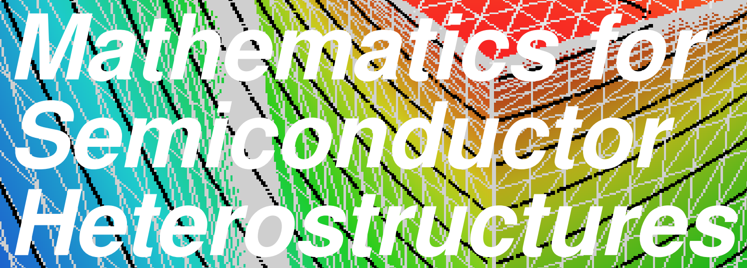

Mathematics for Semiconductor Heterostructures

Modeling, Analysis, and Numerics

Weierstrass Institute for
Applied Analysis and Stochastics
September 24 – 28, 2012

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Cover figure: Computed 3D temperature distribution in an organic semiconductor device containing a thin layer sequence of n-doped / intrinsic / n-doped C_{60} between crossbar metal electrodes *(Organic Electronics, Vol. 13, No. 11, 2012)*.

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International Workshop on

Mathematics for Semiconductor Heterostructures

— Modeling, Analysis, and Numerics —

Organizers

Klaus Gärtner	Weierstrass Institute
Annegret Glitzky	Weierstrass Institute
Hans-Christoph Kaiser	Weierstrass Institute
Francis Nier	Université de Rennes 1

Local Organizers

Olga Kuphal
Marion Lawrenz
Matthias Liero

Support

German Research Foundation (DFG) & Weierstrass Institute, Berlin (WIAS)

Scope

The aim of this workshop is to bring together applied mathematicians and scientists from semiconductor physics and to give them the opportunity to discuss analytical and numerical aspects of relevant semiconductor models including the design of efficient numerical algorithms.

Topics:

- Modeling of micro-, nano-, and optoelectronic devices
- Classical drift-diffusion and energy models
- Semi-classical and quantum transport models
- Asymptotic models
- Organic semiconductors
- Spintronics
- Quantum dots, wires, wells, and waveguides
- Simulation of real-world devices

Monday, 24.09.2012, 08:00 - 17:10

Time	Event
08:00 - 09:00	REGISTRATION
09:00 - 09:30	OPENING
09:30	Virtual Experiments with High Power Semiconductor Devices along and beyond the Rim of the Safe Operating Area **Gerhard Wachutka**
10:20 - 10:50	COFFEE BREAK
10:50	Using gradient structures for modeling semiconductors **Alexander Mielke**
11:30	Asymptotic analysis of a 1D KP system **Francis Nier**
12:10 - 14:00	LUNCH BREAK
14:00	The Oskar3 project **Klaus Gärtner**
14:40	Semi-classical modeling of quantum dot lasers with microscopic treatment of Coulomb scattering **Thomas Koprucki**
15:20 - 15:50	COFFEE BREAK
15:50	Electron transport in strongly confined nanostructures: Modeling and simulation **Paola Pietra**
16:30	Asymptotic models for the transport of an electron gas strongly confined in a slab **Fanny Delebecque**

Tuesday, 25.09.2012, 09:00 - 17:10

Time	Session
09:00	WKB-schemes for Schrödinger-type equations **Anton Arnold**
09:40	On the moment problem for quantum hydrodynamics **Olivier Pinaud**
10:20 - 10:50	COFFEE BREAK and POSTER PRESENTATION **Carolin Kreisbeck** and **Leo Bonato**
10:50	A plane-wave based, generalised formulation of continuum elasticity and multiband kp-models **Oliver Marquardt**
11:30	Optical Recombination in Semiconductor Nanostructures **Eoin O'Reilly**
12:10 - 14:00	LUNCH BREAK
14:00	The Gateable Feature of DEPFET Sensor Arrays **Rainer Richter**
14:40	Physics and modeling of strain effects in SiGe heterojunction bipolar transistors **Holger Rücker**
15:20 - 15:50	COFFEE BREAK
15:50	WIAS-TeSCA simulations in photovoltaics for a point contact concept of heterojunction thin film solar cells **Reiner Nürnberg**
16:30	Application of WIAS-TeSCA to the analysis of the power limits of semiconductor lasers **Hans Wenzel**

Wednesday, 26.09.2012, 09:00 - 21:00

09:00	Artificial interface conditions in quantum transport models **Andrea Mantile**
09:40	Modeling boundary conditions for solving stationary Schrödinger equations **Matthias Ehrhardt**
10:20 - 10:50	COFFEE BREAK and POSTER PRESENTATION **Carolin Kreisbeck** and **Leo Bonato**
10:50	Discretization of Time Dependent Quantum Systems: The Evolution Operators **Joseph Jerome**
11:30	Linear and non-linear eigensolver-based techniques for quantum modeling and simulations: Applications to carbon-based materials **Eric Polizzi**
12:10 - 14:00	LUNCH BREAK
14:00	Modeling Spintronic Effects in Silicon **Siegfried Selberherr**
14:50 - 15:15	COFFEE BREAK
15:45 - 18:00	GUIDED TOUR AT NEUES MUSEUM
18:30 - 21:00	DINNER AT “CUM LAUDE”

Thursday, 27.09.2012, 09:00 - 17:10

09:00	Development and experimental validation of a predictive electrical model of organic light-emitting diodes **Reinder Coehoorn**
09:40	Problems with the Gaussian density of states in organics: Definite solution, ambiguous, and hardly any solution **Gernot Paasch**
10:20 - 10:50	COFFEE BREAK and POSTER PRESENTATION **Carolin Kreisbeck** and **Leo Bonato**
10:50	Drift-Diffusion-Recombination Models for Excitonic Organic Photovoltaic Devices **Klemens Fellner**
11:30	Multiscale Modeling of Heterojunction Organic Photovoltaic Devices **Matteo Porro**
12:10 - 14:00	CONFERENCE PHOTO and LUNCH BREAK
14:00	An electronic model for solar cells taking into account active interfaces **Annegret Glitzky**
14:40	On a model of magnetization switching driven by a spin current: Modeling and numerical simulations **Clément Jourdana**
15:20 - 15:50	COFFEE BREAK
15:50	Bilinear control of Schrödinger equations **Karine Beauchard**
16:30	Some approximate controllability results for bilinear systems **Sylvain Ervedoza**

Friday, 28.09.2012, 09:00 - 16:00

09:00	An application of the Landauer-Büttiker formula to photon emitting and absorbing systems **Hagen Neidhardt**
09:40	A new decomposition for the Schrödinger equation in the semiclassical asymptotics and an associated AP numerical scheme **Florian Méhats**
10:20 - 10:50	COFFEE BREAK
10:50	Plane waveguides with corners in the small angle limit **Nicolas Raymond**
11:30	Quantum transport in semiconductor nano-heterostructures **Paul Racec**
12:10 - 14:00	LUNCH BREAK
14:00	Utilizing Wavelets for the Solution of High-Dimensional Semiconductor Transport Equation **Vincent Peikert**
14:40	Numerical Simulation of Hetero Nanowire Tunnel Field Effect Transistors **Andreas Schenk**
15:20 - 15:30	CLOSING
15:30 - 16:00	COFFEE BREAK

WKB-schemes for Schrödinger-type equations

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We are concerned with the numerical integration of ODEs of the form $\epsilon^2\psi_{xx} + a(x)\psi = 0$ for given $a(x) \geq \alpha > 0$ in the highly oscillatory regime $0 < \epsilon \ll 1$ (appearing as a stationary Schrödinger equation or 1D Helmholtz equation, e.g.). In two steps we derive an accurate finite difference scheme that does not need to resolve each oscillation: 1) With a WKB-ansatz the dominant oscillations are "transformed out", yielding a much smoother ODE. 2) For the resulting oscillatory integrals we devise an asymptotic expansion both in ϵ and h. In contrast to existing strategies, the presented method has (even for a large spatial step size h) the same weak limit (in the classical limit $\epsilon \to 0$) as the continuous solution. Moreover, it has an error bound of the order $O(\epsilon^3 h^2)$. We shall give applications to k·p-Schrödinger systems and to the simulation of semiconductor-nanostructures.

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Bilinear control of Schrödinger equations

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We consider a quantum particle in a potential and an electric field, represented by a Schrödinger equation. It is a control system in which the state is the wave function of the particle and the control is the electric field: one wants to steer the quantum particle from a given initial state, to a desired target state, by applying a suitable control. In the dipolar moment approximation, the control acts bilinearly on the state in the equation. The goal of this talk is to propose an overview of results and technics concerning this problem. We address several questions: exact and approximate controllability, feedback stabilization, influence of the dimension, existence of a positive minimal time required for controllability. First, we recall methods introduced in finite dimension (for ODEs), relying on iterated Lie brackets and discuss their adaptation in infinite dimension (for PDEs). Concerning exact controllability, we propose negative and positive results, depending on the functional frame, the dimension of the space and the assumption on the dipolar moment. Then, we discuss their generalizations. Concerning feedback stabilization, first, we present powerful methods in finite dimension (for ODEs), relying on Lyapunov functions and LaSalle invariance principle; then, we propose adaptations in infinite dimension (for PDEs).

