COUPLING PROBLEMS IN MICROELECTRONIC DEVICE SIMULATION

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Abstract

The cost-effective design of electronic microstructures requires an advanced modeling and coupled simulation of various physical effects. The classical isothermal approach leads to the basic drift-diffusion model for semiconductor device simulation. In the stationary case, it represents a coupled nonlinear system consisting of a Poisson equation for the electric potential and two continuity equations for the electron and hole flow. We discuss various discretization schemes with special emphasis on mixed finite element methods and we further address efficient numerical solution techniques including adaptive multilevel methods. Finally, to allow for ambient conditions such as external magnetic fields we consider consistent extensions of the classical model and discuss perspectives for their numerical treatment.

1. Introduction

The numerical simulation of microelectronic devices is an integral part of the Computer Aided Design of integrated microsystems. It consists of three main stages: The first stage is concerned with the simulation of the fabrication processes and comprises structure defining processing steps such as lithography, etching, decomposition and thermal oxidation as well as the processing steps of ion implantation and dopand diffusion (cf. e.g. [23]).
The second stage deals with the simulation of the physical behavior of the devices within a unified framework which takes into account not only the electrical behavior but also thermal, magnetic and optical effects depending on what the device is aimed for (cf. e.g. [30], [31]).
The third stage represents the simulation of the global behavior of networks of microstructures under operating conditions of interest (cf. e.g. [19]).

In this paper, the emphasis is on concepts for microelectronic device simulation allowing an efficient and reliable numerical solution of the underlying physical equations. A common feature of the physical modeling is the coupled simulation of carrier and energy transport and the proper incorporation of ambient conditions such as electromagnetic radiation fields (power laser diodes) or galvanomagnetic efforts in the presence of an external quasistatic magnetic field (magnetotransistors).

It has to be noted that in the modeling community there is a controversial debate what such advanced device models should be based on. One common approach uses the so-called hydrodynamic model resulting from a momentum expansion of the Boltzmann equation truncated after the second-order moments (cf. e.g. [20]). Another approach, advocated for example by Wachutka [30], uses the principles of irreversible phenomenological thermodynamics to provide an extended thermodynamic model as a comprehensive framework for a unified treatment which allows a tailored modeling of specific microelectronic devices. The model is such that in the absence of mechanical, thermal, magnetic and optical effects it reduces to the description of the interaction between the electric field

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and the particle transport as given by the classical drift-diffusion model in semiconductor device simulation. In this sense the drift-diffusion model represents, so-to-say, the kernel of the extended model and any numerical approach for the extended model has to rely on an efficient solution of the drift-diffusion equations.

In this paper, we will advocate the use of mixed finite elements with special emphasis on a technique called mixed hybridization allowing the simultaneous computation of the current densities and the carrier concentrations. We will also indicate its relationship to other widely used discretization techniques with the celebrated Scharfetter-Gummel scheme at prominent place. Further, we will present tools for adaptive grid generation within a mixed finite element approach and give some numerical results for a MOSFET. Finally, we will shortly address the numerical treatment of an extended model incorporating external magnetic fields.

2. Mixed finite element discretization of the drift-diffusion model

In the stationary case, the classical drift-diffusion model describing the distribution of the electron and hole densities n and p under the influence of an electric field consists of two continuity equations for the current densities $\mathbf{j}_n$ and $\mathbf{j}_p$ coupled with a Poisson equation for the electric potential Ψ.

$$\begin{aligned} -\epsilon\Delta\Psi &= q(D+n-p), \\ \operatorname{div}\mathbf{j}_n &= qR(n,p)+f_1, \\ \operatorname{div}\mathbf{j}_p &= -qR(n,p)+f_2 \end{aligned} \tag{2.1}$$

where

$$\begin{aligned} \mathbf{j}_n &= q\mu_n(U_T\operatorname{grad} n - n\operatorname{grad}\Psi), \\ \mathbf{j}_p &= -q\mu_p(U_T\operatorname{grad} p + p\operatorname{grad}\Psi). \end{aligned}$$

Here, D stands for the dopand profile, $R(n,p)$ for the recombination/generation rate and f_1, f_2 are the source terms. Further, ϵ, q, U_T and μ_n, μ_p denote the dielectric permittivity, the elementary charge, the thermal voltage and the mobilities, respectively. We consider (2.1) in a bounded polyhedral domain $\Omega \subset \mathbb{R}^3$ with boundary conditions of Dirichlet type at the Ohmic contacts Γ_D and of homogeneous Neumann type at the isolating part Γ_N of the device.

$$\begin{aligned} &\Psi = \Psi_D,\ \ n = n_D,\ \ p = p_D \quad \text{on } \Gamma_D, \\ &\tfrac{\partial\Psi}{\partial\nu} = 0,\ \ \nu\cdot\mathbf{j}_n = 0,\ \ \nu\cdot\mathbf{j}_p = 0 \quad \text{on } \Gamma_N. \end{aligned} \tag{2.2}$$

