

Physical Models of Semiconductor Quantum Devices

Ying Fu

Physical Models of Semiconductor Quantum Devices

Second Edition

 Springer

Ying Fu
Royal Institute of Technology
Stockholm, Sweden

ISBN 978-94-007-7173-4

ISBN 978-94-007-7174-1 (eBook)

DOI 10.1007/978-94-007-7174-1

Springer Dordrecht Heidelberg New York London

Library of Congress Control Number: 2013946430

© Springer Science+Business Media Dordrecht 1999, 2014

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law.

The use of general descriptive names, registered names, trademarks, service marks, 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.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

The history of technology development is epitomized in Moore's law. Industrial deep-submicron and laboratorial nanometer process technologies have already been fabricating electronic and optical components containing only a few active electrons, and the geometrical sizes of these components are comparable with the characteristic wavelength of the electrons. However, the advanced multimedia infrastructure and service in the future demand further developments in the chip's capability.

Photonic integrated circuits (PICs) are currently orders of magnitude larger in physical dimensions than their microelectronic counterparts. Field-effect-type transistors have reached lengths on the order of 50 nm, while in contrast, passive optical devices, also those based on photonic crystals, have sizes on the order of one photon wavelength. The sizes of active devices are even larger, essentially depending on the matrix element of the interaction. In order to pursue the steady increase in integration density in photonics such that it rivals the microelectronic footprint size, nanostructure-based high index of refraction and metallic behavior (negative epsilon) are two mostly studied fundamental issues to shrink optical component sizes and to tackle the sub-wavelength limit.

Nanotechnology has been named as one of the most important areas of forthcoming technology because they promise to form the basis of future generations of electronic and optoelectronic devices. From the point view of technical physics, all these developments greatly reduce the geometric sizes of devices, and thus the number of active electrons in the system. Quantum mechanical considerations about electronic states, electron transports and various scattering processes including light-matter interaction, are thus crucial. However, the theoretical study is extremely difficult. My first numerical simulation work about a three-dimensional energy band structure calculation in 1995 took more than 6 months to complete for one bias-configuration of a nanoscale metal-oxide-semiconductor field-effect transistor (MOSFET). With today's computation workstations the CPU time is reduced to be less than 24 hours.

In general, today's experimental and theoretical works are very much separated. The laboratory works are still largely based on try-and-error, while the theoretical models are over simplified as compared with the complexity of real devices. Ideally to be cost effective, experimental and theoretical works are to be coordinated in

such a complementary way that we try to analyze and understand the experimental results, then use the understanding to guide further experimental works, which in their turn serve as the feedback to modify and improve the theoretical model. By this, we expect an optimized device and a valid as well as effective theoretical device model.

The main purpose of the book is to discuss electrons and photons in and through nanostructures by the first-principles quantum mechanical theories and fundamental concepts (a unified coverage of nanostructured electronic and optical components) behind nano-electronics and optoelectronics, the material basis, physical phenomena, device physics, as well as designs and applications. The combination of viewpoints presented within the book can help to foster further research and cross-disciplinary interaction needed to surmount the barriers facing future generations of technology design.

Many specific technologies are presented, including quantum electronic devices, resonant tunneling devices, single electron devices, heterostructure bipolar transistors (HBTs) and high electron mobility transistors (HEMTs), detectors, and infrared sensors, lasers, optical modulators. It contains essential and detailed information about the state-of-the-art theories, methodologies, the way of working and real case studies, helping students and researchers to appreciate the current status and future potential of nanotechnology as applied to the electronics and optoelectronics industry.

In nanophotonics we will concentrate on local electromagnetic interactions between nanometric objects and optical fields (non-linear optics in nano- and microstructured photonic crystals) at the level of systems of nanostructures, into larger density on interfaces, which in turn leads to intriguing collective effects, such as plasmonics or multiple reflection and refraction phenomena.

The major task here is that the system at working condition is no longer static. Rather, it can only properly be described by including dynamic Maxwell and time-dependent Schrödinger equations. Furthermore, because the numbers of atoms and electrons in the real devices are huge, while the quantum mechanical Monte Carlo simulation requires too much computer memory and computer time, we will introduce top-down and bottom-up numerical ways that fundamentally we emphasize the quantum mechanical Monte Carlo simulation, while at the same time, we apply the large-system (cluster) tight-binding numerical method to study the device performance property (where the input parameters in the tight-binding method come from the study of bridging nano to micro scales).

Finally we will examine the processing—structure relationship. The state of nanostructures during the period that one monolayer exists—before being buried in the next layer—determines the ultimate structure of the nanostructure, and thus its properties. This part of the book takes into consideration the following potential influencing factors in solid-state growth techniques such as metalorganic vapour phase epitaxy (MOVPE): crystal defects, void structure, grain structure, interface structure in epitaxial films, reaction-induced structure, strain-induced self-formed quantum dot structures, through the use of MOVPE to produce quantum structured semiconductors.

This book provides a solid foundation for the understanding, design, and simulation of nano-electronic and optoelectronics devices. It will be of interest to researchers and specialists in the field of solid state technology, electronics and optoelectronics. It can also serve as a textbook for graduate students and new entrants in the exciting field. This book takes the reader from the introductory stage to the advanced level of the construction, principles of operation, and application of these devices, and puts readers immediately in a position to take their first steps in the field of computational nano-engineering and design. Results and conclusions of detailed nano-engineering studies are presented in an instructive style. Numerous references, illustrations, basic computation subroutines provide further support in this fast-emerging field. This book is designed as a self-contained introduction to both the understanding and solution of theoretical and practical design problems in nano devices.