Deep-Level Transient Spectroscopy for QD Localization Energy

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Nowadays, the main limitation of so-called “nonvolatile memory devices” is the long time needed to access data. For example, Flash memory can store data for longer than 10 years, but writing data requires about 1μs. On the other hand, “volatile memory devices” like DRAM have data access times shorter than 15ns, but can only retain information for microseconds [1]. A device able to combine the virtues of volatile and nonvolatile memory would be the “Holy Grail of memory devices”.

The QD-Flash project aims to realize such a device by using quantum dots (QDs) as storage element, embedding them in a MODFET (Modulation-Doping Field Effect Transistor) in order to read and write data. The viability of this concept has been already demonstrated on a prototype showing write times of 80ns, erase times of 350ns and 1.6s storage time at room temperature [2]. The current goal is increasing the storage time, which depends on the localization energy of the QDs [3]. The localization energy depends on the material combination used to manufacture the heterostructure and can be determined by Deep Level Transient Spectroscopy, a technique originally developed for traps in semiconductors [4]. However, a simulation method able to take into account all the complex effects generated in the heterostructures and to provide a reliable estimate of the localization energy is still missing.

The poster presents the results obtained for the localization energy and storage time of GaSb QDs in a GaAs matrix, GaSb QDs in GaAs with one or two AlGaAs barriers and InGaAs QDs in GaP, relating them to the expected values obtained from the theoretical dependence of the storage time on the localization energy. The poster also describes the advantages that could be obtained from mathematical simulations of the devices and the related challenges to be overcome.

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Development and experimental validation of a predictive electrical model of organic light-emitting diodes

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OLEDs are large-area light sources with potentially unique applications, e.g. as very thin light-emitting foils with every desired color. The light-emitting layer is only approximately 100 nm thick, and consists of a large number of organic semiconductor sub-layers, each with a different function. The physics which describes the opto-electronic processes is radically different from that in inorganic LEDs, due to the presence of strong disorder. Three-dimensional Monte-Carlo simulations show that the current density is therefore filamentary. In the first part of the talk, it is shown that such 3D calculations can now be used to obtain the 3D current density and recombination profile, without the need to develop for each layer and each charge carrier one-dimensional expressions for the mobility function [1]. Although such calculations are computer-time-intensive, they provide information about the 3D spatial distribution of the charge-carrier density and the exciton density, and at a 3D-level about the charge-exciton and exciton-exciton quenching processes which determine the efficiency and lifetime at high current densities. Whereas this is still work-in-progress, it is shown how such studies can already now be used to evaluate the sensitivity of the OLED properties to materials parameters and OLED stack design changes. In the second part of the talk, it is discussed how the results of 3D calculations can be accurately "translated" to one-dimensional mobility models. The following situations concerning transport and recombination in white multilayer OLEDs are considered:

- A novel view on the effects of Gaussian disorder on the mobility [2].
- Accuracy and limitations of parameter extraction methods [3].
- Transport of in an electric field at interfaces and in the presence of trap states [4].
- Modelling of time-dependent transport, as in the case of impedance or dark-injection experiments, including a realistic description of the process of charge-carrier relaxation [5].
- Modelling of transport in systems with very thin layers, and with emissive dyes.
- Modelling of charge-carrier recombination in disordered systems [6].
- Experimental validation using emission profile reconstruction [7].

In an outlook, several open issues, where a 3D-to-1D translation has yet to be realized, are discussed.

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Asymptotic models for the transport of an electron gas strongly confined in a slab

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The first model is a 3D Schrödinger Poisson system in the whole 3D space, singularly perturbed by a strong confinement potential acting on one direction. The obtained asymptotic model is a simple 2D Schrödinger equation coupled with a Poisson equation on whole density, concentrated on the transport plane. In a second model, the confinement is ensured by homogenous boundary conditions on both the wave function and Poisson potential. I will present time averaging technics used to get rid of the strong time oscillations due to the confinement.

Modeling boundary conditions for solving stationary Schrödinger equations

Xavier Antoine [1], **Christophe Besse** [2], **Matthias Ehrhardt** [3], **and Pauline Klein** [1]

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In this talk we present some novel absorbing boundary conditions (ABCs) for modeling the solution of linear and nonlinear variable potentials one-dimensional stationary Schrödinger equations. Using pseudodifferential calculus and factorization theorems we construct a hierarchy of novel ABCs and generalize the well-known quantum transmitting boundary condition of Kirk and Lentner to the case of space-dependent potential. Moreover, we propose a rapidly converging iterative method based on finite elements suitable for computing scattering solutions and bound states. The accuracy of our new absorbing boundary conditions is investigated numerically for two different situations. The first problem is related to the computation of linear scattering problems. The second application concerns the computation of energies and ground-states for linear and nonlinear Schrödinger equations. It turns out that these absorbing boundary conditions and their variants lead to a higher accuracy than the usual Dirichlet boundary condition. Finally, our approach also offers the possibility to construct ABCs for higher dimensional problems.

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Some approximate controllability results for bilinear systems

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This talk is complementary to the one of Karine Beauchard. Here, I will present a brief overview on approximate controllability results for bilinear systems. I will mainly focus on three approaches:

- a Lyapunov approach, developed by Nersesyan and Beauchard-Nersesyan;
- an approach based on the control properties of Galerkin approximations of the system, developed by Boscain, Caponigro, Chambrion, Mason, Sigalotti;
- an approach based on the control properties of an easy approximate system deduced by using the scales of the equation, based on the works by S.E., Puel.

Drift-Diffusion-Recombination Models for Excitonic Organic Photovoltaic Devices

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Joint work with Dan Brinkman, Peter Markowich (DAMTP, University of Cambridge) and Marie-Therese Wolfram (University of Vienna).

We present some recent results and ongoing work on drift-diffusion-reaction systems modelling organic photovoltaic devices. While classical semiconductors show recombination typically throughout the whole device feature organic photovoltaic devices significant charge generation only in the very proximity of an interface between two different organic polymers. We discuss basic questions of modelling, existence and stationary states and current voltage characteristics. Moreover, we present some interesting asymptotic approximations and discuss the use of entropy.

The Oskar3 project

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The main goal of the project is to improve algorithms for 3d semiconductor device simulation by exploiting the nice properties of the analytic problem. Main areas of interest from the algorithmic point of view are:

a) discretizations, especially cases requiring non Boltzmann statistics;
b) solving linear systems;
c) construction of anisotropic Delaunay grids (Gajewski: "The best convergence acceleration is a good grid").

The goal is understanding and solving selected application problems of research interest. Collaborative, true experts in the special field of application and extreme requirements with respect to at least one of the points a) to c) are essential ingredients of a good obstacle course training brains. We use

A) silicon sensors for high energy and astro physics (high precision, huge volumes, every design is very different and time scales allow discussions - related to b, c);
B) VCSEL hetero structures (representatives of complex heterostructures with exotic materials, mainly related to a);
C) organic semiconductors (the hope for a black paint producing electricity over five years with 10 % efficiency at nearly no cost—for the presently used models no limit of practical interest results in the Boltzmann case, hence a)

to adjust the focus.

A discussion of the used and unused mathematical properties will be given, some examples will help to judge the status reached at WIAS.

An electronic model for solar cells taking into account active interfaces

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In the talk we discuss an electronic model for solar cells taking into account heterostructures with active interfaces and energy resolved volume and interface trap densities. The model introduced by [1] consists of continuity equations for electrons and holes with thermionic emission transfer conditions at the interface and of ODEs for the trap densities with energy level and spatial position as parameters, where the right hand sides contain generation-recombination as well as ionization reactions. This system is coupled with a Poisson equation for the electrostatic potential.

We study the thermodynamic correctness of the model and motivate a priori estimates for the solutions to the evolution system. Moreover, existence and uniqueness results of weak solutions of the problem are presented. For the existence proof regularized problems have to be solved and bounds of the corresponding solution not depending on the regularization level have to be verified, for details see [2].

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Discretization of Time Dependent Quantum Systems: The Evolution Operators

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We discuss time dependent quantum systems. Our emphasis is on the linear problem, but our work may be viewed as a framework for several models, including linear iterations involved in time dependent density functional theory (TDDFT), the Hartree-Fock model, or other quantum models. A key aspect of the analysis of the algorithms is the use of time-ordered evolution operators, which allow for both a well-posed problem and its approximation. We discuss the available theory at the outset, and proceed to apply the theory systematically, via approximations. We discuss rigorous use of the rectangular and Gauss quadrature rules. Our work is consistent with first-principle, real-time propagation of electronic states, aimed at finding the non-linear responses of quantum systems. Given the increasing importance of quantum modeling in applications, we are attempting to identify some of the basic issues to be addressed analytically.

On a model of magnetization switching driven by a spin current: modeling and numerical simulations

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This is a joint work with Naoufel Ben Abdallah, Elise Fouassier and David Sanchez.