Typically, the dopand profile D is strongly varying causing a pronounced layer behavior of the electric potential Ψ. Consequently, we may expect local areas with significant change in magnitude of the gradient of Ψ. In view of the constitutive relations for the current densities, the convective transport is dominant in such areas so that the continuity equations represent convection-dominated diffusion-convection problems. It is well known that the numerical solution of such problems requires utmost care in the discretization process. Apart from upwinding techniques for methods based on the primal variational approach (cf. e.g. [4]), finite volume techniques are widely used, because they are based on the principle of current conservation. Related techniques are provided by mixed finite element discretizations allowing the simultaneous computation of the current densities and the carrier concentrations. For simplicity, we consider the continuity equation for only one minority carrier in the following scaled and linearized form

$$\operatorname{div}(\exp(\Psi)\operatorname{grad} u) - \exp(\Psi)Ru = f$$

where we have introduced the Slotboom variable $u = \exp(-\Psi)n$ and R stands for the differential net recombination/generation rate. The mixed approach is based on the dual formulation of the problem which can be obtained by introducing the current density $\mathbf{j} = \exp(\Psi)\mathrm{grad}\, u$ as an additional unknown. In this way, the second order elliptic partial differential equation can be formally written as a first order system. In contrast to the primal approach we rely on the weak formulation of the relationship between he current density $\mathbf{j}$ and the Slotboom variable u whereas the continuity equation is treated in the strong L^2-sense. This gives rise to a system of two variational equations:

Find $(\mathbf{j}, u) \in H_{\Gamma_N}(\mathrm{div}\,;\Omega) \times L^2(\Omega)$ such that

$$\begin{aligned} \int_\Omega \exp(-\Psi)\mathbf{j}\cdot\mathbf{q}\,dx + \int_\Omega \mathrm{div}\,\mathbf{q}\,u\,dx &= \int_{\Gamma_D} \exp(-\Psi)n_D\nu\cdot\mathbf{q}\,d\sigma,\ \mathbf{q}\in H_{\Gamma_N}(\mathrm{div}\,;\Omega) \\ \int_\Omega \mathrm{div}\,\mathbf{j}\,v\,dx - \int_\Omega \exp(\Psi)Ruv\,dx &= \int_\Omega fv\,dx,\ v\in L^2(\Omega) \end{aligned} \tag{2.3}$$

where $H_{\Gamma_N}(\mathrm{div}\,;\Omega) = \{\mathbf{q}\in (L^2(\Omega))^3 \mid \mathrm{div}\,\mathbf{q}\in L^2(\Omega),\ \nu\cdot\mathbf{q}|_{\Gamma_N} = 0\}$.

In the following we will focus on an approach called dual or mixed hybridization which takes advantage of ideas from domain decomposition and can be carried out both in the continuous and discrete setting of the problem. We will concentrate on the discrete setting and refer to [16] for a treatment of the continuous case. For that purpose we consider the standard mixed discretization by means of the lowest order Raviart-Thomas approximation. Given a simplicial triangulation $\mathcal{T}_h$ of Ω, the Slotboom variable u will be approximated by piecewise constants resulting in the ansatz space

$$W_0(\Omega;\mathcal{T}_h) = \{v_h\in L^2(\Omega) \mid v_h|_K \in P_0(K),\ K\in\mathcal{T}_h\}$$

where $P_k(K)$, $k\geq 0$, denotes the polynomials of degree $\leq k$ on K. An associated approximation of the dual variable $\mathbf{j}$ can be obtained by requiring the divergence of the discrete flux to be piecewise constant, too. This requirement leads in a natural way to the lowest order Raviart-Thomas element $RT_0(K) = P_0(K)^3 + \mathbf{x}P_0(K)$, $\mathbf{x} = (x_1,x_2,x_3)^T$. We note that any vector field from $RT_0(K)$ is uniquely determined by 4 degrees of freedom which can be chosen as the normal component of the flux in the center of gravity of the faces of K. Setting

$$RT_{0;\Gamma_N}(\Omega;\mathcal{T}_h) = \{\mathbf{q}_h\in H_{\Gamma_N}(\mathrm{div}\,;\Omega) \mid \mathbf{q}_h|_K\in RT_0(K),\ K\in\mathcal{T}_h\},$$

the mixed discretization requires the computation of a pair $(\mathbf{j}_h, u_h)\in RT_{0;\Gamma_N}(\Omega;\mathcal{T}_h)\times W_0(\Omega;\mathcal{T}_h)$ as the solution of (2.3) when restricted to $RT_{0;\Gamma_N}(\Omega;\mathcal{T}_h)$ and $W_0(\Omega;\mathcal{T}_h)$, respectively. The concept of mixed hybridization originally due to Fraeijs de Veubeke [11] (cf. also [7]) is to decompose the saddle point problem arising from the standard mixed approach into less bulky pieces by considering the "broken" Raviart-Thomas ansatz space

$$RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h) = \{\mathbf{q}_h\in \prod_{K\in\mathcal{T}_h} RT_0(K) \mid \nu\cdot\mathbf{q}_h|_{\Gamma_N} = 0\}.$$

