$$-\frac{1}{2}\partial_{zz}\chi_p + (V + V_{\text{ext}})\chi_p = \epsilon_p \chi_p\,, \tag{2a}$$

$$\chi_p(t,x,\cdot) \in H^1_0(0,1)\,, \quad \int_0^1 \chi_p \chi_q \, dz = \delta_{pq}\,, \tag{2b}$$

$$-\Delta V = \sum_{p\geq 1} |\chi_p|^2 \int_{\mathbb{R}^d} f_p \, dv\,. \tag{3}$$

Existence and uniqueness results are shown in the bounded domain and whole space case. Energy estimates as well as relative entropy inequalities are shown for the above model as well as for the diffusive subband model. The results have been obtained jointly with Florian Méhats, Géraldine Quinio and Nicolas Vauchelet (MIP Laboratoire CNRS, Toulouse).

Mean Field Models for Self-Gravitating Particles

Piotr Biler (Wrocław)

We consider in this lecture parabolic-elliptic systems of the form

$$n_t = \nabla \cdot (D_*(\nabla p + n\nabla\varphi)) \,, \tag{1}$$

$$\Delta\varphi = n \,, \tag{2}$$

which appear in statistical mechanics as hydrodynamical *mean field* models for self-interacting particles, cf. e.g. [4] and other papers by P.-H. Chavanis.

Here $n = n(x,t) \geq 0$ is the density function defined for $(x,t) \in \Omega\times\mathbb{R}^+$, $\Omega \subset \mathbb{R}^d$, $\varphi = \varphi(x,t)$ is the Newtonian potential generated by the particles of density n, and the pressure $p \geq 0$ is determined by the density-pressure relation with a sufficiently regular function $p = p(n,\vartheta)$. The parameter $\vartheta > 0$ plays the role of the temperature, and $D_* > 0$ is a diffusion coefficient which may depend on n, ϑ, x, ...

Such systems can be studied either in the *canonical ensemble* (i.e. the *isothermal* setting), when ϑ = const is fixed, or in the *microcanonical ensemble* with a variable temperature: $\vartheta = \vartheta(t)$, and the energy

$$E = \frac{d}{2}\int_\Omega p\,dx + \frac{1}{2}\int_\Omega n\varphi\,dx = \text{const} \,, \tag{3}$$

which, for a given n, defines $\vartheta = \vartheta(t)$ in an implicit way.

In this work we consider examples of density-pressure relations

$$p(n,\vartheta) = \vartheta^{d/2+1} P\left(\frac{n}{\vartheta^{d/2}}\right)$$

more general than Maxwell–Boltzmann, Fermi–Dirac and polytropic.

Interesting questions are:

- existence of entropy functionals and entropy production rates,
- existence of steady states with prescribed mass and temperature, or prescribed mass and energy,
- nonexistence of global in time solutions and their blow up,
- continuation of local in time solutions with polytropic density-pressure relations.

These results have been obtained in collaboration with Tadeusz Nadzieja (Zielona Góra), Philippe Laurençot (Toulouse), and Robert Stańczy (Łódź and Wrocław).

References

[1] P. Biler, Ph. Laurençot, T. Nadzieja, On an evolution system describing self-gravitating Fermi–Dirac particles, *Adv. Diff. Eq.*, 1–31, to appear.

[2] P. Biler, T. Nadzieja, R. Stańczy, Nonisothermal systems of self-interacting Fermi–Dirac particles, *Proceedings of the Conference "Nonlocal Elliptic and Parabolic Problems" 2003*, Banach Center Publications, 1–20, to appear.

[3] P. Biler, R. Stańczy, Parabolic-elliptic systems with general density-pressure relations, in preparation.

[4] P.-H. Chavanis, J. Sommeria, R. Robert, Statistical mechanics of two-dimensional vortices and collisionless stellar systems, *Astrophys. J. 471*, 385–399 (1996).

Plasma Instabilities in the Ionosphere

Pierre Degond (Toulouse)

The ionospheric plasma is subject to strong instabilities (the gradient-drift instabilities) which produce fairly complex dynamical patterns, the so-called ionospheric irregularities or striations. In a first part, we will introduce the audience to to the modeling of ionospheric plasmas and their instabilities.

Then, we will concentrate on the mathematical study of this instability in the framework of the so-called dynamo model. We will prove that situations which lead to a linear instability are indeed nonlinear unstable (joint work with C. Besse, H. J. Hwang and R. Poncet).

The growth of the instability leads to a very chaotic dynamics, for which we will propose a model inspired from the statistical approach to turbulence in fluid mechanics. Numerical simulation of the original and of the 'turbulent' dynamo model will be presented to illustrate our considerations (joint work with C. Besse, J. Claudel, F. Deluzet, G. Gallice and C. Tessieras).

