Lecture Notes in Mathematics

1823

Editors: J.–M. Morel, Cachan F. Takens, Groningen B. Teissier, Paris

Subseries: Fondazione C.I.M.E., Firenze Adviser: Pietro Zecca

Springer Berlin

Berlin Heidelberg New York Hong Kong London Milan Paris Tokyo A. M. Anile W. Allegretto C. Ringhofer

Mathematical Problems in Semiconductor Physics

Lectures given at the C.I.M.E. Summer School held in Cetraro, Italy, July 15-22, 1998

With the collaboration of G. Mascali and V. Romano

Editor: A. M. Anile







Authors and Editors

Angelo Marcello Anile Dipartimento di Matematica Università di Catania Viale A. Doria 6 95125 Catania, Italy *e-mail: anile@dmi.unict.it*

Walter Allegretto Department of Mathematical and Statistical Sciences Alberta University Edmonton AB T6G 2G1 Canada

 $e\mbox{-mail: retl} @retl.math.ualberta.ca$

Christian Ringhofer Department of Mathematics Arizona State University Tempe, Arizona 85287-1804, USA

e-mail: ringhofer@asu.edu

Cataloging-in-Publication Data applied for

Bibliographic information published by Die Deutsche Bibliothek

Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the Internet at http://dnb.ddb.de

Mathematics Subject Classification (2000): 82D37, 80A17, 65Z05

ISSN 0075-8434 ISBN 3-540-40802-9 Springer-Verlag Berlin Heidelberg New York

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer-Verlag. Violations are liable for prosecution under the German Copyright Law.

Springer-Verlag Berlin Heidelberg New York a member of BertelsmannSpringer Science + Business Media GmbH

springer.de

© Springer-Verlag Berlin Heidelberg 2003 Printed in Germany

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Typesetting: Camera-ready TEX output by the authors

SPIN: 10952481 41/3142/du - 543210 - Printed on acid-free paper

Preface

The increasing demand on ultra miniturized electronic devices for ever improving performances has led to the necessity of a deep and detailed understanding of the mathematical theory of charge transport in semiconductors. Because of their very short dimensions of charge transport, these devices must be described in terms of the semiclassical Boltzmann equation coupled with the Poisson equation (or some phenomenological consequences of these equations) because the standard approach, which is based on the celebrated driftdiffusion equations, leads to very inaccurate results whenever the dimensions of the devices approach the carrier mean free path.

In some cases, such as for very abrupt heterojunctions in which tunneling occurs it is even necessary to resort to quantum transport models (e.g. the Wigner-Boltzmann-Poisson system or equivalent descriptions).

These sophisticated physical models require an appropriate mathematical framework for a proper understanding of their mathematical structure as well as for the correct choice of the numerical algorithms employed for computational simulations.

The resulting mathematical problems have a broad spectrum of theoretical and practical conceptually interesting aspects.

From the theoretical point of view, it is of paramount interest to investigate wellposedness problems for the semiclassical Boltzmann equation (and also for the quantum transport equation, although this is a much more difficult case). Another problem of fundamental interest is that of the hydrodynamical limit which one expects to be quite different from the Navier-Stokes-Fourier one, since the collision operator is substantially different from the one in rarefied gas case.

From the application viewpoint it is of great practical importance to study efficient numerical algorithms for the numerical solution of the semiclassical Boltzmann transport equation (e.g spherical harmonics expansions, Monte Carlo method, method of moments, etc.) because such investigations could have a great impact on the performance of industrial simulation codes for TCAD (Technology Computer Aided Design) in the microelectronics industry.

The CIME summer course entitled **MATHEMATICAL PROBLEMS IN SEMICONDUCTOR PHYSICS** dealt with this and related questions. It was addressed to researchers (either PhD students, young post-docs or mature researchers from other areas of applied mathematics) with a strong interest in a deep involvement in the mathematical aspects of the theory of carrier transport in semiconductor devices.

The course took place in the period 15-22 July 1998 on the premises of the Grand Hotel San Michele di Cetraro (Cosenza), located at a beach of astounding beauty in the Magna Graecia part of southern Italy. The Hotel facilities were more than adequate for an optimal functioning of the course. About 50 "students", mainly from various parts of Europe, participated in the course. At the end of the course, in the period 23-24 July 1998, a related workshop of the European Union TMR (Training and Mobility of Researchers) on "Asymptotic Methods in Kinetic Theory" was held in the same place and several of the participants stayed for both meetings. Furthermore the CIME course was considered by the TMR as one of the regular training schools for the young researchers belonging to the network.