We note that $RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h)$ is not a subspace of $H_{\Gamma_N}(\mathrm{div}\,;\Omega)$, since the continuity of the normal components $\nu\cdot\mathbf{q}_h$ of vector fields $\mathbf{q}_h\in RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h)$ across the interelement boundaries of the triangulation is no longer guaranteed. Instead, the continuity constraints are taken care of by appropriate Lagrangian multipliers. Denoting by $\mathcal{F}_h$ the set of faces of $\mathcal{T}_h$ an appropriate multiplier space is given by

$$M_{0;\Gamma_D}(\Omega;\mathcal{T}_h) = \{\mu_h\in L^2(\mathcal{F}_h) \mid \mu_h|_F\in P_0(F),\ F\in\mathcal{F}_h,\ \mu_h|_F = 0,\ F\in\mathcal{F}_h\cap\Gamma_D\}.$$

Then, in terms of the original primal variable n_h the mixed hybridization requires the computation of a triple $(\mathbf{j}_h, n_h, \lambda_h) \in RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h) \times W_0(\Omega;\mathcal{T}_h) \times M_{0;\Gamma_D}(\Omega;\mathcal{T}_h)$ such that

$$\begin{aligned}
&\sum_{K\in\mathcal{T}_h} \int_K \exp(-\Psi)\mathbf{j}_h \cdot \mathbf{q}_h \, dx + \sum_{K\in\mathcal{T}_h} \int_K \operatorname{div} \mathbf{q}_h \exp(-\Psi) n_h \, dx \\
&- \sum_{K\in\mathcal{T}_h} \int_{\partial K} \exp(-\Psi)\lambda_h \nu \cdot \mathbf{q}_h \, d\sigma \;=\; \sum_{K\in\mathcal{T}_h} \int_{\partial K\cap\Gamma_D} \exp(-\Psi) n_D \nu \cdot \mathbf{q}_h \, d\sigma, \;\; \mathbf{q}_h \in RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h), \\
&\sum_{K\in\mathcal{T}_h} \int_K \operatorname{div} \mathbf{j}_h v_h \, dx - \sum_{K\in\mathcal{T}_h} \int_K R n_h v_h \, dx \;=\; \int_\Omega f v_h \, dx, \;\; v_h \in W_0(\Omega;\mathcal{T}_h), \\
&\sum_{K\in\mathcal{T}_h} \int_{\partial K} \mu_h \nu \cdot \mathbf{j}_h \, d\sigma \;=\; 0, \;\; \mu_h \in M_{0;\Gamma_D}(\Omega;\mathcal{T}_h).
\end{aligned} \tag{2.4}$$

The purely local character of the bases of $RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h)$ and $W_0(\Omega;\mathcal{T}_h)$ strongly suggests static condensation of both the discrete flux $\mathbf{j}_h$ and the discrete carrier concentration n_h resulting in the Schur complement system

$$S_h \lambda_h = t_h. \tag{2.5}$$

Theorem 2.1 *The Schur complement S_h can be assembled from its local contributions S_h^K, $K \in \mathcal{T}_h$, resulting from static condensation on the elements' level. For interior elements $K \in \mathcal{T}_h \cap \Omega$ we obtain*

$$S_h^K = -D_K^1(\alpha_K^{-1} U_K + \beta_K T_K) D_K^2 \tag{2.6}$$

where D_K^1, D_K^2, U_K and T_K are the 4×4 matrices

$$\begin{gathered}
D_K^1 = (|F_i|\delta_{ij})_{i,j=1}^4, \;\; D_K^2 = \left(\left(\int_{F_i} \exp(-\Psi)\, d\sigma \right) \delta_{ij} \right)_{i,j=1}^4, \;\; U_K = (\nu_i \cdot \nu_j)_{i,j=1}^4 \\
T_K = \eta_K \eta_K^T, \;\; \eta_{K,i} = \mathbf{p} \cdot \nu_i - \alpha_K^{-1} \int_K \exp(-\Psi) \mathbf{x} \cdot \nu_i \, dx, \;\; \mathbf{p} \in F_i, \, 1 \le i \le 4
\end{gathered}$$

and the constants α_K, β_K are given by

$$\begin{gathered}
\alpha_K = \int_K \exp(-\Psi)\, dx, \;\; \beta_K = (\gamma_K \int_K R \, dx + 9\alpha_K |K|)^{-1} \int_K R \, dx, \\
\gamma_K = \int_K \exp(-\Psi) \xi_K \cdot \xi_K \, dx, \;\; \xi_K(x) = \mathbf{x} - \alpha_K^{-1} \int_K \exp(-\Psi) \mathbf{x}' \, dx'.
\end{gathered}$$

For elements $K \in \mathcal{T}_h$ attached to the boundary Γ_D obvious modifications apply.

Proof: Since the Schur complement does not depend on the choice of the bases in $RT^{-1}_{0;\Gamma_N}(\Omega;\mathcal{T}_h)$ and $W_0(\Omega;\mathcal{T}_h)$, we pick a local basis $\mathbf{q}_K^{(i)}$, $1 \le i \le 4$, of the discrete flux space according to $\mathbf{q}_K^{(i)} = \mathbf{e}_i$, $1 \le i \le 3$, $\mathbf{q}_K^{(4)} = \xi_K$ where $\mathbf{e}_i$ stands for the i-th canonical basis vector of $\mathbb{R}^3$. Observing that the $\mathbf{q}_K^{(i)}$ are orthogonal with respect to the inner product $(\mathbf{p}_K, \mathbf{q}_K) = \int_K \exp(-\Psi) \mathbf{p}_K \cdot \mathbf{q}_K \, dx$ and that $\operatorname{div} \mathbf{q}_K^{(i)} = 0$, $1 \le i \le 3$, $\operatorname{div} \mathbf{q}_K^{(4)} = 3$, the representation (2.6) follows from straightforward, but tedious computations. □

It can be immediately seen from (2.6) that the matrix $-S_h^K$ is an M-matrix provided the element K has no obtuse angle. Obviously, this property carries over to the global Schur complement $-S_h$.