Harmonic Maps as Tools for Grid Improvement

Gerhard Dziuk (Freiburg)

Parametric methods for the numerical solution of free boundary problems have the advantage that the dimension of the finite element algorithm coincides with the dimension of the free boundary. But these methods are such that the moving grid degenerates easily. Grid improvement can be achieved by conformal parametrization. This leads to the computation of harmonic maps from the surface into the sphere. We discuss discretization, convergence and application. This is joint work with U. Clarenz (Duisburg).

L^p-Estimates for the Convective Terms of Compressible Fluids

Jens Frehse (Bonn)

A new method obtaining refined L^p-estimate is presented. The technique relies on estimates with singular weights and interpolation between Sobolev–Morrey spaces.

Dissipative Discretization Schemes for Drift-Diffusion and Phase Separation Models with Applications

Klaus Gärtner (Berlin)

For the classical van Roosbroeck equations and a binary phase separation model with global interaction and a finite number of sites finite volume discretizations on Delaunay simplex grids in two and three space dimensions are investigated.

The goal is to give a weak discrete formulation and to reproduce the essential stability properties of the analytic problems for any spatial step size h and time step τ, hence not introduce smallness assumptions on the solution variation on neighboring vertices. The main results are:

The Euler backward scheme in time and the Scharfetter–Gummel discretization of the van Roosbroeck system yields a dissipative discrete problem. Moreover for reduced equations a discrete maximum principle for the quasi Fermi potentials holds.

For the phase separation problem a Crank–Nicholson scheme in time is dissipative. Using this result and the requirement of dissipativity determine the space discretization. For that scheme a priori bounds can be proved using a weak discrete maximum principle.

The discrete equilibrium solutions for both problems are characterized by constant Fermi potentials, too. This fact can be used to simplify a numerical bifurcation analysis for the phase separation model.

Finally some numerical examples of a three dimensional semiconductor sensor are discussed, too. Here the weak form of the discretization can be used for instance to reduce the error in the functional central for that application: the contact currents. This is a joint work with Herbert Gajewski (WIAS).

Numerical and Analytical Investigation of the Fermi Surfaces for the Periodic Schrödinger Equation with a Magnetic Field

Vladimir Geyler (Berlin)

The shape of the Fermi surface determines the kinetic and equilibrium properties of the electron gas in the crystal matter as well as the dynamics of a single electron in the crystal. However, a uniform magnetic field changes drastically the translation properties of an electron in the crystal lattice: the appearance of a new length scale (the magnetic length) leads to the famous phenomena related to the *commensurability-incommensurability* transitions. In particular, a fractal structure arises in the spectral diagrams describing the dependence of the two-dimensional electron spectrum on the magnetic flux (Azbel'–Hofstadter butterfly [1]). The translation symmetry of the Bloch electron in a uniform magnetic field is determined by the magnetic translation group [2], which has more complicated structure in comparison with the translation group without the field. Therefore, a modification of the definition of the Fermi surface at high magnetic fields is required [3]. In the present work, we propose a method of building and investigation of the Fermi surfaces in the magnetic Brillouin zone for the three-dimensional Landau operator perturbed by a periodic point potential [4]. Using our previous results concerning the spectrum of this operator [5], we investigate the Fermi surfaces for various types of crystalline lattices and study the dependence of the surface shape on orientation and strength of the magnetic field. Note that the case of simple-cubic lattice was considered earlier in [6].

These results have been obtained in collaboration with Jochen Brüning and Valery Demidov (HU Berlin). The work was supported by Grants of INTAS 00-257, DFG 436 RUS 113/572/0-2, and RFBR 02-01-00804.

References

[1a] M. Za. Azbel', *Sov. Phys. ZhETP. 19*, 634 (1964).

[1b] D. R. Hofstadter, *Phys. Rev. B 14*, 2239 (1976).

[2] J. Zak, *Phys. Rev. A 134*, 1602 (1964).

[3] V. Ya. Demikhovskii, A. A. Perov, D. V. Khomitsky, *Phys. Lett. A 267*, 408 (2000).

[4a] Y. Avishai, M. Ya. Azbel', S. A. Gredeskul, *Phys. Rev. B 48*, 17280 (1993).

[4b] V. A. Geyler, V. V. Demidov, *Theor. Math. Phys. 103*, 561 (1995).

[5] J. Brüning, V. V. Demidov, V. A. Geyler, *Phys. Rev. B 69*, 033202 (2004)

[6] J. Brüning, V. V. Demidov, V. A. Geyler, `cond-mat/0310501`, to be published in *Int. J. Nanoscience.*

BiCMOS Integration of High Performance SiGe:C HBTs

Bernd Heinemann (Frankfurt (Oder))

Over the last years, SiGe heterojunction bipolar transistors (HBT) have been accepted as a value devices for very-high-data-rate wired and wireless communication systems (e.g. WLAN in the 60 GHz ISM band, automotive radar at 77 GHz). As these systems continue to mature, they create an increasing need for higher integration levels to improve the functionallity, to reduce cost and power dissipation. The development of a SiGe:C HBT technology at IHP contributed to a new perspective for SiGe BiCMOS technologies to fulfills this need by providing high integration capability and high performance levels.

