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Final Report for AFOSR Grant Nbr. WH-85<sup>2</sup>240

'Mathematical Models for VLSI Device Simulation'

Principal Investigator: Christian Ringhofer

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### 1. Introduction

The research supported under this grant was concerned with analytical and numerical investigations on the basic semiconductor equations.

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	$\Im_{p} = -\Im_{p} \nabla_{p} - \mu_{p} p \nabla_{\psi}$

The research, as outlined in the original proposal, was grouped into two areas, an analysis of the mathematical structure of solutions via a singular perturbation approach, and the development of numerical methods for the transient problem. The analytical part was divided into several subcategories. First, the transient problem was analyzed in the case when the mobilities were only functions of position. Then velocity saturation effects were included so the more complicated case, when the mobilities depend on the electric field, was treated. This was done for one-dimensional problems first and later on extended to the two-dimensional case. In the numerical part difference schemes were developed which incorporate the information, obtained in the first part, about the structure of the inverse constructs. Later on, the stability properties of these schemes were analyzed in the schemes the general progress in the area before explaining these to construct the more detail.

## 2. General Progress

Several results have been published in the last two years regarding the existence of solutions and the validity of the singular perturbation approach in the steady state case. In [7] the existence of solutions to the time dependent problem has been shown. In [1] the convergence of the solution to that of the steady state problem has been proven in the one-dimensional case and convergence rates have been derived. In [6] this has been extended to the multidimensional case. Since this result is derived using Schauder arguments, however, it does not provide convergence rates. A singular perturbation approach of a slightly different flavor has been introduced in [3], [4]. It is suited for reverse biased devices and allows the calculation of the boundary of the charge free region via the solution of an obstacle problem. In [2] a difference method for the transient problem has been developed which has features simular to the one developed under this contract (i.e., second order and L-stable).

#### 3. Achievements and Publications

# Analysis:

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In [A] and [B] the proposed asymptotic analysis has been carried out in the case of one space dimension and field independent mobilities. While in [A] a symmetry assumption had been made, which simplified the analysis, [B] deals with the more practical case of a strongly asymmetric doping concentration. In [C] the mobilities have been made dependent on the field in the usual way such that the velocities  $\mu_n \nabla \psi$ ,  $\mu_p \nabla \psi$  'saturate' (approach a limit) for  $|\nabla \psi| + \infty$ . This causes some technical difficulties in the derivation of the asymptotic expansions and introduces an additional time scale, which lies in between the diffusion time and the dielectric relaxation time. Numerical experiments have confirmed the presence of this timescale. In [D] this analysis has been extended to the two-dimensional model of an MOS transistor. Existence proofs for the solutions of the reduced problem have been given in the case of reverse biased or very moderately forward biased devices. It should be pointed out that in the case of field dependent mobilities the layer equations fail to have a solution if the currents become too large.

### Numerical Methods:

As a first step, in order to justify the use of standard methods like backward differences (BDF), the linearized eigenvalue problem has been analyzed in (E). Extending previous results by Mock, it has been shown that eigenvalues can have positive real parts away from steady states. These real parts are bounded from above, however, by moderate quantities proportional to the size of the currents. Using this, one immediately can derive stepsize criteria for BDF methods which guarantee linearized Von Neumann stability. In [F] and [C] a time

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differencing scheme has been introduced and analyzed which exploits the special structure of the stiffness of the basic semiconductor equations. Similar to the method developed in [2] it is L-stable and of second order as long as the timesteps are much larger than the dielectric relaxation time. However, in contrast with the method in [2], it requires the solution of only one nonlinear system per timestep. The task of performing a nonlinear stability and convergence analysis of this method has proven too difficult so far. However, using the analysis of E a linearized stability analysis has been performed. Although not directly related to the subject of this grant, the first steps have been carried out in [H] to develop a new decoupled iterative method for the solution of the nonlinear systems arising from the discretization of the basic semiconductor equations. The underlying concept is to extend Gummel's method in the framework of approximate Newton methods using singular perturbation ideas to approximate the Jacobian. In [H] numerical experiments have been performed with the simplest version of this concept. They show a significant improvement over the convergence properties of Gummel's method for unipolar devices.

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### 4. Conferences Attended

 'International Conference on Computational Methods in Applied Science', Paris, France, December 1985.

Title of talk: 'Numerical Methods for the Tansient Semiconductor Device Equations', (invited).

- (2) 'Conference on Semiconductor Devices and Processes', Swansea, UK, July 1986.
- (3) IEEE conference on 'Numerical Analysis of Processes and Devices', Santa Clara, November 1986.

Title of talk: 'An Improved Decoupling Algorithm for Unipolar Device Simulation'.

(4) AMS summer seminar on 'Mathematical Methods in VLSI', Minneapolis, April 1987.

Title of talk: 'The Shape of Solutions of the Semiconductor Device Equations', (invited).

(5) 'International Conference on Industrial and Applied Mathematics', Paris, France, June 1987.

Title of talk: 'Simulation of Tunneling Effects in Semiconductors'.

### 5. Papers Published Under This Grant

- [A] "An Asymptotic Analysis of a Transient P-N Junction Model", SIAM J. App. Math. Vol. 147 Nr. 3, pp. 624-642 (1987).
- [B] "A Singular Perturbation Analysis for An Asymmetric Diode" to apear in IMA J. Appl. Math., jointly with P. Markowich and C. Schmeiser.
- [C] "A Singular Perturbation Analysis for the Transient Semiconductor Device Equations in One Space Dimension", to appear in IMA J. Appl. Math.
- [D] "The Shape of Solutions to the Basic Semiconductor Device Equations", to appear in "Lectures in Applied Mathematics."
- [E] "Stability for the Transient Semiconductor Device Equations" Zeitschrift Fuer Angewandte Mahtematik und Mechanik (ZAMM) 67, Nr. 7, 319-332, (1987), jointly with P. Markowich.
- [F] "Difference Methods for Transient Device Simulation", in Computational Methods in Applied Science" R. Glowinski ed. (1986).
- [G] "A Second Order Difference Method for Transient Semiconductor Device Simulation," to appear in Trans. Com. Sim.
- [H] "An Improved Gummel Algorithm for the Semiconductor Device Equations," to appear in IEEE Trans. on CAD, jointly with D. Schmeiser.

# 6. References

- Alabeau, F.: 'Asymptotic Analysis of the Semiconductor Equations', preprint, INRIA.
- [2] Bank, R. E., et al.: 'Transient Simulation of Silicon Devices and Circuits', IEEE Trans. Electr. Dev. Ed. 32 Nr. 10, pp. 1992-2007, 1985.
- [3] Brezzi, F., Marini, D.: 'A Singular Perturbation Analysis for the Basic Semiconductor Equations', Proc. 'International Conference on Computational Methods in Applied Science', R. Glowinski, ed., North Holland, 1986.
- [4] Cafarelli, L., Friedman, A.: 'A Singular Perturbation Problem for Semiconductors', preprint.
- [5] Haensch, W.: 'Carrier Transport in Semiconductor Devices of Very Small Dimensions', Proc. 'Two-Dimensional Systems: Physics and Devices', Mauterndorf, FRG, 1986.
- [6] Henry, J., Louro, B.: 'Singular Perturbation Theory Applied to Electrochemistry Equations', preprint, INRIA.
- Seidman, T.: 'Time Dependent Solution of a Nonlinear System Arising in Semiconductor Theory', Nonlinear Analysis, Theory, Meth. and Appl., Vol. 10, #5, pp. 491-502 (1986).