Following the same line of arguments as in the previous theorem, the right hand side of the Schur complement system can be similarly assembled from local load vectors t_h^K, $K \in \mathcal{T}_h$.

Moreover, the inhomogeneous Dirichlet data can be incorporated into the multiplier by setting $\lambda_h|_F = (\int_F \exp(-\Psi)\,d\sigma)^{-1} \int_F \exp(-\Psi) n_D\,d\sigma$, $F \in \mathcal{F}_h \cap \Gamma_D$.

Though in the process of mixed hybridization we have discarded the discrete current densities $\mathbf{j}_h$ and the discrete carrier concentrations n_D, they can be easily retrieved from the values of the Lagrangian multiplier λ_h. In particular, denoting by $\mathbf{j}_h^K$ the vector of fluxes through the faces of $K \in \mathcal{T}_h$ we find that $\mathbf{j}_h^K$ is readily available as the residual of the local Schur complement equation:

$$\mathbf{j}_h^K = t_h^K - S_h^K \lambda_h^K, \quad K \in \mathcal{T}_h.$$

Note that the residual in general does not vanish, since the actual value of λ_h results from the solution of the global Schur complement system and thus inherits contributions from the other elements.

An important implementational aspect of mixed hybridization - in particular with respect to the construction of iterative solvers - is that the Schur complement system can be shown to be equivalent to a nonconforming Petrov-Galerkin scheme of inverse average type. That equivalence has been observed, among others, by Brezzi, Marini and Pietra [8], [9] and has been exploited, for example, by Bachmann [2] and Reusken [24] in a multigrid approach to the continuity equation. To be more precise, let us denote by Ψ_K^i, $1 \le i \le 4$, the local canonical basis of the lowest order nonconforming Crouzeix-Raviart element $CR_1(K)$ and by $\tilde{\Psi}_K^i$ the scaled basis functions

$$\tilde{\Psi}_K^i = s_i \Psi_K^i, \quad s_i = |F_i|^{-1} \int_{F_i} \exp(-\Psi)\,d\sigma, \ 1 \le i \le 4$$

spanning the scaled element $\widetilde{CR}_1(K)$. We choose

$$\begin{aligned} \widetilde{CR}_{1;\Gamma_D}(\Omega;\mathcal{T}_h) \;=\; & \{v_h \in L^2(\Omega) \mid v_h|_K \in \widetilde{CR}_1(K),\ K \in \mathcal{T}_h, \\ & v_h|_{F_i} = s_i^{-1} \exp(-\Psi) n_D,\ F_i \in \mathcal{F}_h \cap \Gamma_D\} \end{aligned}$$

as the ansatz space and

$$CR^0_{1;\Gamma_D}(\Omega;\mathcal{T}_h) = \{v_h \in L^2(\Omega) \mid v_h|_K \in CR_1(K),\ K \in \mathcal{T}_h,\ v_h|_{\Gamma_D} = 0\}$$

as the test space in a modified nonconforming Petrov-Galerkin approach to the primal variational formulation of the continuity equation where the modification consists in replacing the coefficient function $\exp(\Psi)|_K$ by its harmonic average over an individual element $K \in \mathcal{T}_h$. Then, the following result can be established where for notational convenience we only consider the case $R = 0$.

Theorem 2.2 *Let $u_h \in \widetilde{CR}_{1;\Gamma_D}(\Omega;\mathcal{T}_h)$ be the solution of the nonconforming Petrov-Galerkin scheme*

$$a_h(u_h, v_h) = l_h(v_h), \quad v_h \in CR^0_{1;\Gamma_D}(\Omega;\mathcal{T}_h) \tag{2.7}$$

where

$$\begin{aligned} a_h(u_h, v_h) \;&=\; \sum_{K \in \mathcal{T}_h} \int_K \left(|K|^{-1} \int_K \exp(-\Psi)\,dx \right)^{-1} \operatorname{grad} u_h \cdot \operatorname{grad} v_h\,dx, \\ l_h(v_h) \;&=\; \sum_{K \in \mathcal{T}_h} (3|K|)^{-1} \int_K f\,dx \int_K \left(\exp(-\Psi) \left(|K|^{-1} \int_K \exp(-\Psi)\,dx' \right)^{-1} - 4 \right) v_h\,dx \end{aligned}$$

Then, if λ_h is the solution of the Schur complement system (2.5) in case $R = 0$ and Π_h denotes the L^2-projection onto the multiplier space, we have $\lambda_h = \Pi_h u_h$.

