

## Optoelectronic Devices

### Design, Modeling, and Simulation

With a clear application focus, this book explores optoelectronic device design and modeling through physics models and systematic numerical analysis.

By obtaining solutions directly from the physics-based governing equations through numerical techniques, the author shows how to design new devices and how to enhance the performance of existing devices. Semiconductor-based optoelectronic devices such as semiconductor laser diodes, electro-absorption modulators, semiconductor optical amplifiers, superluminescent light-emitting diodes and their integrations are all covered.

Including step-by-step practical design and simulation examples, together with detailed numerical algorithms, this book provides researchers, device designers, and graduate students in optoelectronics with the numerical techniques to solve their own structures.

**Xun Li** is a Professor in the Department of Electrical and Computer Engineering at McMaster University, Hamilton. Since receiving his Ph.D. from Beijing Jiaotong University in 1988, he has authored and co-authored over 160 technical papers and co-founded Apollo Photonics, Inc., developing one of the company's major software products, "Advanced Laser Diode Simulator". He is a Member of the OSA and SPIE, and a Senior Member of the IEEE.

# Optoelectronic Devices

## Design, Modeling, and Simulation

XUN LI

Department of Electrical and Computer Engineering  
McMaster University  
Hamilton, Ontario



CAMBRIDGE  
UNIVERSITY PRESS

Cambridge University Press  
978-0-521-87510-3 — Optoelectronic Devices  
Xun Li  
Frontmatter  
[More Information](#)

---

## CAMBRIDGE UNIVERSITY PRESS

University Printing House, Cambridge CB2 8BS, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314-321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi - 110025, India

103 Penang Road, #05-06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of the University of Cambridge.

It furthers the University's mission by disseminating knowledge in the pursuit of education, learning and research at the highest international levels of excellence.

[www.cambridge.org](http://www.cambridge.org)

Information on this title: [www.cambridge.org/9780521875103](http://www.cambridge.org/9780521875103)

© Cambridge University Press 2009

This publication is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2009

*A catalogue record for this publication is available from the British Library*

ISBN 978-0-521-87510-3 Hardback

Cambridge University Press has no responsibility for the persistence or accuracy of URLs for external or third-party internet websites referred to in this publication, and does not guarantee that any content on such websites is, or will remain, accurate or appropriate.

Contents

|   |                                                                                         |                |
|---|-----------------------------------------------------------------------------------------|----------------|
|   | <i>Preface</i>                                                                          | <i>page xi</i> |
| 1 | <b>Introduction</b>                                                                     | 1              |
|   | 1.1 The underlying physics in device operation                                          | 1              |
|   | 1.2 Modeling and simulation methodologies                                               | 1              |
|   | 1.3 Device modeling aspects                                                             | 3              |
|   | 1.4 Device modeling techniques                                                          | 3              |
|   | 1.5 Overview                                                                            | 5              |
| 2 | <b>Optical models</b>                                                                   | 6              |
|   | 2.1 The wave equation in active media                                                   | 6              |
|   | 2.1.1 Maxwell equations                                                                 | 6              |
|   | 2.1.2 The wave equation                                                                 | 8              |
|   | 2.2 The reduced wave equation in the time domain                                        | 9              |
|   | 2.3 The reduced wave equation in the space domain                                       | 11             |
|   | 2.4 The reduced wave equation in both time and space domains – the traveling wave model | 12             |
|   | 2.4.1 The wave equation in fully confined structures                                    | 12             |
|   | 2.4.2 The wave equation in partially confined structures                                | 17             |
|   | 2.4.3 The wave equation in periodically corrugated structures                           | 21             |
|   | 2.5 Broadband optical traveling wave models                                             | 31             |
|   | 2.5.1 The direct convolution model                                                      | 32             |
|   | 2.5.2 The effective Bloch equation model                                                | 34             |
|   | 2.5.3 The wavelength slicing model                                                      | 37             |
|   | 2.6 Separation of spatial and temporal dependences – the standing wave model            | 40             |
|   | 2.7 Photon rate and phase equations – the behavior model                                | 47             |
|   | 2.8 The spontaneous emission noise treatment                                            | 48             |
| 3 | <b>Material model I: Semiconductor band structures</b>                                  | 54             |
|   | 3.1 Single electron in bulk semiconductors                                              | 54             |
|   | 3.1.1 The Schrödinger equation and Hamiltonian operator                                 | 54             |
|   | 3.1.2 Bloch’s theorem and band structure                                                | 57             |