Here, we report about the integration of high performance SiGe:C HBT modules into an industry-standard CMOS process. The talk is focused on aspects related to the devices design as well as to the technological mplementation of SiGe HBTs. In particular, we demonstrate how imulation and modeling capabilities were used to support the HBT development. Requirements for future simulation tools are discussed in the context of HBT design. This is a joint work with Holger Rücker (IHP Frankfurt (Oder)).

Analysis and Simulation of Quantum Diffusion Models for Semiconductor Devices

Ansgar Jüngel (Mainz)

Usually, quantum systems are described by microscopic quantum models, like SCHRÖDINGER's or WIGNER's equation. However, the numerical solution of these models is computationally very expensive. Alternative models are given by the computational less expensive quantum diffusion models, like (viscous) quantum hydrodynamic and quantum drift-diffusion models.

In this talk we sketch the derivation of these models and give some results on the mathematical analysis of the equations. In particular, the fourth-order parabolic part of the quantum drift-diffusion model is analyzed in detail (existence, uniqueness, long-time behavior of the solutions). Finally, some numerical results for a one-dimensional resonant tunneling diode, simulated by different models, are given.

Global and Exploding Solutions in a Model of Self-Gravitating Systems

Tadeusz Nadzieja (Zielona Góra)

We study properties of solutions of the system

$$\begin{aligned} u_t &= \nabla \cdot (\vartheta \nabla u + u \nabla \varphi)\,, \\ \Delta \varphi &= u\,, \\ E &= M\vartheta + \frac{1}{2}\int_\Omega u\varphi\, dx\,. \end{aligned}$$

This system was proposed by Chavanis, Sommeria and Robert for description of evolution of density of a system of gravitating particles. In physical interpretation $u(x,t)$, $\varphi(x,t)$ are the density and the gravitational potential, respectively. The temperature $\vartheta(t)$ is uniform in the domain Ω, where the problem is considered. M is the total mass and E is the energy of the particles. We are interested in the existence of global solutions, blow-up phenomena and stationary solutions of our system.

The results have been obtained jointly with Piotr Biler (Uniwersytet Wrocławski) and Ignacio Guerra (Universidad de Chile).

References

[1] P. Biler, T. Nadzieja, Global and exploding solutions in a model of self-gravitating systems, *Rep. Math. Phys. 52*, 205–225 (2003).

[2] P.-H. Chavanis, J. Sommeria, R. Robert, Statistical mechanics of two-dimensional vortices and collisionless stellar systems, *Astrophys. J. 471*, 385–399 (1996).

[3] I. Guerra, T. Nadzieja, Convergence to stationary solutions in a model of self-gravitating systems, *Coll. Math. 98*, 39-47 (2003).

Nonequilibrium Green's Functions Theory for Intersubband Optics

Mauro F. Pereira (Cork)

Intersubband transition based devices like the quantum cascade laser (qcl) are now important in the infrared spectral region, with interesting perspectives for applications in the THz regime. Recent detailed comparisons between theory and experiments have clearly demonstrated that many body effects are required to explain the intersubband optical absorption of quantum wells. However, the gain spectra of more complicated qcl structures have been explained relatively well without those effects. Our nonequilibrium KELDYSH–GREEN's functions microscopic approach explains the apparent contradiction. We apply our theory to two limiting cases: qcl's, characterized by WANNIER–STARK states and parabolic in-plane dispersion relations and coupled band quantum wells with strongly nonparabolic bandstructure and k-dependent transition dipole moments.

In the qcl structure, we demonstrate that the many-body effects depend essentially in the occupations of the subbands and on the detailed COULOMB matrix elements that describe the overlap of electronic wavefunctions. The combination of large population differences and occupation factors with large COULOMB matrix elements lead to strong COULOMB corrections on the THz region (absorption). However, in the mid-infra-red (gain) region, the COULOMB overlap integrals are small or the dominating gain transition. That explains the apparent contradiction, which requires the actual nonequilibrium distribution and realistic wavefunctions and COULOMB matrix elements, in contrast to simplifying approximations that are relatively successful for quantum wells, which fail in the more complex qcl superlattice scenario. Only transitions with TM polarization are possible.