Proof: The proof is the 3D analogue of that one given in [16; Thm. 4.2] in the 2D case (cf. also [15; Satz 3.2.2]). □

As said before, the equivalence with the nonconforming Petrov-Galerkin scheme (2.7) can be used by taking advantage of efficient multilevel iterative solvers designed for nonconforming finite element discretizations (cf. e.g. [6]). In the sequel, we will not follow this aspect but instead elaborate on the relationship between mixed methods and the Scharfetter-Gummel box method widely used in device simulation.

3. Mixed discretization and the Scharfetter-Gummel scheme

It is well known that mixed finite element methods are closely related to finite volume techniques. Such box methods are also appropriate candidates for the discretization of the drift-diffusion model, since they are based on the principle of current conservation. The most prominent box method in device simulation is the Scharfetter-Gummel scheme which is used in many existent program packages (cf. e.g. [10], [27], [28]). In order to establish the relationship between mixed methods and the Scharfetter-Gummel scheme, let us consider the mixed discretization of the continuity equation by means of the lowest order Raviart-Thomas approximation with respect to a hexahedral triangulation. In this case, the Raviart-Thomas element $RT_{[0]}(K)$, $K \in \mathcal{T}_h$, is given by

$$RT_{[0]}(K) = Q_{1,0,0}(K) \times Q_{0,1,0}(K) \times Q_{0,0,1}(K)$$

where $Q_{\nu_1,\nu_2,\nu_3}(K) = \{p \mid p(x) = \sum_{|\alpha_i| \le \nu_i} \gamma_\alpha x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3},\ \mathbf{x} \in K\}$. Any vector field from $RT_{[0]}(K)$ is uniquely determined by six degrees of freedom which are again chosen as the normal components in the centers of gravity of the faces of K. As for simplicial triangulations the primal variable is approximated by piecewise constants. Denoting by $RT_{[0];\Gamma_N}(\Omega;\mathcal{T}_h)$ and $W_0(\Omega;\mathcal{T}_h)$ the associated global ansatz spaces, we have to compute $(\mathbf{j}_h, n_h) \in RT_{[0];\Gamma_N}(\Omega;\mathcal{T}_h) \times W_0(\Omega;\mathcal{T}_h)$ as the solution of

$$\begin{aligned} &\int_\Omega \exp(-\Psi)\mathbf{j}_h \cdot \mathbf{q}_h\, dx + \int_\Omega \exp(-\Psi)\mathrm{div}\,\mathbf{q}_h\, n_h\, dx = \int_{\Gamma_D} \exp(-\Psi) n_D \nu \cdot \mathbf{q}_h\, d\sigma, \\ &\int_\Omega \mathrm{div}\,\mathbf{j}_h\, v_h\, dx - \int_\Omega R n_h v_h\, dx = \int_\Omega f v_h\, dx, \quad v_h \in W_0(\Omega;\mathcal{T}_h),\ \mathbf{q}_h \in RT_{[0];\Gamma_N}(\Omega;\mathcal{T}_h). \end{aligned} \tag{3.8}$$

By regular refinement we subdivide each element $K \in \mathcal{T}_h$ with vertices P_ν, $1 \le \nu \le 8$, into eight subelements K_ν, $1 \le \nu \le 8$, and evaluate the integrals $\int_K \exp(-\Psi)\mathbf{j}_h \cdot \mathbf{q}_h\, dx$ in (3.8) by means of the quadrature formula

$$\sum_{\nu=1}^{8} (\mathbf{p}_h \cdot \mathbf{q}_h)(P_\nu) \int_K \exp(-\Psi)\, dx. \tag{3.9}$$

Theorem 3.3 *The mixed method (3.8) in combination with the quadrature formula (3.9) is equivalent to the Scharfetter-Gummel discretization of the continuity equation.*

Proof: Considering the 2×2 block coefficient matrix which represents the algebraic formulation of (3.8), the first diagonal block obviously reduces to a diagonal matrix when using (3.9). Then, the equivalence can be easily established by static condensation of the discrete fluxes. □

Another finite volume technique that has been proposed for device simulation is the Baliga-Patankar scheme (cf. e.g. [3], [29]). However, as has been shown in [21], small carrier concentrations cannot be computed in a numerically stable way due to the influence

of rounding-off errors.

4. Adaptive grid refinement

As we have already pointed out, for most devices the dopand profile is such that we are faced with a pronounced layer behavior of both the electric potential and the carrier concentrations. An efficient resolution of such layers requires the use of highly nonuniform grids which can be generated by means of adaptive grid refinement. For mixed finite element discretizations of the drift-diffusion model, more or less heuristic criteria for grid refinement based on the gradient of the solutions have been used by Hemker and Molenaar [14] and by van Nooyen [22]. However, for mixed hybridization an efficient and reliable a posteriori error estimator is at hand which can be implemented very cheaply (cf. [17], [18]). This estimator is motivated by a superconvergence result for mixed hybridization due to Arnold and Brezzi [1] which states that under the same regularity assumptions the nonconforming extension $\hat{n}_h$ of the Lagrangian multiplier λ_h from the mixed hybrid approach approximates the primal variable n of a higher order than does n_h. This superconvergence result supports the following saturation assumption