|          |                                                                       |            |
|----------|-----------------------------------------------------------------------|------------|
| vi       | <b>Contents</b>                                                       |            |
|          |                                                                       |            |
|          | 3.1.3 Solution at $\vec{k} = 0$ : Kane's model                        | 65         |
|          | 3.1.4 Solution at $\vec{k} \neq 0$ : Luttinger–Kohn's model           | 71         |
|          | 3.1.5 Solution under $4 \times 4$ Hamiltonian and axial approximation | 76         |
|          | 3.1.6 Hamiltonians for different semiconductors                       | 80         |
|          | 3.2 Single electron in semiconductor quantum well structures          | 80         |
|          | 3.2.1 The effective mass theory and governing equation                | 80         |
|          | 3.2.2 Conduction band (without degeneracy)                            | 84         |
|          | 3.2.3 Valence band (with degeneracy)                                  | 85         |
|          | 3.2.4 Quantum well band structures                                    | 87         |
|          | 3.3 Single electron in strained layer structures                      | 91         |
|          | 3.3.1 A general approach                                              | 91         |
|          | 3.3.2 Strained bulk semiconductors                                    | 93         |
|          | 3.3.3 Strained layer quantum well structures                          | 95         |
|          | 3.3.4 Semiconductors with the zinc blende structure                   | 96         |
|          | 3.4 Summary of the k–p theory                                         | 98         |
| <b>4</b> | <b>Material model II: Optical gain</b>                                | <b>102</b> |
|          | 4.1 A comprehensive model with many-body effect                       | 102        |
|          | 4.1.1 Introduction                                                    | 102        |
|          | 4.1.2 The Heisenberg equation                                         | 103        |
|          | 4.1.3 A comprehensive model                                           | 104        |
|          | 4.1.4 General governing equations                                     | 109        |
|          | 4.2 The free-carrier model as a zeroth order solution                 | 122        |
|          | 4.2.1 The free-carrier model                                          | 122        |
|          | 4.2.2 The carrier rate equation                                       | 123        |
|          | 4.2.3 The polariton rate equation                                     | 126        |
|          | 4.2.4 The susceptibility                                              | 127        |
|          | 4.3 The screened Coulomb interaction model as a first order solution  | 128        |
|          | 4.3.1 The screened Coulomb interaction model                          | 128        |
|          | 4.3.2 The screened Coulomb potential                                  | 129        |
|          | 4.3.3 Solution under zero injection and the exciton absorption        | 133        |
|          | 4.3.4 Solution under arbitrary injection                              | 137        |
|          | 4.4 The many-body correlation model as a second order solution        | 140        |
|          | 4.4.1 The many-body correlation model                                 | 140        |
|          | 4.4.2 A semi-analytical solution                                      | 141        |
|          | 4.4.3 The full numerical solution                                     | 144        |
| <b>5</b> | <b>Carrier transport and thermal diffusion models</b>                 | <b>151</b> |
|          | 5.1 The carrier transport model                                       | 151        |
|          | 5.1.1 Poisson and carrier continuity equations                        | 151        |
|          | 5.1.2 The drift and diffusion model for a non-active region           | 152        |
|          | 5.1.3 The carrier transport model for the active region               | 154        |
|          | 5.1.4 Simplifications of the carrier transport model                  | 158        |