In the multiple quantum well case, with conduction and valence subband contributions, the evolution of TM and TE modes is remarkably different and extra peaks can appear in the TE spectra due to the COULOMB interaction. Furthermore weak, but possibly resolvable conduction band contributions can be found in the TE spectra and their strength is increased by a combination of bandcoupling and COULOMB corrections, also demonstrated here for the first time. Moreover, the spectral positions and broadening, number of peaks and their relative oscillator strengths of the spectra calculated with and without COULOMB effects are radically different, further highlighting the relevance of our calculations

In summary, our fully quantum mechanical microscopic modeling of transport and optics of quantum cascade lasers demonstrates how to control the overall strength of COULOMB corrections by modifying the wavefunction overlap and thus the COULOMB matrix elements by means of an external bias. Our equilibrium calculations for nonparabolic subband quantum wells demonstrate strong interplays between bandstrcuture and many-body effects that can be relevant for the predictive simulations of possible new devices based on both conduction and valence subband transitions. These result have been obtained in collaboration with ANDREAS WACKER (Lund) and HANS WENZEL (FBH Berlin).

Entropy Estimates for a Fully Discretized Fokker–Planck Equation

Robert Plato (Berlin)

An initial value problem for a Fokker–Planck equation is discretized in time by an implicit Euler scheme and in space by a Galerkin scheme. It is shown that this scheme conserves mass, positivity and decay of the entropy. The approximation properties are investigated and numerical experiments are provided.

Application of R-Matrix Formalism in Modeling of Semiconductor Nanostructures

Paul N. Racec (Cottbus)

We show how the R-matrix formalism can be used for characterizing the transport properties of open quantum nanostructures. It gives a practical method for calculating the resonances of the open systems using the poles of the S-matrix. Applications at self-consistent calculations, capacitance characteristics and leakage current in MIS-type nanostructures are shown. New idea for calculation of the leakage current based on the decaying probabilities of the resonances will be discussed. These result have been obtained jointly with E.R. Racec and U. Wulf.

Newton Iteration Procedure and Nonlinear Elliptic Boundary Value Problems with Non-Smooth Data

Lutz Recke (Berlin)

The lecture concerns boundary value problems for quasilinear second order elliptic equations and systems with non-smooth data. Here *non-smooth data* means that the domain can be non-smooth, that the boundary conditions can change type (mixed boundary conditions, where the DIRICHLET and the NEUMANN boundary parts can touch) and that the coefficients of the equations and the boundary conditions can be discontinuous with respect to the space variable x (but they have to be smooth with respect to the unknown function u and its gradient ∇u). The equations are of divergence type (this is joint work with K. GRÖGER) as well as of non-divergence type (joint work with D. PALAGACHEV and L. SOFTOVA).

The aim is to state conditions which imply results of the following type: Let u_0 be a weak solution such that the formally linearized (in $u = u_0$) boundary value problem has no nontrivial solution. Let u_1 be sufficiently close to u_0 in $L^\infty(\Omega) \cap W^{1,2}(\Omega)$ (in the case of divergence type equations) or in $W^{1,\infty}(\Omega)$ (in the case of non-divergence type equations), respectively, and let u_2, u_3, ... be the NEWTON iterations determined by means of the formally linearized (in $u = u_1$, u_2, ...) boundary value problem. Then $u_l \to u_0$ in $L^\infty(\Omega) \cap W^{1,2}(\Omega)$ (in the case of divergence type equations) or in $W^{1,\infty}(\Omega)$ (in the case of non-divergence type equations), respectively.

Transport in Semiconductors at Saturated Velocities

Christian Schmeiser (Wien)

A model for the transport of electrons in a semiconductor is considered, where the electrons travel with saturation speed in the direction of the driving force computed self consistently from the POISSON equation. Since the velocity is discontinuous at zeroes of the driving force, an interpretation of the model in the distributional sense is not necessarily possible. For a spatially one-dimensional model existence of distributional solutions is shown by passing to the limit in a regularized problem corresponding to a scaled drift-diffusion model with a velocity saturation assumption on the mobility. Several explicit solutions of the limiting problem will be presented and illustrated by the results of numerical computations. A model for the transport of electrons in a semiconductor is considered, where the electrons travel with saturation speed in the direction of the driving force computed self consistently from the POISSON equation. Since the velocity is discontinuous at zeroes of the driving force, an interpretation of the model in the distributional sense is not necessarily possible. For a spatially one-dimensional model existence of distributional solutions is shown by passing to the limit in a regularized problem corresponding to a scaled drift-diffusion model with a velocity saturation assumption on the mobility. Several explicit solutions of the limiting problem will be presented and illustrated by the results of numerical computations. This is a joint work with JAN HASKOVEC (Charles University Prague).