$$\|n - \hat{n}_h\|_0 \leq \beta \|n - n_h\|_0, \quad 0 \leq \beta < 1 \tag{4.10}$$

where $\|\cdot\|_0$ stands for the standard L^2-norm. In practice, instead of λ_h and n_h we only have some iterative approximations $\tilde{\lambda}_h$ and $\tilde{n}_h$ at hand. If we denote by $\hat{\tilde{n}}_h$ the nonconforming extension of $\tilde{\lambda}_h$ and further assume

$$\|n - n_h\|_0 \leq \sigma \|n - \tilde{n}_h\|_0, \quad 0 \leq \sigma,\ \beta\sigma < 1, \tag{4.11}$$

then from (4.10) and (4.11) we can easily deduce the following two-sided estimate of the total error $\|n - \tilde{n}_h\|_0$:

$$\begin{array}{rcl} \|n - \tilde{n}_h\|_0 & \geq & (1 + \beta\sigma)^{-1} \left(\|\hat{\tilde{n}}_h - \tilde{n}_h\|_0 - C\|n_h - \tilde{n}_h\|_0 \right), \\ \|n - \tilde{n}_h\|_0 & \leq & (1 - \beta\sigma)^{-1} \left(\|\hat{\tilde{n}}_h - \tilde{n}_h\|_0 + C\|n_h - \tilde{n}_h\|_0 \right). \end{array} \tag{4.12}$$

For adaptive grid refinement we use the easily computable elementwise contributions of $\|\hat{\tilde{n}}_h - \tilde{n}_h\|_0$, determine the mean value and mark an element for refinement, if the local contribution exceeds the mean value by a certain problem-dependent margin. The refinement process itself is performed according to the strategy proposed by Bornemann et al. [5].

5. Numerical results for a MOSFET

For an illustration of the application of adaptive grid refinement in device simulation let us consider the results of the mixed hybrid approach to the drift-diffusion model in case of a MOSFET.

As shown in Figure 1, the MOSFET is a three layer device consisting of two highly doped n regions equipped with the source and drain contacts and a lower doped p region called bulk. Between source and drain the semiconductor material is coated with a thin oxide layer equipped with the gate contact. If a sufficiently high voltage is applied to the gate, an inversion layer is created in the bulk region close to the interface between the silicon and the oxide. In case of a potential difference between source and drain there is a current from source to drain in the n-channel whose magnitude can be controlled by the voltage

applied at the gate.

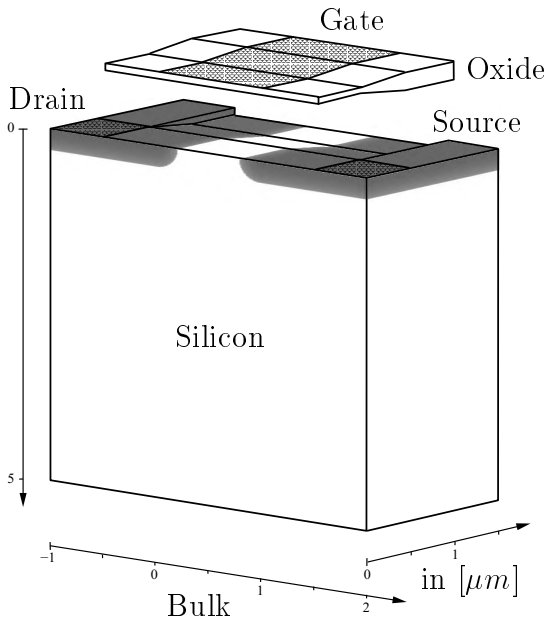

Fig. 1: Typical geometry of a MOSFET

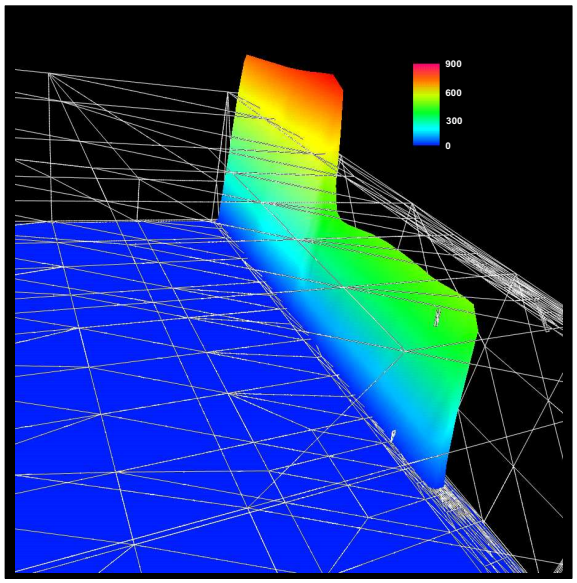

Fig. 2: Scaled electron density in a vicinity of an n-channel MOSFET

The drift-diffusion equations have been solved by an approximate Newton method, namely the well-known Gummel iteration. The resulting linearized problems have been treated by mixed hybridization with respect to an adaptively generated hierarchy of simplicial triangulations along the lines described in the previous sections.
Figure 2 represents a visualization of the electron density and the underlying triangulation in a vicinity of the n-channel. The layer behavior is clearly visible as it is the pinch-off point close to the drain region. Moreover, we observe that the layer is neatly resolved by the adaptively generated triangulation.