The course developed as follows:

- W. Allegretto delivered 6 lectures on analytical and numerical problems for the drift-diffusion equations and also on some recent results concerning the electrothermal model. In particular he highlighted the relationship with integrated sensor modeling and the relevant industrial applications, inducing a considerable interest in the audience.
- F. Poupaud delivered 6 lectures on the rigorous derivation of the quantum transport equation in semiconductors, utilizing recent developments on Wigner measures introduced by Gérard, in order to obtain the semiclassical limit. His lectures, in the French style of pure mathematics, were very clear, comprehensive and of advanced formal rigour. The lectures were particularly helpful to the young researchers with a strong background in Analysis because they highlighted the analytical problems arising from the rigorous treatment of the semiclassical limit.
- C. Ringhofer delivered 6 lectures which consisted of an overview of the state of the art on the models and methods developed in order to study the semiclassical Boltzmann equation for simulating semiconductor devices. He started his lectures by recalling the fundamentals of semiconductor physics then introduced the methods of asymptotic analysis in order to obtain a hierarchy of models, including: drift-diffusion equations, energy transport equations, hydrodynamical models (both classical and quantum), spherical harmonics and other kinds of expansions. His lectures provided comprehensive review of the modeling aspects of carrier transport in semiconductors.

d) D. Levermore delivered 6 lectures on the mathematical foundations and applications of the moment methods. He presented in detail and depth the concepts of exponential closures and of the principle of maximum entropy. In his lectures he gave several physical examples of great interest arising from rarefied gas dynamics, and pointed out how the method could also be applied to the semiclassical Boltzmann equation. He highlighted the relationships between the method of moments and the mathematical theory of hyperbolic systems of conservation laws.

During the course several seminars on specialized topics were given by leading specialists. Of particular interest were these of P. Markowich (co-director of the course) on the asymptotic limit for strong fieds, of P. Pietra on the numerical solution of the quantum hydrodynamical model, of A. Jungel on the entropy formulation of the energy transport model, of O. Muscato on the Monte Carlo validation of hydrodynamical models, of C. Schmeiser on extended moment methods, of A. Arnold on the Wigner-Poisson system, and of A. Marrocco on the mixed finite element discretization of the energy transport model.

A. M. Anile

CIME's activity is supported by:

Ministero dell'Università Ricerca Scientifica e Tecnologica; Consiglio Nazionale delle Ricerche; E.U. under the Training and Mobility of Researchers Programme.

Contents

Recent Developments in Hydrodynamical Modeling of Semiconductors

| Α. | M. | Anile, G. Mascali and V. Romano | 1 |
|----|-----------------|---|----|
| 1 | Intr | oduction | 1 |
| 2 | Gen | eral Transport Properties in Semiconductors | 2 |
| 3 | H-T | heorem and the Null Space of the Collision Operator | 5 |
| 4 | roscopic Models | 7 | |
| | 4.1 | Moment Equations | 7 |
| | 4.2 | The Maximum Entropy Principle | 8 |
| 5 | App | lication of MEP to Silicon | 11 |
| | 5.1 | Collision Term in Silicon | 11 |
| | 5.2 | Balance Equations and Closure Relations | 13 |
| | 5.3 | Simulations in Bulk Silicon | 15 |
| | 5.4 | Simulation of a $n^+ - n - n^+$ Silicon Diode | 21 |
| | 5.5 | Simulation of a Silicon MESFET | 26 |
| 6 | App | lication of MEP to GaAs | 34 |
| | 6.1 | Collision Term in GaAs | 34 |
| | 6.2 | Balance Equations and Closure Relations | 36 |
| | 6.3 | Simulations in Bulk GaAs. | 38 |
| | 6.4 | Simulation a GaAs $n^+ - n - n^+$ Diode | 43 |
| | 6.5 | Gunn Oscillations | 45 |
| Re | eferer | nces | 54 |
| _ | | | |
| D | rift-l | Diffusion Equations and Applications | |
| W | . All | egretto | 57 |
| 1 | The | Classical Semiconductor Drift-Diffusion System | 57 |
| | 11 | Derivation | 57 |

| | 1.1 | Derivation | 97 |
|---|-----|-------------------------------|----|
| | 1.2 | Existence | 58 |
| | 1.3 | Uniqueness and Asymptotics | 63 |
| 2 | Ot | her Drift-Diffusion Equations | 66 |
| | 2.1 | Small Devices | 66 |

| 70 70 |
|----------|
| 70 |
| 10 |
| 70 |
| 73 |
| |
| 74 |
| 80 |
| 82 |
| 89 |
| |

Kinetic and Gas – Dynamic Models for Semiconductor Transport

| Christian Ringhofer |)7 | | |
|--|----|--|--|
| 1 Multi-Body Equations and Effective Single Electron Models | 98 | | |
| 1.1 Effective Single Particle Models – The BBGKY Hierarchy 10 |)1 | | |
| 1.2 The Relation Between Classical and Quantum Mechanical Models10 |)4 | | |
| 2 Collisions and the Boltzmann Equation |)7 | | |
| 3 Diffusion Approximations to Kinetic Equations | 1 | | |
| 3.1 Diffusion Limits: The Hilbert Expansion | 3 | | |
| 3.2 The Drift Diffusion Equations: | 4 | | |
| 3.3 The Energy Equations: | 5 | | |
| 3.4 The Energy Transport – or SHE Model | .6 | | |
| 3.5 Parabolicity | 8 | | |
| 4 Moment Methods and Hydrodynamic Models | 20 | | |
| References | | | |
| | | | |