We study a model, introduced in [1], of magnetization switching induced by a spin polarized current without applying an external magnetic field. It consists of a coupled system for the local magnetization (that satisfies a Landau-Lifshitz equation with an additional spin torque) and for the spin density (that satisfies a diffusion equation with a term for the procession phenomenon around the magnetization).

We first write the one dimensional model in an adimensionalized form, using a small parameter ϵ. We then explain the various time and space scales involved in the studied phenomena. Taking into account these scales, we construct an appropriate numerical scheme, that allows us to recover numerically various results of physical experiments. Finally, we perform a formal asymptotic study as ϵ tends to 0. We thus obtain an approximate limit model that we compare with the original model via numerical simulations.

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Semi-classical modeling of quantum dot lasers with microscopic treatment of Coulomb scattering

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Drift-diffusion models provide a semi-classical description of the carrier transport in semiconductor devices. Self-consistently coupled to equations for the optical field they are established models for the simulation of semiconductor lasers. We consider quantum dot lasers with optically active regions consisting of quantum dots grown on a wetting layer. We present a drift-diffusion based modeling approach for the simulation of quantum dot lasers which uses a multi-species description of the carriers along the quantum dot active region and includes microscopically determined scattering rates describing the capture of the carriers into the quantum dots by Coulomb scattering. The presented results are joint work with U. Bandelow, K. Gärtner, A. Wilms, and A. Knorr (TU Berlin).

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Asymptotic spectral analysis in quantum waveguides with heterogeneous fibers

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In recent years nanowires have become an active field of research in the physics community. We discuss two settings in which heterogeneous structures affect propagation through a quantum waveguide, highlighting their interaction with curvature and torsion.

First, we analyze the macroscopic behavior of a wire made of composite fibers with microscopic periodic texture. Mathematically, this amounts to determining the asymptotic behavior of the spectrum of an elliptic Dirichlet eigenvalue problem with finely oscillating coefficients in a three-dimensional tube with shrinking cross section. This two-scale problem is treated in a variational framework performing homogenization and 3d-1d dimension reduction by means of Γ-convergence. We show that the effective one-dimensional limit problem is of Sturm-Liouville type and give an explicit formula for the underlying potential.

Second, for a waveguide with inhomogeneous cross section that does not oscillate as before but shrinks along with the wire in the limit process one observes qualitatively different behavior. Stable propagation through such a modulated wire can be guaranteed by imposing symmetry on the inhomogeneities. In the non-symmetric case, localization is in general the dominant effect. We prove, however, that propagation does happen if a specific relation between the shape of the waveguide and its transversal inhomogeneities holds. Thus, propagation can be enforced by simple geometrical operations, i.e. bending and twisting, which provides a theoretical concept for the building of quantum switching devices.

Artificial interface conditions in quantum transport models

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In a recent collaboration with F. Nier and A. Faraj, it has been shown that a simple modification of the Laplacian through artificial interface conditions allows an alternative approach to the adiabatic evolution of quantum resonances. The use of this modified framework, may hopefully provide with effective equations for the non-linear dynamics of Schrödinger-Poisson systems in the regime of quantum wells in a semiclassical island. In this perspective, it is important to control the deformations effects introduced on the spectrum and on the time propagator by such interface conditions. In particular we are interested in uniform-in-time estimates of the perturbed semigroup. The main difficulty is due to the non-selfadjoint character of our class of operators involving a lack of accretivity for the corresponding generator of the quantum dynamics. In this framework, a standard approach would only provide with finite-time estimates for the dynamical system. Our approach consists in constructing interwining operators leading to a dynamical comparison between the modified non-selfadjoint model and the corresponding “physical” Hamiltonian.

A plane-wave based, generalised formulation of continuum elasticity and multiband k·p-models

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Multiband k·p-models have been used successfully for the theoretical modelling of semiconductor nanostructures of different shapes, sizes, and for a wide range of materials. These models offer a computationally efficient approach to the electronic properties of quantum dots, wires, and wells on the basis of a continuum representation of the system under consideration. We will present a general formulation of k·p-models, that allows to study arbitrary nanostructure geometries, sizes, and material compositions employing an n-band Hamiltonian. The details of the Hamiltonian as well as the nanostructure geometry and composition are defined in user-generated input files, which adds great flexibility to taylor the calculation to the question of interest. In this manner, simulations using the well-established eight-band k·p-model as well as more sophisticated 14-band approaches or simple one-band effective mass models are straightforwardly possible. To account for elastic and piezoelectric properties, a continuum elasticity model has also been implemented. The resulting strain and piezoelectric potentials can then be considered in the calculation of the electronic properties. Both the continuum elasticity model as well as the multiband k·p-formalism were implemented in a plane-wave framework within the existing S/PHI/nX physics simulation package. This allows to make use of existing, highly efficient minimisation algorithms and to apply a reciprocal space representation for gradient operations, allowing for a significant boost in efficiency. The specific issues that occur in a plane-wave based implementation of these two continuum models will be furthermore discussed in example simulations that have been performed with our approach.

A new decomposition for the Schrödinger equation in the semiclassical asymptotics and an associated AP numerical scheme

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This is a joint work with Ch. Besse and R. Carles. We propose a new decomposition “à la Grenier” for linear and nonlinear Schrödinger equations, which leads to a locally well-posed problem, independently of the semiclassical parameter. Based on this formulation, we give a numerical scheme which is Asymptotic Preserving in the semiclassical limit (before caustics). The performances of this method will be compared with the ones of the standard splitting method.

Using gradient structures for modeling semiconductors

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Joint work with Annegret Glitzky and Matthias Liero (WIAS Berlin).

We show that classical energy-drift-diffusion systems used for modeling of semiconductor devices can be written as gradient systems in the form

$$\partial_t \mathbf{u} = -\mathcal{K}(\mathbf{u})\mathrm{D}\Phi(\mathbf{u}),$$

where $\mathbf{u}$ is a vector of densities of the different species and possibly the temperature (or the internal energy), cf. [Mie11]. While the potential Φ is the free energy in the isothermal case and the negative entropy in the temperature-dependent case, the Onsager operator $\mathcal{K}(\mathbf{u}) = G(\mathbf{u})^{-1}$ is the inverse of the metric tensor $\mathcal{G}$ and has an additive split into the different dissipation mechanics:

$$\mathcal{K}(\mathbf{u})\boldsymbol{\xi} = \mathcal{K}_{\text{diff}}(\mathbf{u})\boldsymbol{\xi} + \mathcal{K}_{\text{react}}(\mathbf{u})\boldsymbol{\xi} = -\mathrm{div}\big(\mathbb{M}(\mathbf{u})\nabla\boldsymbol{\xi}) + \mathbb{K}(\mathbf{u})\boldsymbol{\xi}.$$

In the case of Fermi-Dirac statistics this modeling lead to new and more consistent modeling of diffusion enhancement and reaction kinetics. In particular, the modeling of semiconductors via gradient system $(\Phi, \mathcal{K})$ yields always thermodynamically consistent models and highlights the different physical aspects of the theory in a clear way.

It is shown in [GlM12, Mie12] that gradient structures can also used effectively to model hybrid models with nontrivial bulk-interface interaction and active interfaces, which are need in photovoltaics. Finally, we discuss how the theory of geodesically λ-convex gradient can be applied in this field, cf. [LiM12].

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An application of the Landauer-Büttiker formula to photon emitting and absorbing systems

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The abstract Landauer-Büttiker formula is applied to a Jaynes-Cummings model coupled to leads. As a result, we obtain formulas for electron and photon currents in terms of the partial cross-sections of a scattering system for which the unperturbed and perturbed Hamiltonians correspond to systems where the leads are either decoupled or coupled to the Jaynes-Cummings model. It is shown that the resolvent difference of the coupled and decoupled Hamiltonians is a trace class operator. The electron and photon currents are analyzed in detail.

The talk is based on a common paper with Horia Cornean, Lukas Wilhelm and Valentin Zagrebnov.

Asymptotic analysis of a 1D KP system

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In this talk we will show how the semiclassical analysis allows to elucidate the complex subband structure of a KP system for bipolar semiconductors.

WIAS-TeSCA simulations in photovoltaics for a point contact concept of heterojunction thin film solar cells

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For a long time 1D simulation software such as SCAPS were the widely used semiconductor simulation tools in photovoltaics because of the relatively simple structure of solar cells. A novel point contact concept is an example for the necessary and useful application of 2D and 3D simulation in this field.

The photovoltaic performance of the wider-band gap chalcopyrite based thin film solar cells is limited by the recombination at the interface between the absorber and the buffer layer. In principle, the heterojunction should exhibit a high density of defect states at this interface due to lattice mismatch. The concept of a point-contact geometry at the front side of thin film chalcopyrite solar cell devices includes (i) an interfacial defect state passivation and (ii) a current transport only through these point contacts that cover a few percent of the device area, while the rest of the surface is electronically passivated by a dielectric coating. The introduction of a point-contact type structure allows for the relaxation of the requirements at the absorber/buffer heterointerface and could dramatically increase performance of heterojunction thin film solar cells.