6. Extended model for galvanomagnetic carrier transport

Integrated bipolar magnetotransistors are semiconductor devices that are used as magnetosensors converting a magnetic field into an electronic signal. The magnetic field sensitivity is caused by galvanomagnetic phenomena which have to be modeled on the basis of the galvanomagnetic carrier transport in semiconductors. The physical modeling of the transport equations describing the flow of the electrons and holes has to incorporate the deflection of the carriers by the Lorentz force in the interior of the device (cf. e.g. [25], [26]). In particular, the constitutive equations for the electron and hole current densities must be augmented by appropriate magnetic field dependent terms. Denoting by $\mathbf{j}_\alpha^0$, $\alpha = n$ or $\alpha = p$, the current densities without magnetic field, by $\mathbf{b}$ the magnetic field vector and by μ_α^* the Hall mobilities, we use

$$\mathbf{j}_\alpha = \mathbf{j}_\alpha^0 + \left(1 + (\mu_\alpha^*|\mathbf{b}|)^2\right)^{-1} \left(\mu_\alpha^* \mathbf{b} \times \mathbf{j}_\alpha^0 + \mu_\alpha^* \mathbf{b} \times (\mu_\alpha^* \mathbf{b} \times \mathbf{j}_\alpha^0)\right). \tag{6.13}$$

The extended model then consists of the system (2.1) with $\mathbf{j}_n, \mathbf{j}_p$ given by (6.13). Further, the boundary conditions (2.2) have to be modified slightly for taking into account the action of the magnetic field on the device (see e.g. [25] for details).

The existence and uniqueness of weak solutions and the stability of the thermal equilibrium have been established by Gajewski and Gröger [12] and by Gajewski and Gärtner [13], respectively. Moreover, as far as the numerical solution by the Scharfetter-Gummel scheme is concerned, for a magnetic field of the form $\mathbf{b} = (0,0,b_z)^T$, in [13] sufficient conditions in terms of the grid geometry and the modulus of the magnetic field have been derived guaranteeing that the scheme is still dissipative and leads to positive solutions. A similar analysis can be carried out for the mixed finite element approach. Observing that for $\mathbf{b} = (0,0,b_z)^T$ the action of the magnetic field can be described by a 3×3 matrix B_α according to $\mathbf{j}_\alpha = B_\alpha \mathbf{j}_\alpha^0$,

$$B_\alpha = \left(1 + (\mu_\alpha^* b_z)^2\right)^{-1} \begin{pmatrix} 1 & -\mu_\alpha^* b_z & 0 \\ \mu_\alpha^* b_z & 1 & 0 \\ 0 & 0 & 1 + (\mu_\alpha^* b_z)^2 \end{pmatrix},$$

the mixed discretization of the continuity equation for e.g. the electron flux requires the computation of $(\mathbf{j}_h, n_h) \in RT_{0;\Gamma_N}(\Omega;\mathcal{T}_h) \times W_0(\Omega;\mathcal{T}_h)$ such that

$$\begin{aligned} &\int_\Omega \exp(-\Psi) B_n^{-1} \mathbf{j}_h \cdot \mathbf{q}_h \, dx + \int_\Omega \exp(-\Psi) \operatorname{div} \mathbf{q}_h n_h \, dx = \int_{\Gamma_D} \exp(-\Psi) n_D \nu \cdot \mathbf{q}_h \, d\sigma, \\ &\int_\Omega \operatorname{div} \mathbf{j}_h v_h \, dx - \int_\Omega R n_h v_h \, dx = \int_\Omega f v_h \, dx, \quad v_h \in W_0(\Omega;\mathcal{T}_h), \ \mathbf{q}_h \in RT_{0;\Gamma_N}(\Omega;\mathcal{T}_h). \end{aligned}$$

Then, if we perform mixed hybridization, in the process of static condensation of the discrete current densities and the discrete carrier concentrations the local Schur complement can be explicitly computed in terms of the local grid geometry and the modulus of the magnetic field. This allows to state conditions under which the M-matrix property of $-S_h$ is retained. Details will be given in a forthcoming paper.

Acknowledgments: The authors wish to thank G. Wachutka for fruitful discussions on the subject.

References

[1] D.N. Arnold and F. Brezzi, *Mixed and nonconforming finite element methods: implementation, post–processing and error estimates.* M^2AN Math. Modelling Numer. Anal. 19, 7-35 (1985)

[2] B. Bachmann, *Adaptive Mehrgitterverfahren zur Lösung der stationären Halbleitergleichungen.* Dissertation, Universität Zürich (1993)

[3] B.R. Baliga and S.V. Patankar, *A new finite-element formulation for convection-diffusion problems.* Numer. Heat Transfer 3, 393-409 (1980)

[4] R. Bank, J.F. Bürgler, W. Fichtner and R.K. Smith, *Some upwinding techniques for finite element approximations of convection-diffusion equations.* Numer. Math. 58, 185-202 (1990)

[5] F. Bornemann, B. Erdmann and Kornhuber, *Adaptive multilevel methods in three space dimensions.* Int. J. Numer. Methods Eng. 36, 3187-3203 (1993)