Nonlinear and Chaotic Spatio-Temporal Dynamics in Semiconductor Nanostructures

Eckehard Schöll (Berlin)

Nonlinear transport in semiconductor nanostructure devices can be modelled on the basis of the spatio-temporal dynamics of charge carriers in combination with the electric field and circuit equations. Negative differential conductivity, current instabilities and self-organized pattern formation may arise in the regime of strong nonlinearities far from thermodynamic equilibrium. In this talk we present simulations of complex and chaotic scenarios of the current density and field distributions in nanostructure devices. In particular, we study two models of semiconductor nanostructures which are of current interest [1]:

(i) Charge accumulation in the quantum-well of a double-barrier resonant-tunneling diode (DBRT) may result in lateral spatio-temporal patterns of the current density. Various oscillatory instabilities in form of periodic or chaotic breathing and spiking current filaments may occur. We demonstrate that unstable current density patterns can be stabilized in a wide parameter range by means of a delayed feedback loop.

(ii) Electron transport in semiconductor superlattices (SL) exhibits complex scenarios including chaotic motion of charge accumulation and depletion fronts under time-independet bias conditions. We show that self-stabilization of current oscillations corresponding to travelling field domain modes is possible by a novel low-pass filtered time delayed feedback control.

References

[1] E. Schöll, *Nonlinear spatio-temporal dynamics and chaos in semiconductors*, Cambridge: Cambridge University Press, 2001.

Advanced Microelectronic Front End Processes, Transistors, and Back End Processes Challenging the Modeling and Simulation of the Semiconductor Processes and Devices

Rolf Stephan (Dresden)

The presentation will give a general overview about advanced microprocessor technologies. The international technology roadmap of semiconductors is used to guide the process and device simulation community through the requirements for FEOL processes, transistor formation, and BEOL processes.

Sub-50 nm SOI technologies are mature at AMD and run in high-volume production. Advanced modules of these technologies are shown to illustrate and to define challenges for the modeling and simulation of semiconductor processes and devices. Appropriate examples are the shallow trench isolation, the manufacturing of ultra-thin gate dielectrics, the gate pattering, and the Cu interconnect using CVD-deposited low-k dielectric.

Forecasting further extendibility and process developments, future requirements for the process and device simulation will be outlined. This is a joint work with G. Burbach, T. Feudel, D. Greenlaw, M. Horstmann, P. Hübler, T. Kammler, S. Krügel, M. Lenski, K. Romero, K. Wieczorek and M. Raab.

Mesh Generation for Three Dimensional Process Simulation

Norbert Strecker (Mountain View)

The three-dimensional simulation of fabrication processes for the semiconductor industry requires a very robust mesh generation algorithm together with a reliable update of the geometry.

While the process description of a single process step remains simple: dry or wet etch with a mask, isotropic, planarizing or selective deposition, oxidation or silicide growth, the complexity of the resulting structure becomes very high, usually already after a few steps. The situation becomes more complicated due to the presence of non-planar thin layers, e.g. in non-volatile memory cells.

In our 1D, 2D and 3D simulator we use an implicit geometry representation given by region-wise level set functions. Each level set function is constructed when defining a new region. If the initial region geometry is defined by one or several geometry objects, then the signed distance function from these objects is used as level set function.

The union and subtraction of objects is done using a combination of several level set functions.

If a new region is defined using a deposit command, the level set function is calculated based on the exposed regions of the existing mesh according to a formula that depends on the process step. If the region geometry is changed, e.g. by etching, a similar analysis of exposed regions and similar mathematical expressions are applied to define the level set functions for the modified regions.

For the simulation of oxidation and silicide growth the solution of level set equations is required to account for the motion of the interfaces. Diffusion-reaction equations are solved for the transport and surface reactions of the oxidant. A viscoelastic stress problem is solved to account for the mechanical deformation of the structure resulting from both initial or old stresses and from the surface reactions. Given the local mechanical displacements and the local material consumption rates, the velocity of the surface of each region is determined and extended into the entire volume. This extension velocity is used to solve the level set equation

$$\frac{\partial \varphi}{\partial t} + v \cdot \nabla \varphi = 0\,.$$

The level set functions for all regions are utilized to construct a boundary fitted mesh: at the end of the entire process step for an etching or deposition process and at the end of each time step for an oxidation or silicide growth process.

Our meshing algorithm combines the tasks of robust mesh generation with the filtering and correction of small scale noise and topology errors that may be present in the input description or the solution of the level set equations. This makes the algorithm well suited for 3D process simulation.

The mesh construction always starts by generating an initial grid. We allow the user to specify grid lines, by default we construct the grid lines by using all coordinates, provided by the user: all corners of geometry objects, mask corners and contact end points.

During the mesh refinement, a binary tree of mesh elements is constructed. If an element satisfies one of the refinement criteria it is split in an edge midpoint along one of the coordinate axes. The values of the level set functions in the corners of an element defines the regions to

which the corner is assigned. If several level set functions provide the same maximum value in a corner, the corner is assigned to several regions. The assignment of corners to regions is used to control refinement at interfaces, to restrict refinements to certain regions and to pick appropriate field values during the data interpolation. Extrapolation of level set functions along edges is used to account for thin regions, since otherwise they might be lost after the meshing is finished.

