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## Design, Modeling, and Simulation

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Department of Electrical and Computer Engineering
McMaster University
Hamilton, Ontario



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## Optoelectronic Devices

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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.

# 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.

# Contents

# 1 Introduction

## 1.1 The underlying physics in device operation

Figure 1.1 shows the major physical processes and their linkages in the operation of optoelectronic devices.

To capture these physical processes, we need the following models and knowledge:

(1) a model that describes wave propagation along the device waveguide (electromagnetic wave theory);
(2) a model that describes the optical properties of the device material platform (semiconductor physics);
(3) a model that describes carrier transport inside the device (quasi-electrostatic theory);
(4) a model that describes thermal diffusion inside the device (thermal diffusion theory).

Therefore, the above four aspects should be included in any model established for simulation of optoelectronic devices.

## 1.2 Modeling and simulation methodologies

There are two major approaches in device modeling and simulation.

(1) Physics modeling: a direct approach based on the first principle physics-based model.

The required governing equations in the preceding four aspects are all derived from first principles, such as the Maxwell equations (including electromagnetic wave theory for the optical field distribution and quasi-electrostatic theory for the carrier transport), the Schrödinger equation (for the semiconductor band structure), the Heisenberg equation (for the gain and refractive index change), and the thermal diffusion equation (for the temperature distribution).

This model gives the physical description of what exactly happens inside the device and is capable of providing predictions on device performance in every aspect, once the device building material constants, the structural geometrical sizes, and the operating conditions are all given.

This approach is usually adopted by device designers who work on developing devices themselves.

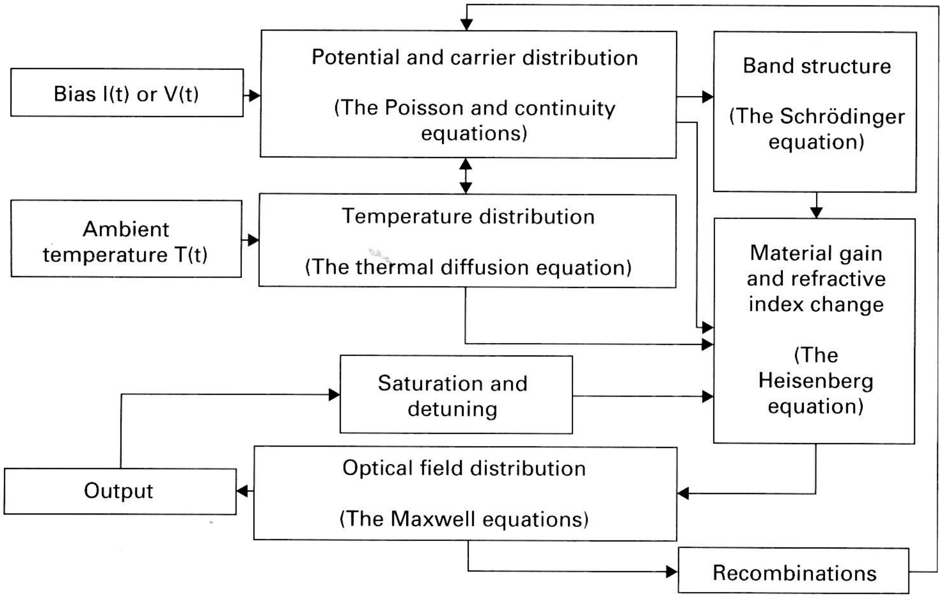


**Fig. 1.1.** The physical processes and their linkages in the operation of optoelectronic devices. Noted in brackets are the first principle equations that govern these processes.

However, such a modeling technique is usually complex and sophisticated numerical tools have to be invoked in solving the equations involved. Computationally it is usually expensive.

(2) Behavior modeling: an indirect approach based on an equivalent or phenomenological model.

The governing equations in the preceding four aspects are extracted from first principles under various assumptions. Hence they are greatly simplified compared with the equations in the physics-based model. Those frequently used methods in the extraction of the simplified equations include: (1) reducing or even eliminating spatial dimensions; (2) neglecting the dependence that causes only relatively slow or small variation; and (3) ignoring the physical processes that have little direct effect on the aspects of interest. Another method is to replace the original local or discrete variable by a global or integrated variable in the description of the physical process, as the latter usually obeys a certain conservation law, hence a corresponding balance equation can be derived in a simple form.

This model does not give the description of what exactly happens inside the device but is capable of providing the same device terminal performance as the physics-based model. Therefore, if the device is treated as a black box, this model will provide the correct output for any given input.

This approach is usually adopted by circuit and system designers who just use rather than develop devices.

Although this modeling technique is usually simple and computationally inexpensive, it has two major drawbacks that prevent its application in device design and development. The first demerit is that it can give hardly any physical insights. Little information can be obtained on how to make a device work better by improving the design. The second demerit is that it often relies on non-physical input parameters, such as effective constants or phenomenologically introduced coefficients, which are usually difficult to obtain.

In optoelectronic device modeling, we normally take a combination of the preceding two approaches. Depending on different simulation requirements, we usually retain a minimum set of the necessary physics-based equations and replace the rest by simplified ones.

## 1.3 Device modeling aspects

In device modeling, we normally look at the following aspects.

(1) Device steady state performance.
No time dependence needs to be considered in this simulation. The device characteristics are usually modeled as functions of the bias.

(2) Device small-signal dynamic performance.
Based on the small-signal linearization, a direct current (DC) at a fixed bias plus a frequency domain analysis are required in this simulation.

(3) Device large-signal dynamic performance.
A direct time-domain analysis is required in the simulation.