Stockholm, Sweden
May 2013

Ying Fu

Contents

1	Semiconductor Materials	1
1.1	Atoms and Solids	3
1.2	Bulk and Epitaxial Crystal Growth	14
1.3	Bloch Theorem of Electrons in Solids	19
1.4	sp^3s^* Tight-Binding Model	21
1.5	Bandedge States	27
1.6	Eight-Band $k \cdot p$ Model	33
1.7	Strain Field in Nanostructures	40
1.8	Heterostructure Material and Envelope Function	49
1.9	Dimensionality and Density of States	56
	References	62
2	Electron Transport	67
2.1	Quantum Mechanical Wave Transport	67
2.2	Scattering Theory	73
2.3	Time-Dependent Perturbation	82
2.4	Acceleration Theorems	84
2.5	Impurities and Fermi Level of Doped Semiconductor	89
2.6	Boltzmann Equation	97
2.7	Drift, Diffusion and Ballistic Transport	100
2.8	Carrier Scatterings	103
2.8.1	Phonon Scattering	103
2.8.2	Carrier-Carrier Interaction	109
2.8.3	Impurity Scattering	110
	References	110
3	Optical Properties of Semiconductors	111
3.1	Electromagnetic Field	111
3.2	Electron in Electromagnetic Field	118
3.3	Optical Spectrum of Nanostructure	126
3.4	Exciton and Its Optical Properties	134

3.5	Exciton in Quantum Well	142
3.6	Colloidal Quantum Dot	146
3.7	Exciton Polariton	157
3.8	Multiphoton Process	168
3.9	Auger Recombination and Impact Ionization	174
	References	181
4	Electronic Quantum Devices	185
4.1	$p - n$ Junction and Field-Effect Transistor	185
4.2	Semiclassical vs Quantum Considerations	191
4.3	Resonant Tunneling Diode	193
4.3.1	$I - V$ Characteristics at Steady State	196
4.3.2	Response to a Time-Dependent Perturbation	203
4.3.3	Phonon-Assisted Tunneling	207
4.4	Heterostructure Barrier Varactor	213
4.4.1	Conduction Current	216
4.4.2	$C - V$ Characteristics	218
4.5	High-Electron-Mobility Transistor	224
4.5.1	Remote Impurity Scattering	226
4.5.2	δ -Doped Field-Effect Transistor	230
4.6	Nano-scale Field-Effect Transistor	233
4.6.1	Wave Characteristics and Threshold Voltage	234
4.6.2	Steady-State Wave Transport	238
4.6.3	Interface Roughness	246
4.6.4	Time-Dependent Wave Packet Transmission	249
4.6.5	Nanometer MOSFET Architectures	253
4.7	Coulombic Blockade and Single-Electron Transistor	257
4.8	Future Perspectives	261
4.8.1	Carbon Nanotubes	261
4.8.2	Molecular Devices	262
4.8.3	Metallic Devices	262
4.8.4	Ferromagnetic Devices	263
	References	263
5	Nanostructured Optoelectronics	271
5.1	Optical Transition and Quantum Selection Rule	271
5.2	Intraband Optical Transition	275
5.3	Optical Grating and Crosstalk	289
5.4	Nanostructure Infrared Photodetector	302
5.4.1	Quantum Well Infrared Photodetector	302
5.4.2	Quantum Wire Infrared Photodetector	307
5.4.3	Quantum Dot Infrared Photodetector	308
5.5	SiGe Heterostructure Internal Emission Infrared Photodetector	313
5.6	Quantum Dot Solar Cell	316
5.7	Exciton-Polariton Photonic Crystal	323
5.8	Resonant Tunneling Light Emitting Diode	335

- 5.9 Nanostructure Laser 342
- 5.10 Light Emission from Highly Strained $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{GaAs}$
 - Quantum Wells by Dipole δ Doping 345
- 5.11 Quantum Dot Biomarker 348
- References 350
- 6 Numerical Recipes 353**
 - 6.1 Fermi-Dirac Integral 353
 - 6.2 Amplitude of Transmitted Wave 356
 - 6.3 Localized State 366
 - 6.4 Local Density of States: Recursion Method 368
 - 6.5 Time-Dependent Wave Packet Transmission 377
 - References 380
- Appendix A Fundamental Constants 381**
- Appendix B Quantum Physics 383**
 - B.1 Black Body Radiation 383
 - B.2 The Compton Effect 383
 - B.3 Electron Diffraction 384
 - B.4 Operators in Quantum Physics 384
 - B.5 The Schrödinger Equation 384
 - B.6 The Uncertainty Principle 386
 - B.7 Parity 386
 - B.8 The Tunneling Effect 387
 - B.9 Harmonic Oscillator 388
 - B.10 Angular Momentum and Spin 388
 - B.11 Hydrogen Atom 390
 - B.12 Interaction with Electromagnetic Fields 391
 - B.13 Time-Independent Perturbation Theory 391
 - B.14 Time-Dependent Perturbation Theory 392
 - B.15 N -Particle System 392
 - B.16 Quantum Statistics 393
- Appendix C Electricity & Magnetism 395**
 - C.1 The Maxwell Equations 395
 - C.2 Force and Potential 396
 - C.3 Electromagnetic Waves 396
- Appendix D Solid State Physics 399**
 - D.1 Crystal Structure 399
 - D.2 Crystal Binding 400
 - D.3 Crystal Vibrations 400
 - D.4 Free Electron Fermi Gas 401
 - D.4.1 Thermal Heat Capacity 401
 - D.4.2 Electric Conductance 402
 - D.5 Energy Bands 402
- Index 405**