Once all refinement is done, the boundary fitted mesh is constructed from the leaf elements of the tree using several stages.

In a first stage refinement is propagated to separate dangling points from unterminated refinements and interfaces: subdivided edges must not be cut by an interface.

In the second stage the edges are cut by interfaces. The sets of regions, identified for the end points of an edge are checked. If the two sets are disjoint, an edge cut is computed, based on the maximum intersection of two level set functions inside the edge. If the intersection point is too close to one of the end points, the level set function values and the regions stored for the end point are adjusted. Otherwise a new mesh point is inserted at the cut. After this step every edge can be assigned to at least one region.

In the third stage faces of the elements are triangulated using a generic triangulation that accounts for all points on the perimeter and inside of the face. The region information, stored for the corners is used to detect if the face is intersected by a triple line (intersection of three regions). The location of the triple line intersection is calculated as the position of the intersection of the three level set functions and is inserted to the face. Additionally the user may assist the mesher by supplying the exact location of ridges and triple lines (very important lines, VIL).

If a point is inserted to a face, it is connected to all points on the perimeter of the face. After this step all faces of the mesh elements can be assigned to at least one region.

The fourth stage consists of testing the volume tessellation of the elements. Based on the regions of the corners, the elements are tested for the presence of intersections of triple lines. If an intersection of triple lines is detected, it will be inserted in the interior of the element. Additionally the user may assist the mesher by supplying the exact location of the triple line intersection or corner (very important point, VIP).

After constructing all elements, a region is assigned to each of the sub-elements. The assignment utilizes available unambiguous region information for corners, edges, faces or the element. If no unambiguous information is available (e.g. on a Null patch), the element is assigned to the region with the maximum level set function in the centroid of the elements.

Once the construction of a boundary fitted mesh is finished, the mesh element quality is enhanced by a Delaunizer. The mesh points on interfaces and the corners of the bricks are transferred to the Delaunizer, the faces of the brick elements are flagged as protected and the faces between elements of different regions are flagged as interface.

The DELAUNAY algorithm establishes first a basic DELAUNAY mesh for the points defined by the mesh. Then it builds a conforming DELAUNAY triangulation by inserting mesh points into the protected faces and interfaces. Special tests are applied that guarantee that the control volumes are properly bounded by the interface faces.

Macromodeling of Microdevices: Virtual Prototyping by Predictive Simulation

Gerhard Wachutka (München)

The rapid progress in microsystems technology is increasingly supported by MEMS-specific modeling methodologies and dedicated simulation tools. These do not only enable the visualization of fabrication processes and operational principles, but they also assist the designer in making decisions with a view to finding optimized microstructures under technological and economical constraints. Currently strong efforts are being made towards simulation platforms for the predictive simulation of microsystems, i.e. the *virtual fabrication* and *virtual experimentation and characterization* on the computer.

We discuss the most important aspects and practicable methodologies for setting up physically-based consistent microdevice and full system models for the effort-economizing and yet accurate numerical simulation of mechatronical microsensors and actuators and microsystems built up of them. In this framework, we demonstrate the consistent treatment of coupled fields and coupled energy and signal domains required for deriving micromechatronical acromodels from the continuous field level, leading to the concept of *full system mixed-level simulation*, and we also address some important issues to be focussed on for the reliable validation and accurate calibration of the models.

The adequate formal representation of the full system description is provided in terms of a finite network description in combination with an appropriate analog hardware description language such as VHDL-AMS or Verilog-A. This makes it possible to code the models of all the individual system components in a generic and uniform way and to assemble the full system model by linking the constituent parts on the same descriptional level.

A multitude of computational results obtained for elementary and complex microstructures such as highly perforated plates are in excellent agreement with accurate 3D-Navier-Stokes FEM calculations and, thus, corroborate the practicality and quality of this approach to predictive simulation.

Simulation of High-Power Semiconductor Lasers with WIAS-TeSCA

Hans Wenzel (Berlin)

High-power semiconductor lasers are needed for a number of applications, such as for pumping of solid-state lasers and optical fiber amplifiers, nonlinear optical frequency conversion, medical treatments and material processing. The different requirements concerning the emission wavelength, optical power, beam quality and spectral purity necessitates the development of a large variety of lasers tailored to the corresponding application. Because state-of-the-art lasers operate at the frontiers which is physical and technological feasible, simulation is a must in order to reach the required electro-optical parameters and to reduce technological cycles.

The two-dimensional simulator `WIAS-TeSCA` has two capabilities built-in to simulate lasers. The first one varies the optical power as an additional parameter in the drift-diffusion equations for the transverse plane and calculates a look-up table to be stored in a file, which is subsequently used by another program (written at HU Berlin and FBH) to calculate the power-current and other characteristics. The second capability is based on the solution of an additional balance equation for a longitudinal-averaged optical power and yields directly the power-current characteristics.