|          | Contents                                                                         | vii        |
|----------|----------------------------------------------------------------------------------|------------|
| 5.1.5    | The free-carrier transport model                                                 | 160        |
| 5.1.6    | Recombination rates                                                              | 162        |
| 5.2      | The carrier rate equation model                                                  | 164        |
| 5.3      | The thermal diffusion model                                                      | 165        |
| 5.3.1    | The classical thermal diffusion model                                            | 165        |
| 5.3.2    | A one-dimensional thermal diffusion model                                        | 168        |
| <b>6</b> | <b>Solution techniques for optical equations</b>                                 | <b>172</b> |
| 6.1      | The optical mode in the cross-sectional area                                     | 172        |
| 6.2      | Traveling wave equations                                                         | 173        |
| 6.2.1    | The finite difference method                                                     | 173        |
| 6.2.2    | The split-step method                                                            | 183        |
| 6.2.3    | Time domain convolution through the digital filter                               | 188        |
| 6.3      | Standing wave equations                                                          | 191        |
| <b>7</b> | <b>Solution techniques for material gain equations</b>                           | <b>200</b> |
| 7.1      | Single electron band structures                                                  | 200        |
| 7.2      | Material gain calculations                                                       | 200        |
| 7.2.1    | The free-carrier gain model                                                      | 200        |
| 7.2.2    | The screened Coulomb interaction gain model                                      | 205        |
| 7.2.3    | The many-body gain model                                                         | 205        |
| 7.3      | Parameterization of material properties                                          | 211        |
| <b>8</b> | <b>Solution techniques for carrier transport and thermal diffusion equations</b> | <b>214</b> |
| 8.1      | The static carrier transport equation                                            | 214        |
| 8.1.1    | Scaling                                                                          | 215        |
| 8.1.2    | Boundary conditions                                                              | 216        |
| 8.1.3    | The initial solution                                                             | 218        |
| 8.1.4    | The finite difference discretization                                             | 218        |
| 8.1.5    | Solution of non-linear algebraic equations                                       | 228        |
| 8.2      | The transient carrier transport equation                                         | 231        |
| 8.3      | The carrier rate equation                                                        | 232        |
| 8.4      | The thermal diffusion equation                                                   | 233        |
| <b>9</b> | <b>Numerical analysis of device performance</b>                                  | <b>236</b> |
| 9.1      | A general approach                                                               | 236        |
| 9.1.1    | The material gain treatment                                                      | 236        |
| 9.1.2    | The quasi-three-dimensional treatment                                            | 238        |
| 9.2      | Device performance analysis                                                      | 240        |
| 9.2.1    | The steady state analysis                                                        | 240        |
| 9.2.2    | The small-signal dynamic analysis                                                | 243        |
| 9.2.3    | The large-signal dynamic analysis                                                | 245        |
| 9.3      | Model calibration and validation                                                 | 246        |