The software WIAS-TeSCA for the numerical simulation of charge transfer processes in semiconductor structures, in principle, is suitable for use in thin film photovoltaics. It is based on the drift-diffusion model and allows for heterostructures. Modeling of the structured passivation layer with point contacts can be simplified by taking a structural unit with cylindrical symmetry so that the modeling is performed in 2D but provides results which will be a good approximation to the 3D structure. In the present model study, especially, the effect of the interfacial defect level and density, and of the point contact radius and area ratio have been investigated.

Optical Recombination in Semiconductor Nanostructures

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Two of the key current challenges in photonics are the development of entangled photon sources and the development of lasers and efficient light sources across the full visible spectrum. There is considerable interest in the use of semiconductor quantum dots (QDs) to achieve both these aims. Here we discuss the issues involved to investigate the piezoelectric potential and electronic structure of III-N wurtzite and of site-controlled (111)-oriented zinc-blende dots. We investigate the single-particle electronic structure of (111)-oriented InGaAs/GaAs QDs by means of an 8-band $k \cdot p$ model. We then discuss how this model needs to be extended in order to identify how best to engineer the dots to give orthogonally polarized exciton states that are degenerate (zero fine structure splitting), thereby supporting the emission of entangled photons. This requires both to treat dots where there are only a few confined electron but many confined hole states, as well as to incorporate the effects of disorder into the system. We highlight that accurate knowledge of physical parameters remains an issue for such dots [1]. We then turn to consider the influence of the built-in potential in wurtzite structures. We first compare the elastic and the first-order piezoelectric tensor of the (111)-zinc-blende systems with the corresponding quantities in a wurtzite structure and point out similarities and differences [2]. We then turn to consider the analysis of the built-in potential and its consequences for polar and for non-polar III-N QDs [3]. We propose that the growth of InGaN/GaN QD structures can lead to a significant reduction in the built-in potential compared to InGaN/GaN quantum well structures, allowing efficient optical emission to longer wavelengths [4]. We also highlight that the calculated field values and their effects are very sensitive to details of the dot shape and composition in such heterostructures.

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Problems with the Gaussian density of states in organics: definite solution, ambiguous, and hardly any solution

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Disordered organic materials are the basis of organic electronics with organic light emitting diodes for displays and lighting, organic field-effect transistors (OFET) and circuits made with them, and organic solar cells. Almost twenty years since the pioneering work of Bässler [1] on hopping transport in disordered organics it is widely accepted that the density of states (DOS) is a Gaussian. From the application of various numerical models for the mobility, a variance of the order of $100\ \mathrm{meV}$ seems to be typical. Although a large number of device modelling using the Gaussian DOS has been published, support of design and technology of devices by full two-dimensional simulation is required. Until recently this possibility was not completely implemented in the simulation programs as sDEVICE [2] or ATLAS [3] due to peculiarities of the Gaussian DOS. We discuss here three problems important for implementation and application.

Fast and efficient numerical simulation requires analytical expressions for the carrier density (as the Fermi integral for the square-root DOS). Alternatively, the numerical integration of the product of the DOS and the Fermi distribution is in principle possible and for some cases of non-parabolic bands available. For the Gaussian DOS we developed an analytical approximation for the carrier density (Gauss-Fermi integral) [4] which is meanwhile implemented in sDEVICE [2]. Detailed testing and comparison with experimental OFET current characteristics is in progress but is also connected with further problems.

For the Gaussian DOS an enormous amount of theoretical work on the mobility has been done and published. The extended Gaussian disorder model (EGDM) [5, 6] (describing the dependence of the mobility on temperature, carrier concentration, and field) was to our opinion a first highlight after Bässler, followed later by the extended correlated disorder model (ECDM). However there exist many other models, also from recent times, with different dependencies. There remain serious ambiguities: Which model is applicable to a given organic material, which parameters should be used or how one can determine them, are the models sufficient for application at high concentrations and high fields?

Most problematic is the question what the band edge is and how to determine it. As a routine method the valence band edge is determined by ultraviolet photoemission (UPS). However, this method probes regions of the DOS which are unoccupied in devices and transport takes place at much lower energies not accessible up to date by UPS. Moreover, the upper part of the UPS spectrum below the gap is rather broad compared with the narrow hopping transport DOS. Thus we do not really know where this DOS is situated. We supposed [7] that the transport DOS is the narrower tail of the broader UPS distribution. With some uncertainty one can then fix the position of the Gaussian transport DOS on the binding energy scale. But there remains a further problem, namely where is the band edge situated relative to the maximum of the Gaussian DOS. The method presented in [7] is not unique and we will discuss several other possibilities, but until now without a definite choice. It might be that the injection into a Gaussian DOS requires a new theoretical treatment and its implementation beyond the traditional one.

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Utilizing Wavelets for the Solutions of High-dimensional Semiconductor Transport Equations

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Introduction. Transport equations (Boltzmann,Wigner) on 6-dimensional phase spaces describe the behavior of charge carriers in semiconductors and form the basis for Technology Computer Aided Design (TCAD) on device level. However, the numerical solution of these high-dimensional equations involves huge matrices which practically limits contemporary direct solvers to problems with only one real space dimension. Since the integral operator in the Wigner transport equation (WTE) produces full matrices, 2-dimensional simulations are only feasible for the Boltzmann transport equation (BTE) so far. Even for the BTE the simulation of 2D devices calls for coarse meshes and geometrical simplicity which sets limitations to the accuracy and the practical application for the new TCAD challenges introduced by the rapidly increasing importance of 3D devices. By far the most established numerical BTE approach is the Spherical Harmonics Expansion Method (SHE) which is based on a representation of the momentum space in spherical coordinates and an expansion of the angular variables in SH. The SH Y_l^m build a dense basis in L_2^S on the sphere: $V_S^0 \subset V_S^1 \subset \ldots V_S^N \subset L_2^S$, with $V_S^N := \mathrm{span}\{Y_l^m : l = 0, \ldots N; m = -l, \ldots, l\}$. Any V_S^k may be decomposed as $V_S^k = W_S^k \oplus V_S^{k-1}$, with $W_S^k \perp V_S^{k-1}$. A special property of SH is that the detail spaces W_S^k are spanned by SH Y_l^m themselves. The SH coefficients only contain the additional detail information to the orders before and decay quickly with the detail order (typically only 7 orders are necessary to simulate silicon transistors). The SH coefficient size has recently been used as an adaptive criterion for a variable order SHE expansion and the feasibility of 3D SHE simulations have been investigated [1].

Multi-Wavelets. All contemporary numerical BTE approaches apply piecewise polynomials (pp) as basis functions. Usually, they apply piecewise constants (pc) in all dimensions (the SHE applies pc in the energy and real space directions). Recently, the Discontinuous Galerkin (DG) method for the BTE has been proposed [2]. The DG method is flux conserving and is (in contrast to SHE) stable with high-order pp in real space and energy directions (hp-stable) and is therefore a promising alternative. Let V_n^k be the space of all one-dimensional pp of the degree less than k on a uniform mesh (to keep the notation simple) with 2^n equidistant intervals within $[0, 1]$. By bisecting the mesh, pp build a dense basis in L_2 and fulfill the nested structure $V_0^k \subset V_1^k \ldots \subset V_n^k \ldots \subset L_2([0, 1])$. It is possible to decompose V_{n+1}^k into V_n^k and a perpendicular space W_n^k which only contains the additional details of V_{n+1}^k compared to V_n^k: $V_n^k \oplus W_n^k = V_{n+1}^k$, with $V_n^k \perp W_n^k$. Recursively, V_n^k can be decomposed by detail spaces $V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus \ldots \oplus W_{n-1}^k$. W_l^k is spanned by $2^{l-1}k$ detail functions $\psi_{l,i,j}$ which are called Multi-Wavelets (MWs) (see [3]) where l indexes the detail order, j indexes the vanishing moment order and i indexes the position.