In my talk, I will address the pros and cons of both methods presenting results on the mode competition in ridge-waveguide lasers as well as the power-current characteristics of broad-area lasers. Comparisons with experimental results will be also given.

Discrete Transparent Boundary Conditions for Time-Dependent Systems of Schrödinger Equations

Andrea Zisowsky (Berlin)

The time evolution of the multi-band electronic states in nano-scale semiconductor heterostructures can be described by a system of time-dependent kp-SCHRÖDINGER equations. Since this coupled system is usually posed on an unbounded domain, we derive *transparent boundary conditions* (TBC) to confine the domain to a finite computational region. In order to maintain stability and to avoid numerical reflections we construct *discrete transparent boundary conditions* (DTBC) using the $\mathcal{Z}$-transformation method on a completely discrete level. Since these exact DTBCs are non-local in time and thus rather costly, we present a sum-of-exponentials ansatz to approximate the DTBCs, that allows a very fast calculation of the boundary terms. These results have been obtained in collaboration with ANTON ARNOLD, MATTHIAS EHRHARDT and THOMAS KOPRUCKI.

List of Participants

Albinus, Günter
Charlottenburger Str. 19
13086 Berlin
Germany

Arnold, Anton
Westfälische Wilhelms-Universität Münster
Institut für Numerische Mathematik
Einsteinstr. 62
48149 Münster
Germany
aarnold@math.uni-muenster.de

Bänsch, Eberhard
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
baensch@wias-berlin.de

Bandelow, Uwe
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
bandelow@wias-berlin.de

Baro, Michael
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
baro@wias-berlin.de

Ben Abdallah, Naoufel
Université Paul Sabatier
Laboratoire MIP
118 route de Narbonne
31062 Toulouse Cedex 4
France
naoufel@mip.ups-tlse.fr

Biler, Piotr
University of Wrocław
Institute of Mathematics
pl. Grunwaldzki 2/4
50384 Wrocław
Poland
biler@math.uni.wroc.pl

Bodestedt, Martin
Technische Universität Berlin
Institut für Mathematik Ma 4-5
Straße des 17. Juni 136
10623 Berlin
Germany
bodestedt@math.tu-berlin.de

Degond, Pierre
Université Paul Sabatier
Laboratoire MIP
118 route de Narbonne
31062 Toulouse Cedex 4
France
degond@mip.ups-tlse.fr

Dziuk, Gerhard
Albert-Ludwigs-Universität Freiburg
Institut für Angewandte Mathematik
Hermann-Herder-Str. 10
79104 Freiburg
Germany
gerd.dziuk@mathematik.uni-freiburg.de

Ehrhardt, Matthias
Technische Universität Berlin
Institut für Mathematik
Straße des 17. Juni 136
10623 Berlin
Germany
ehrhardt@math.tu-berlin.de

Farshbaf Shaker, Mohammed Hassan
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
shaker@wias-berlin.de

Frehse, Jens
Rheinische Friedrich-Wilhelms-Universität Bonn
Institut für Angewandte Mathematik
Beringstr. 6
53115 Bonn
Germany
erdbeere@iam.uni-bonn.de

Gärtner, Klaus
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
gaertner@wias-berlin.de

Gajewski, Herbert
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
gajewski@wias-berlin.de

Geyler, Vladimir
Humboldt Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
geyler@mathematik.hu-berlin.de

Glitzky, Annegret
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
glitzky@wias-berlin.de

Griepentrog, Jens André
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
griepent@wias-berlin.de

Gröger, Konrad
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
groeger@wias-berlin.de

Grund, Friedrich
Dianastr. 22
16552 Schildow
Germany

Heinemann, Bernd
IHP (Innovations for High Performance microelectronics)
Im Technologiepark 25
15236 Frankfurt (Oder)
Germany
heine@ihp-ffo.de

Hömberg, Dietmar
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
hoemberg@wias-berlin.de

Hoffmann, Karl-Heinz
Stiftung Caesar
Ludwig-Erhard-Allee 2
53175 Bonn
Germany
hoffmann@caesar.de

Hofmann, Viktor
Humboldt-Universität zu Berlin
Unter den Linden 6
10099 Berlin
Germany

Hünlich, Rolf
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
huenlich@wias-berlin.de

Jäger, Willi
Ruprecht-Karls-Universität Heidelberg
Institut für Angewandte Mathematik
Im Neuenheimer Feld 294
69120 Heidelberg
Germany
jaeger@iwr.uni-heidelberg.de

Jüngel, Ansgar
Johannes-Gutenberg-Universität Mainz
FB Mathematik und Informatik
Saarstr. 21
55099 Mainz
Germany
juengel@mathematik.uni-mainz.de

Kaiser, Hans-Christoph
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
kaiser@wias-berlin.de