|           |                                                                                             |            |
|-----------|---------------------------------------------------------------------------------------------|------------|
| viii      | <b>Contents</b>                                                                             |            |
| <b>10</b> | <b>Design and modeling examples of semiconductor laser diodes</b>                           | <b>251</b> |
| 10.1      | Design and modeling of the active region for optical gain                                   | 251        |
| 10.1.1    | The active region material                                                                  | 251        |
| 10.1.2    | The active region structure                                                                 | 255        |
| 10.2      | Design and modeling of the cross-sectional structure<br>for optical and carrier confinement | 259        |
| 10.2.1    | General considerations in the layer stack design                                            | 259        |
| 10.2.2    | The ridge waveguide structure                                                               | 260        |
| 10.2.3    | The buried heterostructure                                                                  | 265        |
| 10.2.4    | Comparison between the ridge waveguide structure and buried<br>heterostructure              | 268        |
| 10.3      | Design and modeling of the cavity for lasing oscillation                                    | 269        |
| 10.3.1    | The Fabry–Perot laser                                                                       | 269        |
| 10.3.2    | Distributed feedback lasers in different coupling<br>mechanisms through grating design      | 271        |
| 10.3.3    | Lasers with multiple section designs                                                        | 281        |
| <b>11</b> | <b>Design and modeling examples of other solitary optoelectronic devices</b>                | <b>288</b> |
| 11.1      | The electro-absorption modulator                                                            | 288        |
| 11.1.1    | The device structure                                                                        | 288        |
| 11.1.2    | Simulated material properties and device performance                                        | 288        |
| 11.1.3    | Design for high extinction ratio and low insertion loss                                     | 292        |
| 11.1.4    | Design for polarization independent absorption                                              | 297        |
| 11.2      | The semiconductor optical amplifier                                                         | 299        |
| 11.2.1    | The device structure                                                                        | 299        |
| 11.2.2    | Simulated semiconductor optical amplifier performance                                       | 300        |
| 11.2.3    | Design for performance enhancement                                                          | 302        |
| 11.3      | The superluminescent light emitting diode                                                   | 305        |
| 11.3.1    | The device structure                                                                        | 305        |
| 11.3.2    | Simulated superluminescent light emitting diode performance                                 | 305        |
| 11.3.3    | Design for performance enhancement                                                          | 306        |
| <b>12</b> | <b>Design and modeling examples of integrated optoelectronic devices</b>                    | <b>313</b> |
| 12.1      | The integrated semiconductor distributed feedback laser and<br>electro-absorption modulator | 313        |
| 12.1.1    | The device structure                                                                        | 313        |
| 12.1.2    | The interface                                                                               | 315        |
| 12.1.3    | Simulated distributed feedback laser performance                                            | 315        |
| 12.1.4    | Simulated electro-absorption modulator performance                                          | 317        |
| 12.2      | The integrated semiconductor distributed feedback<br>laser and monitoring photodetector     | 321        |
| 12.2.1    | The device structure                                                                        | 321        |

|                                                                    | Contents | ix  |
|--------------------------------------------------------------------|----------|-----|
| 12.2.2 Simulated distributed feedback laser performance            |          | 325 |
| 12.2.3 Crosstalk modeling                                          |          | 326 |
| <b>Appendices</b>                                                  |          | 332 |
| A Lowdin’s renormalization theory                                  |          | 332 |
| B Integrations in the many-body gain model                         |          | 334 |
| C Cash–Karp’s implementation of the fifth order Runge–Kutta method |          | 347 |
| D The solution of sparse linear equations                          |          | 348 |
| D.1 The direct method                                              |          | 349 |
| D.2 The iterative method                                           |          | 351 |
| <i>Index</i>                                                       |          | 356 |



## Preface

Over the past 30 years, the world has witnessed the rapid development of optoelectronic devices based on III-V compound semiconductors. Past effort has mainly been directed to the theoretical understanding of, and the technology development for, these devices in applications in telecommunication networks and compact disk (CD) data storage. With the growing deployment of such devices in new fields such as illumination, display, fiber sensor, fiber gyro, optical coherent tomography, etc., research on optoelectronic devices, especially on those light emitting components, continues to expand with the pursuit of many experimental explorations on new materials such as group-III nitride alloys and II-VI compounds and novel structures such as quantum wires, dots, and nanostructures.

As the manufacturing technology becomes mature and standardized and few uncertainties are left, design and simulation become the major issue in the performance enhancement of existing devices and in the development of new devices. Recent progress in numerical techniques as well as computing hardware has provided a powerful platform that makes sophisticated computer-aided design, modeling, and simulation possible. So far, the development of optoelectronic devices seems to replicate the history of electronic devices: from discrete to integrated, from technology intensive to design intensive, from trial-and-error experiments to computer-aided simulation and optimization.

The purpose of this book is to bridge the gap between the theoretical framework and the solution to real-world problems, or, more specifically, to bridge the gap between our knowledge acquired on electromagnetic field theory, quantum mechanics, and semiconductor physics and optoelectronic device design and modeling through advanced numerical tools.