Multi-Wavelet Discontinuous Galerkin Method. Instead of using pp$\in V_n^k$ (nodal DG: NDG), the solution of the BTE Φ could be expanded in tensor products of one-dimensional MW bases (Multi-Wavelet Discontinuous Galerkin method: MWDG):

$$\Phi(x, y, z, \mu, \phi, \omega) = \sum_{I,J,K,L} \alpha_{I,J,K,L} \psi_I^{x,y,z} \psi_J^{\mu} \psi_K^{\phi} \psi_L^{\omega}$$

(multi-indexes I are used for $\{l, i, j\}$). x, y, z are the real space coordinates, μ is the cosine of the polar angle, ϕ is the azimuthal angle and ω is the energy. Note that a tensor product is only build within the momentum space and with the real space. Within the real space, unstructured grids are typically necessary and the construction of MWs x, y, z on unstructured grids can be done following the procedure in [4]. A strongly growing community utilizes the detail and vanishing moment properties of wavelets for the adaptive compression for different complex problems. For the solution of PDEs, hierarchical bases build the "driving force" behind modern adaptive solvers and pre-conditioners. However, of particular interest are the properties of wavelet tensor bases. The coefficient decay (as a property of the detail nature of wavelets) is strongly enhanced in multi-dimensional tensor bases so that most wavelets can be canceled. This is referred to as high-dimensional wavelets compression (HWC) here and is called adaptive sparse grids in literature [5]. Preliminary work on adaptive sparse grids concentrated on FEM formulations and on scalar wavelets rather than on the flux conserving formulations that are necessary for the solution of transport equations. Furthermore, in contrast to scalar wavelets, MWs have an additional vanishing moment hierarchy within each detail to represent high order pp and compression leads to some kind of super sparse grid. This is referred to as vanishing moment compression (VMC) here. Preliminary work on DG and MWs (e.g. [6]) use MW coefficients as adaption criterion, but always keep a full grid so that the MWDG and the NDG stay equivalent. MWDG simulations of 1D devices with pc MWs in [7] show that adaptive HWC can compress the basis by about 99%. Furthermore, MWDG simulations of 1D devices with higher-order polynomials in [8] perform significantly better even for uncompressed MWDG (up to 96% saving for only 1.4% error in the current) and HWC and VMC can compress the basis by additional 90%. Future Work. Even larger compression rates are expected for future full hp-adaptive MWDG simulations of 3D devices. A drawback of MWs is the higher coupling of difference operators compared to a conventional pp basis which can reduce the advantages of MWs compression. However, the product structure of the BTE within the momentum space and with the real space enables (in combination with the corresponding product basis above) to decompose the system matrix into a Kronecker product $M = M_{x,y,z} \otimes M_\mu \otimes M_\phi \otimes M_\omega$. Utilizing the distributive property enables to calculate a matrix vector product without building up the matrix M and with a complexity that scales with the number of unknowns only (undirectional principle [9]). Hence, an iterative solver in combination with a multi-level pre-conditioner make the problem independent of the couplings within the subdimensions. If quantum mechanical effects become important, the WTE has to be solved. Since the solution of the BTE and the WTE stay similar, similar high MW compression rates are expected for the WTE. MWs are advantageous for the discretization of integral operators such as the Wigner potential, since the matrices show a quasi-sparse structure. Additionally, the product structure of the Wigner potential enables the undirectional principle so that 3D MWDG WTE solvers could become feasible in the future.

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Electron transport in strongly confined nanostructures: modeling and simulation

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We present an effective mass model, derived in [1], describing the ballistic transport of electrons in ultra-scaled confined nanostructures. Due to the strong confinement, the crystal lattice is considered periodic only in the one dimensional transport direction and an atomistic description of the entire cross–section is given. The model consists of a sequence of 1D device dependent Schrödinger equations, one for each energy band, which retain the effects of the confinement and of the transversal crystal structure. In order to model field effect transistors, self-consistent computations include the resolution, in the whole 3D domain, of a Poisson equation. Simulations of the electron transport in semiconducting single-walled carbon nanotubes are presented, using a classical-quantum hybrid strategy. The ballistic effective mass model is used only in the active region, and it is coupled to a drift-diffusion model (derived for strongly confined nanostructures in [2]) in the source and drain regions. Appropriate current preserving interface conditions (as in [3]) are used.

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On the moment problem for quantum hydrodynamics

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We address the following inverse problem in quantum statistical physics: does the quantum free energy (von Neumann entropy + kinetic energy) admit a unique minimizer among the density operators having a given local density n(x)? We give a positive answer in various configurations and characterize the minimizer in dimension one. The problem is related to a recent theory developed by P. Degond and C. Ringhofer concerning the derivation of quantum hydrodynamics models. This is joint work with F. Mehats.

Linear and non-linear eigensolver-based techniques for quantum modeling and simulations: applications to carbon-based materials

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In a recent article [Phys. Rev. B 79, 115112, (2009)], the FEAST algorithm has been presented as a general purpose eigenvalue solver which combines accuracy, robustness, high-performance and (linear) parallel scalability. Here, FEAST will be presented beyond the “black-box” solver as a fundamental modeling framework for the electronic structure problem spanning the research fields of solid-state physics and quantum chemistry.

First, it will be shown that FEAST can naturally address the original numerical complexity of the electronic structure problem as formulated by Slater in 1937 [Phys. Rev. 51, 846-851, (1937)]. The non-linear eigenvalue problem of type $\mathbf{A}(\lambda)\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$ arising from the muffin-tin decomposition of the real-space domain is first derived and then reformulated to be solved exactly within the FEAST framework. This new framework is presented as a fundamental and practical solution for performing both accurate and scalable electronic structure calculations, bypassing the various issues of using traditional approaches such as linearization and pseudopotential techniques.

Second, we present a modification of the FEAST algorithm that solves the full non-linear eigenvector problem of type $\mathbf{A}(\mathbf{x})\mathbf{x} = \lambda\mathbf{B}\mathbf{x}$ (i.e. Schrödinger/Poisson) as an efficient and robust alternative to traditional self-consistent field method (such as Newton-Broyden, Anderson mixing, direct inversion of the iterative subspace and mixed Pulay techniques). The resulting approach is potentially one order of magnitude faster than conventional iterative methods, and it converges to the correct solution regardless of the choice of initial guess.

Finally, we present and discuss FEAST-based time-domain propagation techniques for time dependent quantum problem. Efficient time-dependent simulations have become increasingly important for characterizing the electron dynamics under time dependent external perturbations such as electromagnetic fields, pulsed lasers, and particle scattering. Using innovative spectral decomposition and discretization of time-ordered evolution operators, we aim to address the traditional limitations in term of trade-off between robustness and performances in such calculations.

In order to illustrate the efficiency of the FEAST framework, numerical examples are provided for various molecules and carbon-based materials using our in-house all-electron finite element implementation for the DFT/Kohn-Sham/LDA problem.

Multiscale Modeling of Heterojunction Organic Photovoltaic Devices

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In this lecture, we present our most recent results in the modeling and simulation of heterojunction organic solar cells [2]. The proposed mathematical model is an extension of that introduced in [1] for planar heterojunction solar cells to treat arbitrary multi-dimensional morphologies. Our approach consists in describing diffusion and transport phenomena of excited states and charge carriers in a heterogeneous domain Ω of $\mathbb{R}^d$, $d = 1, 2, 3$, constituted by two non-overlapping subdomains Ω_i, $i = 1, 2$, using mass balance equations supplied with the Drift-Diffusion model for flux densities. Charge dissociation and recombination phenomena occurring in a thin region around the $(d-1)$-interface are lumped with a scale transition procedure into flux transmission conditions. This approach is twofold beneficial since it allows to account for the local dependence of dissociation on the orientation of the electric field and to reduce the computational effort compared to previous multi-dimensional models [5, 6]. The resulting system of fully coupled nonlinear PDEs/ODEs is faced with Rothe's method using a quasi-Newton technique for linearization, the Edge-Average Finite Element method studied in [7] for spatial discretization and adaptive BDF schemes for time advancement. Simulations are extensively discussed to validate the model against realistic data and results available in the literature. In the final part of the lecture, we show that the proposed model can be used also for investigating the behavior of different classes of devices, *e.g.* the photoactivated light harvesting capacitor proposed in [3] or the sensing substrate used for neuronal photostimulation in [4].

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Quantum transport in semiconductor nano-heterostructures

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In this talk we review some mathematical challenges and our solutions arising from modeling of semiconductor nanodevices. Often, the active part of a nanodevice is a quantum system to which electrical contacts are attached such that there is an open quantum system on hand. The scattering theory is suitable for describing such systems. A practical method for computing the scattering matrix, even for 2D and 3D systems, is the R-matrix formalism. For this, one solves the Wigner-Eisenbud eigenvalue problem, i.e. the single-band effective mass Schrödinger equation on the scattering region with mixed Dirichlet/Neumann boundary conditions. Using the finite volume method one may take into account even a position dependent effective mass inside the heterostructure. The R-matrix formalism also yields the scattering wave functions inside the scattering region. Applications of this formalism to nanowire heterostructures will be provided.

As a consequence of opening the quantum system its discrete spectrum becomes a continuous spectrum with resonances. The practical computation of resonances as poles of the scattering matrix is also possible within R-matrix formalism. Furthermore, it allows for a systematic expansion in case of interacting resonances. We obtain a qualitative description of the peaks and dips in the linear conductance of a single electron transistor by Fano lines, where the complex asymmetry parameter is computed explicitly.

In order to compute the physical observables, one needs to know the density matrix of the system. The Landauer-Büttiker formalism provides an ansatz for the density matrix for open quantum systems. In the last years, a detailed analysis has been done in our group in order to mathematically justify the above ansatz.

Finally we discuss future challenges of a realistic modeling of semiconductor nanodevices, like many-particle description and dissipative interaction.

This is a joint work with Hans-Christoph Kaiser, Hagen Neidhardt and Roxana Racec.