(4) Noise performance.
Either a semi-analytical frequency domain analysis or a numerical time-domain analysis is required in this simulation.

## 1.4 Device modeling techniques

A typical procedure for optoelectronic device modeling and simulation includes:

(1) input geometrical structures;
(2) input material constants;
(3) set up meshes;
(4) initialize solvers (pre-processing);
(5) input operating conditions;
(6) scale variables (physical to numerical);
(7) start looping;
(8) call carrier solver;
(9) call temperature solver;
(10) call material solver;
(11) call optical solver;

(12) go back to step 7 until convergence;
(13) scale variables (numerical to physical);
(14) output assembly (post-processing).

To start this procedure, however, one must have an initial device structure, which relies on one's understanding of the device physics and on one's experience accumulated from analysis and interpretation of the results obtained from device design, modeling and simulation practice.

Other than the initial structure, we still need to collect all the input parameters required by the numerical solvers. These parameters are usually obtained from open literature, experiment, or calibration.

The following are a number of numerical techniques that are often involved in optoelectronic device modeling:

(1) partial differential equation (PDE) solvers (boundary value and mixed boundary and initial value problems);
(2) ordinary differential equation (ODE) solvers (initial and boundary value problems);
(3) algebraic eigenvalue problem solvers;
(4) linear and non-linear system of algebraic equations solvers;
(5) root searching routine;
(6) minimization or maximization routine;
(7) function evaluations, interpolation and extrapolation routines;
(8) numerical quadratures;
(9) fast Fourier transform (FFT) and digital filtering routines;
(10) pseudo-random number generation.

The key issue in device modeling is to establish numerical solvers for PDEs, which usually follows a procedure as shown below.

(1) Scale the variables in given PDEs.
(2) Set up computation window and mesh grids.

(These two steps translate a physical problem into a numerical problem.)

(3) Equation discretization through, e.g., finite difference (FD) scheme.
(4) Boundary processing.

(These two steps translate PDEs into a system of algebraic equations.)

(5) Start Newton's iteration for the system of non-linear algebraic equations.

(This step translates the system of non-linear algebraic equations into a system of linear algebraic equations.)

(6) Find solution to the system of linear algebraic equations.
Direct method (for moderate size or dense coefficient matrix).
Iterative method (for large size sparse coefficient matrix).
Convergence acceleration (for iterative method).

(7) Convergence acceleration for Newton's iteration.

(The numerical solution will be obtained after this step.)

(8) Scale variables and post processing.

(A physical solution will be obtained after this step.)

## 1.5 Overview

This book is divided into three parts. The first part, comprising Chapters 2, 3, 4, and 5, is on the derivation and explanation of governing equations that model the closely coupled physics processes in optoelectronic devices. The second part, Chapters 6, 7, 8, and 9, is devoted to numerical solution techniques for the governing equations arising from the first part and explains how these techniques are jointly applied in device simulation. Chapters 10, 11, and 12 form the third part, which provides real-world design and simulation examples of optoelectronic devices, such as Fabry–Perot (FP) and distributed feedback (DFB) LDs, EAMs, SOAs, SLEDs, and their monolithic integrations.

# 2 Optical models

## 2.1 The wave equation in active media

### 2.1.1 Maxwell equations

The behavior of the optical wave is generally governed by the Maxwell equations

$$\nabla \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t}\vec{B}(\vec{r}, t), \tag{2.1}$$

$$\nabla \times \vec{H}(\vec{r}, t) = \frac{\partial}{\partial t}\vec{D}(\vec{r}, t) + \vec{J}(\vec{r}, t), \tag{2.2}$$

$$\nabla \cdot \vec{D}(\vec{r}, t) = \rho(\vec{r}, t), \tag{2.3}$$

$$\nabla \cdot \vec{B}(\vec{r}, t) = 0, \tag{2.4}$$

where $\vec{E}$ and $\vec{H}$ indicate the electric and magnetic fields in V/m and A/m, respectively, $r$ and $t$ represent the space coordinate vector and time variable, respectively, $\vec{D}$ the electric flux density in C/m$^2$, $\vec{B}$ the magnetic flux density in Wb/m$^2$, $\vec{J}$ the current density in A/m$^2$, and $\rho$ the charge density in C/m$^3$.

In semiconductors, the constitutive relation reads

$$\vec{D}(\vec{r}, t) = \int_{-\infty}^{t} \varepsilon(\vec{r}, t-\tau)\vec{E}(\vec{r}, \tau)\mathrm{d}\tau, \tag{2.5}$$

$$\vec{B}(\vec{r}, t) = \mu_0 \vec{H}(\vec{r}, \tau), \tag{2.6}$$

with $\varepsilon$ and $\mu_0$ denoting the time domain permittivity of the host medium and permeability in a vacuum in F/m and H/m, respectively.

Noting that

$$\varepsilon(\vec{r}, t) = \varepsilon_0[\delta(t) + \chi(\vec{r}, t)], \tag{2.7}$$

with $\varepsilon_0$ denoting the permittivity in a vacuum in F/m and $\chi$ the dimensionless time-domain susceptibility of the host medium, equation (2.5) can also be written as

$$\vec{D}(\vec{r}, t) = \varepsilon_0 \int_{-\infty}^{t} [\delta(t-\tau) + \chi(\vec{r}, t-\tau)]\, \vec{E}(\vec{r}, \tau)\mathrm{d}\tau = \varepsilon_0\vec{E}(\vec{r}, t) + \vec{P}(\vec{r}, t), \tag{2.8}$$