Koprucki, Thomas
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
koprucki@wias-berlin.de

Langmach, Hartmut
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
langmach@wias-berlin.de

Lichtner, Mark
Humboldt-Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
lichtner@mathematik.hu-berlin.de

Lobanov, Igor
Humboldt Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
lobanov@mathematik.hu-berlin.de

Manzini, Chiara
Scuola Normale Superiore Pisa
Piazza dei Cavalleri 7
Pisa
Italy
c.manzini@sns.it

Matthes, Daniel
Johannes-Gutenberg-Universität Mainz
Fachbereich 17 - Mathematik & Informatik
Staudingerweg 9
55128 Mainz
Germany
matthes@mathematik.uni-mainz.de

Milišić, Josipa-Pina
Johannes-Gutenberg-Universität Mainz
FB Mathematik und Informatik
Staudingerweg 9
55099 Mainz
Germany
milisic@mathematik.uni-mainz.de

Nadzieja, Tadeusz
University of Zielona Góra
Institute of Mathematics
ul. prof. Z. Szafrana 4a
65516 Zielona Góra
Poland
T.Nadzieja@im.uz.zgora.pl

Neidhardt, Hagen
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
neidhard@wias-berlin.de

Niethammer, Barbara
Humboldt-Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
niethamm@mathematik.hu-berlin.de

Nürnberg, Reiner
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
nuernberg@wias-berlin.de

Pereira, Mauro F.
University College Cork
National Microelectronic Research Center, Photonics Theory Group
Prospect Row, Lee Maltings
Cork
Ireland
mpereira@nmrc.ucc.ie

Plato, Robert
Technische Universität Berlin
Institut für Mathematik Ma 6-3
Straße des 17. Juni 135
10623 Berlin
Germany
plato@math.tu-berlin.de

Racec, Paul N.
Brandenburgische Technische Universität Cottbus
Lehrstuhl für Theoretische Physik
Postfach 101344
03013 Cottbus
Germany
racec@physik.tu-cottbus.de

Recke, Lutz
Humboldt-Universität zu Berlin
Institut für Mathematik
Unter den Linden 6
10099 Berlin
Germany
recke@mathematik.hu-berlin.de

Rehberg, Joachim
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
rehberg@wias-berlin.de

Richter, Rainer
MPI Halbleiterlabor
Otto-Hahn-Ring 6
81739 München
Germany
rar@hll.mpg.de

Röpke, Wilfried
Strausberger Platz 14
10243 Berlin
Germany

Schmeiser, Christian
Technische Universität Wien
Institut für Angewandte und Numerische Mathematik
Wiedner Hauptstr. 8-10
1040 Wien
Austria
schmeise@deana.math.tuwien.ac.at

Schmidt, Gunther
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
schmidt@wias-berlin.de

Schöll, Eckehard
Technische Universität Berlin
Institut für Theoretische Physik
Hardenbergstr. 36
10623 Berlin
Germany
schoell@physik.tu-berlin.de

Schulte, Maike
Westfälische Wilhelms-Universität Münster
Institut für Numerische Mathematik
Einsteinstr. 62
48149 Münster
Germany
Maike.Schulte@math.uni-muenster.de

Sprekels, Jürgen
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
sprekels@wias-berlin.de

Stephan, Holger
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
stephan@wias-berlin.de

Stephan, Rolf
AMD Saxony Limited Liability Company & Co.KG
Wilschdorfer Landstr. 101
01109 Dresden
Germany
rolf.stephan@amd.com

Strecker, Norbert
Synopsys, Inc.
700 E. Middlefield Road
Mountain View, CA 94043
USA
norbert.strecker@synopsys.com

Tiba, Dan
Weierstraß-Institut
Mohrenstr. 39
10117 Berlin
Germany
tiba@wias-berlin.de

Tischendorf, Caren
Technische Universität Berlin
Institut für Mathematik Ma 4-5
Straße des 17. Juni 136
10623 Berlin
Germany
tischend@math.tu-berlin.de

Wachutka, Gerhard
Technische Universität München
Lehrstuhl für Elektrophysik
Arcisstr. 21
80290 München
Germany
wachutka@tep.ei.tum.de

Wenzel, Hans
Ferdinand-Braun-Institut für Höchstfrequenztechnik Berlin
Gustav-Kirchhoff-Str. 4
12489 Berlin
Germany
wenzel@fbh-berlin.de

Wilke, Hermann
Institut für Kristallzüchtung Berlin
Max-Born-Str. 2
12489 Berlin
Germany
wilke@ikz-berlin.de

Zacharias, Klaus
Clara-Zetkin-Str. 23
16562 Bergfelde
Germany

Zisowsky, Andrea
Technische Universität Berlin
Institut für Mathematik
Straße des 17. Juni 136
10623 Berlin
Germany
zisowsky@math.tu-berlin.de