Plane waveguides with corners in the small angle limit

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The plane waveguides with corners considered here are infinite V-shaped strips with constant thickness. They are parametrized by their sole opening angle. We study the eigenpairs of the Dirichlet Laplacian in such domains when their angle tends to 0. We provide multi-scale asymptotics for eigenpairs associated with the lowest eigenvalues. For this, we investigate the eigenpairs of a one-dimensional model which can be viewed as their Born-Oppenheimer approximation. We also investigate the Dirichlet Laplacian on triangles with sharp angles. The eigenvalue asymptotics involve powers of the cube root of the angle, while the eigenvector asymptotics include simultaneously two scales in the triangular part, and one scale in the straight part of the guides.

Particle Detection with DEPFET Arrays in Gated Mode

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Arrays of Depleted Field effect Transistors (DEPFET) are mostly operated in rolling shutter mode. During this CCD like operation scheme one pixel row is read our while the others are collecting signals. For the very compact pixel design used for the Belle II pixel detector we found a very simple procedure to switch off the signal collection for the entire matrix preserving the information already stored in the pixel. In this way we are able to mask out the noise which may occur during and after bunch injection in the accelerator. The talk will cover the device related aspects of this new operation mode. 3D-device-simulations are used to gain an insight into the device and to optimize the pixel design. The feasibility of this very promising approach is demonstrated by laser and tests beam data taken on a Belle II test matrix.

The DEPFET (DEPleted Field Effect Transistor) is a semiconductor detector concept which combines detection and amplification within one device. A p-channel MOSFET is integrated onto a silicon detector substrate, which becomes fully depleted by a sufficiently high negative voltage applied to a p+ contact on the backside. A potential minimum is formed by sideward depletion, which is shifted directly underneath the transistor channel at a depth of about 1 μm by an additional phosphorus implantation underneath the external gate. Incident particles generate electron-hole pairs within the fully depleted bulk. While the holes drift into the back contact, electrons are accumulated in the potential minimum, called the internal Gate. If the transistor is switched on the electrons modulate the channel current. An amplification of more than 500pA per signal electron can be achieved with the technology currently available.

The removal of the signal charge and thermally generated electrons from the internal gate is called Clear. An n+ contact neighboring to the internal Gate is pulsed at a positive voltage providing a reach-through into the internal Gate. There is no any reset noise if the entire charge is completely removed. The probably most important feature of the DEPFET is the very small capacitance of the internal gate resulting in a low noise performance, even at room temperature and high operation speed. DEPFET arrays are usually operated in rolling shutter mode. Since only the addressed row is consuming power the rolling shutter mode is the most power efficient mode to operate a DEPFET array. In an accelerator particle bunches have to be refreshed by additional injections. Since new bunches cannot be injected in the same phase space volume they have to cool by synchrotron radiation which leads to noisy bunches. Due to rolling shutter scheme any junk charge introduced by noisy bunches which hits the detector spoils the entire detector array. According to pessimistic estimations more than 20% of the data could be affected due to this phenomena at Belle II. Noisy bunches may appear every 10μs – the revolution time at Belle - in a well defined time window.

The pixel detector can be protected from noisy bunches if the DEPFET can be 'gated' into an insensitive (blind) mode during that time. Signals already collected in those pixel which were not yet readout have to be preserved during this blind phase. The basic idea of the 'gated mode' operation is to temporary provide an electrode which is much more attractive for electrons then the internal Gate. In the Belle DEPFET design the clear region is very large compared to Gate and the internal Gate beneath (see Fig. 1 and 2). The Figures illustrate the completely different charge collection behavior for Clear_{hi} =18V and $\text{Clear}_{\text{low}}$ = 3V. During the noisy bunch phase the Clear lines of the entire matrix are raised at Clear_{hi} to protect the internal Gates from being hit. Related system aspects like high peak currents and cross talk are still under investigation.

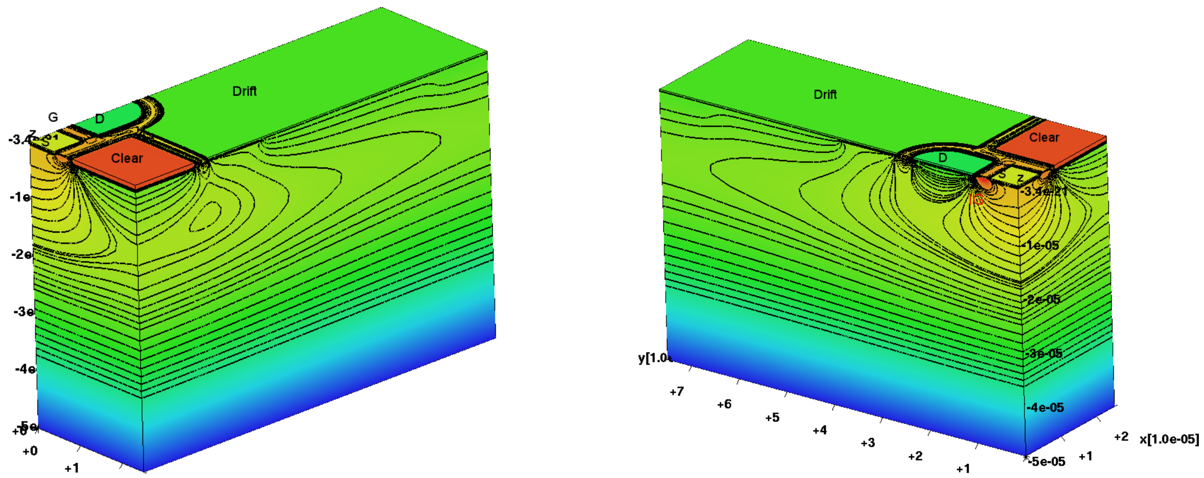

Fig. 1: 3D potential distributions of the 'collection state'. View on Clear and Drift regions (left) and on Drift, Drain (D), Source (S) and Gate (right). Clear is in off state (3V). Generated electrons drift into the internal Gate (IG). The simulation make use of Neumann boundary conditions. Every lateral boundary is a symmetric plane thus one half of a pixel is shown.

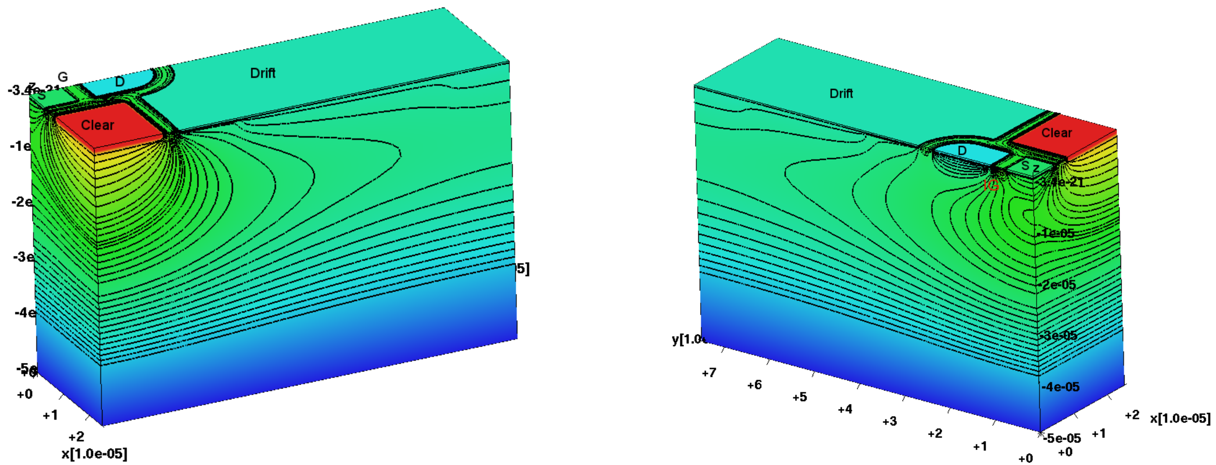

Fig. 2: 3D potential distributions of the 'blind state'. View on Clear and Drift regions (left) and on Drift, Drain (D), Source (S) and Gate (right). Clear is in on state (18V). Generated electrons drift into the Clear. The internal Gate (IG) is separated by potential barriers.

The selectivity to the actual *Clear* process is given by the external Gate. During Clear the external Gate has to be switched to the on state (current is flowing). This provides the most possible negative potential of the internal Gate and the biggest potential difference between the Clear region and the internal Gate. Electrons can be emitted over the potential barrier inbetween. If the external Gate is switched off the hole channel at the surface disappears and the strong capacitive coupling between external and internal Gate leads to a much more positive potential in the latter one. Fig. 3 drafts the resulting potential slopes between internal Gate and Clear. Fig. 4. shows a measurement during blind mode. The removed charge is plotted versus the external Gate voltage. The Clear suppression works very well.