Advanced optoelectronic devices are built on compound semiconductor material systems with complicated geometrical structures; they are also operated under varying conditions. For this reason, we can find hardly any easy, intuitive, and analytical solutions to the first-principle-based governing equations that accurately describe the closely coupled physical processes inside such devices. Although solutions are relatively easy to obtain from the equations derived from the phenomenological model, assumptions have to be made in such a model, which often ignores some important effects and fails to achieve quantitative agreement between theoretically predicted and practically measured results.

Therefore, obtaining the solution directly from the physics-based governing equations through numerical techniques seems to be a promising approach to bridge the gap as mentioned above, as not only a qualitative, but also a quantitative matching between

the theory and experiment is achievable. This book is intended for readers who want to link their understanding of the device physics through the theoretical framework they have already acquired to the design, modeling and simulation of real-world devices and innovative structures.

This book will focus on semiconductor-based optoelectronic devices such as laser diodes (LDs), electro-absorption modulators (EAMs), semiconductor optical amplifiers (SOAs), and superluminescent light emitting diodes (SLEDs) in various applications. Numerical methods will be used throughout the analysis of these devices.

Derived from physics-based first principles, governing equations will be given for the description of different physical processes, such as light propagation, optical gain generation, carrier transport and thermal diffusion, and their interplays inside the devices. Different numerical techniques will be discussed in detail along with the process of seeking the solution to these governing equations. Discussions on device design optimizations will also be followed, based on the interpretation of the numerical solutions.

The methodology introduced in this book hopefully will help its readers to learn (1) how to extract the governing equations from first principles for the accurate description of their devices; and more importantly, (2) how to obtain the numerical solution to those governing equations once derived. Practical design and simulation examples are also given to support the approaches used in this book.

I am in debt to my colleague and friend, Professor W.-P. Huang, who showed me the prospect of computer-aided design, modeling and simulation in this field 15 years ago, and with whom I had countless stimulating discussions on almost every topic involved in this book, from the material physics to waveguide theory, from the model establishment to result interpretation, and from the modeling methodology to numerical algorithm. I would like to thank Dr. T. Makino (former Nortel), Dr. K. Yokoyama (former NTT), Dr. T. Yamanaka (NTT), Dr. C.-L. Xu (RSoft Inc.), Dr. J. Hong (Oplink Inc.), Dr. A. Shams (former Photonami Inc.), Professor S. Sadeghi (University of Alabama at Huntsville), Professor W. Li (University of Wisconsin at Platteville), Professor Y. Luo (Tsinghua University), Professor Y.-H. Zhang (Arizona State University), Ms. T.-N. Li (InPhenix Inc.), Ms. N. Zhou (AcceLink Co.), Mr. M. Mazed (IP Photonics Inc.), Professor T. Luo (University of Minnesota), Professor C.-Q. Xu (McMaster University), Professor M. Dagenais (University of Maryland at College Park), Dr. J. Piprek (former University of California at Santa Barbara), and many other colleagues and friends in this field, for numerous insightful and inspiring discussions and interactions on various subjects in this book, during and after our research collaborations. I am grateful to Ms. Y.-P. Xi, who helped me with the simulation of SOAs and SLEDs, and Mr. Q.-Y. Xu, who helped me with the simulation of crosstalks in the integrated DFB laser and monitoring photodetector. I am also grateful to Professor S.-H. Chen (Huazhong University of Sci. and Tech.) and her graduate students, who helped me to create most of the schematic diagrams in the first eight chapters and all the three-dimensional device structure drawings in Chapters 10 and 12. I would also like to thank my graduate students and many other graduate students in the Department of Electrical and Computer Engineering at McMaster University who took my course on this subject, for their valuable comments and suggestions. Finally, I appreciate the constant help and great patience of Dr. J. Lancashire and Ms. S. Koch.