[6] D. Braess and R. Verfürth, *Multigrid methods for nonconforming finite element methods.* SIAM J. Numer. Anal. 27, No. 4, 979-986 (1990)

[7] F. Brezzi and M. Fortin, *Mixed and Hybrid Finite Element Methods.* Springer, Berlin–Heidelberg–New York, 1991

[8] F. Brezzi, L.D. Marini and P. Pietra, *Two dimensional exponential fitting and application to drift-diffusion models.* SIAM J. Numer. Anal. 26, 1347-1355 (1989)

[9] F. Brezzi, L.D. Marini and P. Pietra, *Numerical simulation of semiconductor devices.* Comp. Math. Appl. Mech. Eng. 75, 493-514 (1989)

[10] J.F. Bürgler, *Discretization and Grid Adaption in Semiconductor Device Modeling.* Hartung-Gorre, Konstanz, 1990

[11] B. Fraeijs de Veubeke, *Displacement and equilibrium models in the finite element method.* In: Stress Analysis, C. Zienkiewicz and G. Holister (eds.), John Wiley and Sons, New York, 1965

[12] H. Gajewski and K. Gröger, *Semiconductor equations for mobilities based on Boltzmann statistics or Fermi-Dirac statistics.* Math. Nachr. 140, 7-36 (1989)

[13] H. Gajewski and K. Gärtner, *On the discretization of van Roosbroeck's equations with magnetic field.* ETH Zürich, Integrated Systems Laboratory, Techn. Rep. No. 94/14 (1994)

[14] P.W.H. Hemker and H. Molenaar, *A multigrid approach for the solution of the 2D semiconductor equations.* IMPACT Comput. Sci. Engrg. 2, 219-243 (1990)

[15] R. Hiptmair, *Gemischte Finite-Elemente-Diskretisierung der Kontinuitätsgleichungen aus der Bauelementsimulation.* Master Thesis, Technische Universität München, 1992

[16] R. Hiptmair and R. H. W. Hoppe, *Mixed finite element discretization of continuity equations arising in semiconductor device simulation.* In: Proc. Conf. Math. Modelling and Simulation of Electrical Circuits and Devices, R.E. Bank et al. (eds.), p. 197-217 Birkhäuser, Basel, 1994

[17] R.H.W. Hoppe and B. Wohlmuth, *Adaptive multilevel techniques for mixed finite element discretizations of elliptic boundary value problems.* Submitted to SIAM J. Numer. Anal.

[18] R.H.W. Hoppe and B. Wohlmuth, *Efficient Numerical Solution of Mixed Finite Element Discretizations by Adaptive Multilevel Methods.* to appear in Apl. Mat.

[19] W. Kampowsky, P. Rentrop and W. Schmidt, *Classification and numerical simulation of electric circuits.* Surv. Math. Ind. 2, 23-65 (1992)

[20] P.A. Markowich, Chr.A. Ringhofer and Chr. Schmeiser, *Semiconductor Equations.* Springer, Berlin-Heidelberg-New York, 1990

[21] F. Montrone, *The method of Baliga-Patankar in 3D device simulation.* In: Proc. Conf. Math. Modelling and Simulation of Electrical Circuits and Devices, R.E. Bank et al. (eds.), p. 251-265 Birkhäuser, Basel, 1994

[22] R.R.P. van Nooyen, *Some aspects of mixed finite element methods for semiconductor simulation.* Ph.D. Thesis, University of Amsterdam, 1992

[23] M. Paffrath, W. Jacobs, W. Klein, E. Rank, K. Steger, U. Weinert and U. Wever, *Concepts and algorithms in process simulation.* Surv. Math. Ind. 3, 149-183 (1993)

[24] A. Reusken, *Multigrid applied to mixed finite elements schemes for current continuity equations.* Preprint, Technical University Eindhoven (1990)

[25] C. Riccobene, G. Wachutka, J.F. Bürgler and H. Baltes, *Two-dimensional numerical modeling of dual-collector magnetotransistors: evidence for emitter efficiency modulation.* Sensors and Actuators A, 31, 210-214 (1992)

[26] C. Riccobene, G. Wachutka, J.F. Bürgler and H. Baltes, *Operating principle of dual collector magnetotransistors studied by two-dimensional simulation.* IEEE Trans. Electron Devices ED-41, 32-43 (1994)

[27] D.L. Scharfetter and H.K. Gummel, *Large-signal analysis of a silicon read diode oscillator.* IEEE Trans Electron Devices ED-16, 64-77 (1969)

[28] S. Selberherr, *Analysis and Simulation of Semiconductor Devices.* Springer, Berlin-Heidelberg-New York, 1984

[29] N. Shigyo, T. Wada and S. Yasuda, *Discretization problem for multidimensional current flow.* IEEE Trans. CAD, CAD-8, 1046-1050 (1989)

[30] G. Wachutka, *Unified framework fir thermal, electrical, magnetic and optical semiconductor device modeling.* COMPEL 10, 311-321 (1991)

[31] G. Wachutka, *Problem-oriented modeling of microtransducers: state of the art and future challenges.* Sensors and Actuators A, 41-42, 279-283 (1994)