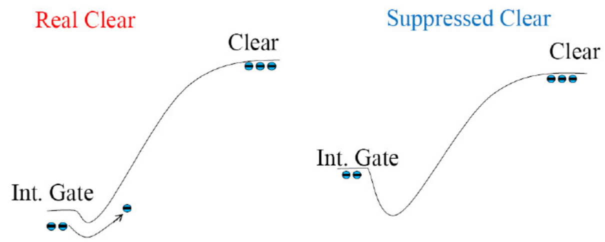

Fig. 3: Principle of the clear selectivity. Maximum potential between internal Gate and Clear during Real Clear and Suppressed Clear (blind mode).

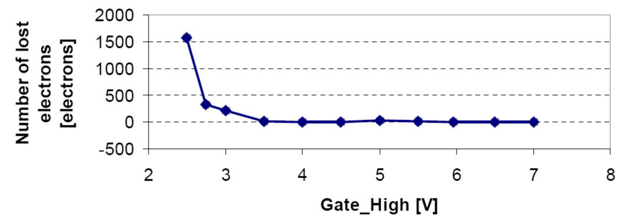

Fig. 4: Number of electrons removed from the internal Gate vs external Gate voltage. 12000 electrons were deposited before (laser illumination).

Physics and Modeling of Strain Effects in SiGe Heterojunction Bipolar Transistors

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Strain engineering is a key technological method for performance enhancement of state-of-the-art CMOS technologies. The effect of strain on the semiconductor band structure is exploited to manipulate carrier transport properties and device characteristics in a beneficial way. Strain plays also an essential role for the electrical behavior of SiGe heterojunction bipolar transistors (HBT). The SiGe base layer experiences a biaxial compression due to its lattice mismatch to the Si substrate. Since this stress is close to the stability limit of the SiGe layer reliability concerns have discouraged the use of further stress enhancement techniques in SiGe HBTs so far. Nevertheless, the device fabrication process imposes significant stresses in addition to the lattice mismatch stress which can have significant impact on device characteristics. In this talk, we study the impact of process induced stress on the electrical characteristics of SiGe HBTs. Particularly large stresses are imposed by metal interconnects. We found experimentally that layout variations of aluminum metallization lines in the vicinity of a HBT can change collector currents by as much as 50% [1]. The main cause for this effect is uniaxial stress in the surface-normal direction imposed by the metal layer stack. The stress field and its effect on device characteristics can be calculated based on known mechanical properties and deformation potential theory.
Stress Simulation: The evolution of stress during the fabrication of a five-layer aluminum metallization was calculated taking into account the full thermal cycle of the process and measured intrinsic stress values of the individual layers. While the structured metal lines are essentially stress free at the deposition temperature (380°C) of the interlayer dielectrics they experience a strong tensile stress normal to the silicon surface when they are covered with oxide and cooled down to room temperature due to the large thermal expansion coefficient of aluminum. As a consequence, tensile stress up to 500 MPa is build up in transistor regions below a stack of 5 metal layers while adjacent Si regions without metal coverage are under compressive stress.
Device Simulation: Electrical characteristics of the strained HBTs were simulated within the drift-diffusion model. The effect of strain is taken into account by the splitting of electron and hole valleys according to deformation potential theory and $k{\cdot}p$ band structure. The mobility model includes modified inter-valley scattering due to strain splitting. The dominating effect of strain on the HBT characteristics is due to the strain dependence of the band gap in the SiGe base. Tensile strain in the surface-normal direction enhances the valley splitting introduced by lattice mismatch stress resulting in a reduced band gap in the base region of the HBT and in enhanced collector currents. The experimentally observed dependence of the collector current on the metal layout is well described by the presented simulation approach.

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Numerical Simulation of Hetero Nanowire Tunnel Field Effect Transistors

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Tunnel Field Effect Transistors (TFETs) are candidates for low-power logic switches with steep (sub-thermal) slope which could enable a strongly reduced supply voltage. Device and circuit simulations of TFETs have shown a 8x smaller delay-energy product at a supply voltage of 0.35V compared to CMOS [1]. To improve the ON/OFF-current ratio, III-V/Si hetero junctions have been proposed [2]. Using nanowires has additional advantages: (i) the possibility of many different material combinations [3], (ii) efficient strain relaxation with shrinking diameter [3], (iii) a good electrostatic control due to the surrounding gate. Simulation results of this presentation are based on experimental data by Tomioka et al. [4, 5, 6] and Björk et al. [7] who advanced the integration of InAs nanowires on Si with nanometerscale hetero epitaxy.

We show how the combined application of a quantum transport solver and a TCAD tool can help to understand the behavior of InAs/Si hetero nanowire Esaki diodes and TFETs leading to design guidelines for the optimization of geometry, doping, gating, and biasing. We used the massively parallel, multi-dimensional, and atomistic quantum transport simulator OMEN [8] which is based on a $sp^3d^5s^*$ tight-binding representation of the band structure. Quantum transport simulation can be done either in the Non-equilibrium Greens Function (NEGF) formalism, if electron-phonon scattering must be included, or using the much faster Wave Function formalism in the ballistic case. OMEN has been applied to direct and phonon-assisted band-to-band tunneling (BTBT) in InAs, Si, and Ge nanowire homo TFETs [9]. The commercial device simulator Sentaurus-Device [10] offers various local and non-local BTBT models. However, neither a theory nor an analytical model for BTBT in a hetero junction between a direct and an indirect semiconductor exist. A practical workaround has to be used with Sentaurus-Device, since a tunnel path across the hetero interface must either belong to a direct (zero-phonon) or to a phonon-assisted tunnel process. Therefore, the *"dynamic nonlocal path BTBT model"* [11], calibrated for InAs, is also used on the silicon side, fitted to experimental data of [12], whereas the calibrated model for Si [13] is also used on the InAs side after proper modifications.

First, the BTBT current of short, unconfined Esaki homo diodes ($\langle 111 \rangle$, 20nm length, abrupt doping) was simulated with OMEN for different materials and doping levels. For the direct materials (InAs, GaSb) and for Ge, where coherent BTBT is dominant [9], the simulation of bulk-like diodes is straightforward. Bulk simulations are needed because of the absence of geometrical confinement in the fabricated nanowire TFETs (diameters in the range 25nm – 100nm). It turns out that InAs has the highest BTBT current density, followed by GaSb and Ge. The upper limit for InAs is $\sim$ 10MA/cm^2. In the case of Si, due to the demanding electron-phonon coupling, at least one-dimensional confinement has to be applied. The estimated bulk limit of Si remains below 100 kA/cm^2, a factor 500 smaller than that of InAs. The doping concentrations at the InAs side of InAs/Si nanowire hetero Esaki diodes produced at IBM Research-Zurich [14, 15] are determined by reverse modeling. Measured InAs/Si nanowire TFET $I_D V_{GS}$ characteristics [6] are then compared with calibrated TCAD simulations. Whereas the measured $I_D V_{GS}$ curves show an almost constant slope over 2-3 orders of magnitude, a very weak ambipolarity, and a strong saturation of the ON-current for each source-drain voltage, simulation yields much higher ON-currents, a strong ambipolarity, curved slopes typical for BTBT, a minimum point slope of

45mV/dec, and no ON-current saturation. The most likely explanation of the measured currents is that they are dominated by defect-assisted tunneling (DAT), either during interface or bulk Shockley-Read-Hall generation. Although multi-phonon coupling parameters of the involved defects in InAs are not known, the shape of the $I_D V_{GS}$ curves can be qualitatively reproduced with a physics-based DAT model [16] in Sentaurus-Device. The apparent absence of BTBT in the measurement could be due to compressive biaxial strain in the highly lattice mismatched system.

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Modeling Spintronic Effects in Silicon

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1. Introduction

The electron spin can change its orientation to opposite very fast by utilizing an amazingly small amount of energy, which offers a unique opportunity to reduce the power per operation in semiconductor logic devices. The spin field-effect transistor (SpinFET) is a switch which employs the spin properties of electrons. The SpinFET is composed of a semiconductor channel region sandwiched between the two ferromagnetic contacts, source and drain (Fig. 5). The source contact injects spin-polarized electrons in the semiconductor region. The gate-voltage-dependent spin-orbit interaction in the channel is used to modulate the current through the SpinFET [1]. It causes the electron spin to precess during the electron propagation through the channel. Only the electrons with their spin aligned to the drain contact magnetization can leave the channel through the drain contact, thus contributing to the current. The spin-orbit interaction is controlled electrically by applying an external gate voltage.

2. Model and Results

To calculate the transport properties of the ballistic spin field-effect transistor schematically shown in Fig. 5 we consider the Hamiltonian in the ferromagnetic regions in the following form [2], [3]:

$$\begin{aligned} H &= \frac{p_x^2}{2m_f^*} + h_0\sigma_z, \quad x < 0, \\ H &= \frac{p_x^2}{2m_f^*} \pm h_0\sigma_z, \quad x > L, \end{aligned} \tag{1}$$

where m_f^* is the effective mass in the contacts, $h_0 = 2PE_F/(P^2{+}1)$ is the exchange splitting energy with P defined as the spin polarization in the ferromagnetic regions, E_F is the Fermi energy, and σ_z is the Pauli matrix; $\pm$ in (1) stands for the parallel (P) and anti-parallel (AP) configuration of the contact magnetization. The effective Hamiltonian in the channel is [2]

$$H = \frac{p_x^2}{2m_s^*} + \delta E_c + \frac{\beta}{\hbar}(p_x\sigma_x - p_y\sigma_y) + \frac{1}{2}g\mu_B B\sigma^*. \tag{2}$$

Here m_s^* is the subband effective mass, δE_c is the band mismatch between the ferromagnetic and the semiconductor region, g is the Landé factor, μ_B is the Bohr magneton, B is the magnetic field, and $\sigma^* \equiv \sigma_x \cos\gamma + \sigma_y \sin\gamma$ with γ defined as the angle between the magnetic field and the transport direction. As it was recently demonstrated [4], [5], the major contribution to the spin-orbit interaction in thin silicon films is due to the interface-induced inversion asymmetry and is mathematically equivalent to the linear Dresselhaus term. The coefficient β of the spin-orbit interaction in silicon heterostructures is a linear function of the gate voltage, which is the key for the current modulation in the channel (Fig. 5): it causes the electron spin to precess during the propagation through the channel. Fig. 6 shows the modulation of the tunnel magnetoresistance $TMR \equiv \frac{G^P - G^{AP}}{G^{AP}}$ defined by the channel conductances in P/AP configuration of the relative source/drain magnetizations on the strength of the spin-orbit interaction β in silicon channels of different length. As the length of the channel decreases, the period of the *TMR* modulation

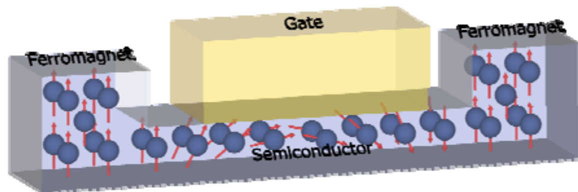

Fig. 5: Illustration of the Datta-Das spin field effect transistor. The spin-orbit interaction with the gate voltage dependent strength alters the spin polarization direction in the channel close to the ferromagnetic drain. Only electrons with the spin direction aligned to the drain magnetization contribute to the current.

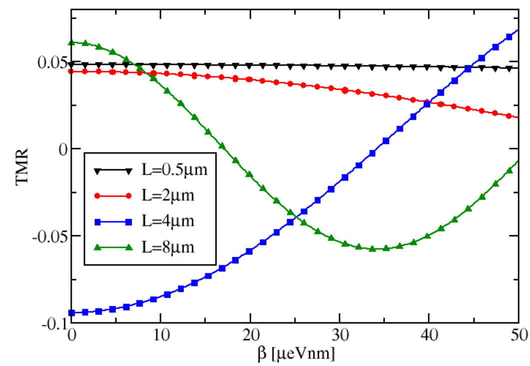

Fig. 6: TMR dependence on the value of the Dresselhaus spin-orbit interaction for $E_F = 2.47$eV, $\delta E_c = 2.154$eV, $z = 1$.

increases. $L = 4\mu$m is sufficient to observe half of the oscillation and thus to modulate the *TMR* by adjusting the strength of the spin-orbit interaction. To facilitate the spin injection into silicon delta-function barriers of strength $z = 2m_F U \,/\, \hbar^2 k_F$ are introduced. As shown in Fig. 7, increasing the barrier leads to a more pronounced *TMR* modulation as a function of β. Fig. 8 shows oscillations of the *TMR* on the value of the bandgap mismatch δE_c. The period of the oscillations is inversely proportional to the length of the channel. Temperature exerts a significant influence on the oscillatory amplitude as shown in Fig. 9. For $L = 0.2\mu$m the oscillatory behavior of the *TMR* completely vanishes for $T = 50$K. The reason is a relatively short period of the *TMR* oscillation with respect to δE_c shown in Fig. 8. For longer channels the period becomes even shorter, hence the shorter channels are needed to preserve the *TMR* modulation at higher temperatures as a function of δE_c. A different option to proceed to room temperature operation is to increase the channel length. Fig. 10 shows a possibility to modulate the *TMR* by changing the value of β even at room temperature, however, the channel length should be a few micrometers for the parameters specified [6]. The non-zero spin-orbit interaction leads to an increased spin relaxation. In quasi-one-dimensional electron structures, however, a suppression of the spin relaxation was predicted [7].

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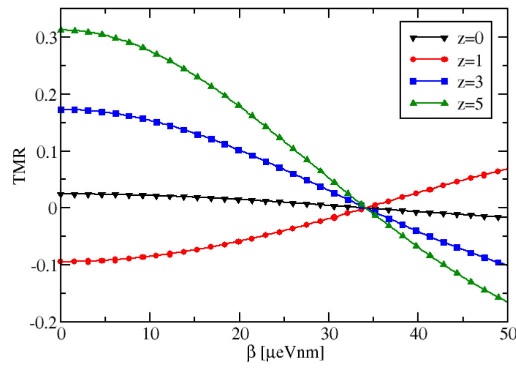

Fig. 7: TMR dependence on the spin-orbit interaction strength for $L = 4\mu$m.

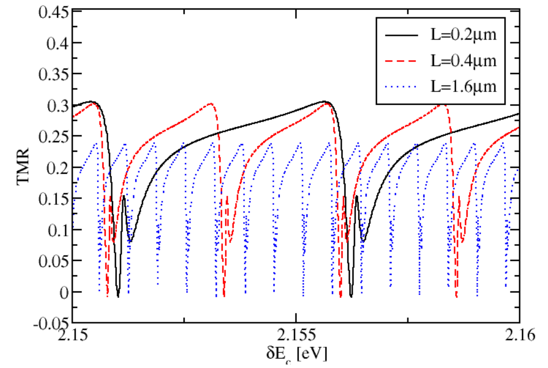

Fig. 8: TMR dependence on the conduction band mismatch for $z = 3$, $\beta = 42.3\mu$eVnm.

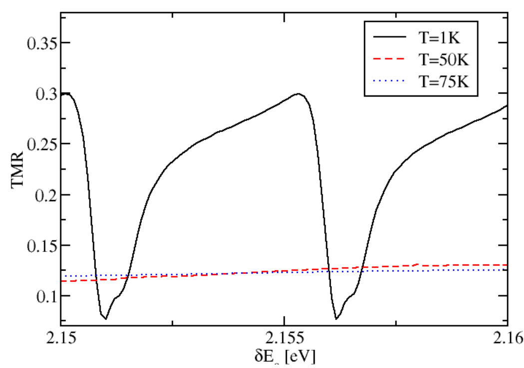

Fig. 9: TMR for different temperatures for the parameters from Fig. 8, and $L = 0.2\mu$m, $V = 1$meV.

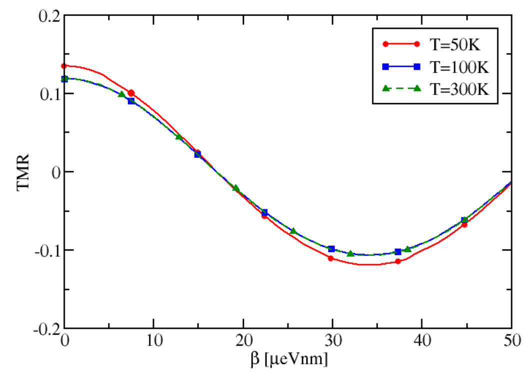

Fig. 10: TMR dependence on β for $L = 8\mu$m. The other parameters are the same as in Fig. 8.

Virtual Experiments with High Power Semiconductor Devices Along and Beyond the Rim of the Safe Operating Area

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Reliability and robustness against harsh operating conditions such as high temperature, hard unclamped switching, irradiation by cosmic particles, or mechanical vibrations are of utmost importance in the design of modern high power semiconductor devices.

Today's challenge is to make virtual experiments and tests on the computer, which are qualitatively correct and quantitatively accurate even for devices that have never been built before, and under operational conditions that very rarely occur as long as the device is kept within the so-called "safe operating area (SOA)". What we are interested in is to explore the rim of the SOA and even to go beyond it in order to study failure and, eventually, destruction mechanisms with a view to improving robustness and reliability of the devices. To this end, predictive high-fidelity computer simulations of "virtual destruction" have to be mastered.

While the physical models (typically energy-domain coupling continuous field models) which underlie the description of the inner life of electronic devices have become more and more elaborate and highly detailed, even under extreme and exceptional operating conditions, the capabilities and the quality of the simulation tools in which they are implemented still needs quite a lot of improvement. We will address these problems with reference to selected real-life examples, leading to a proclamation of improvements to be made towards a more judicious interpretation of numerical simulations w.r.t. accuracy, reliability and, hence, predictiveness.

Application of WIAS-TeSCA to the analysis of the power limits of semiconductor lasers

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The factors that limit both the continuous wave and the pulsed output power of broad-area laser diodes driven at very high currents are investigated theoretically and experimentally. The decrease in the gain due to self-heating under CW operation and spectral holeburning under pulsed operation as well as heterobarrier carrier leakage and longitudinal spatial holeburning limit the maximum achievable output power.

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