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.

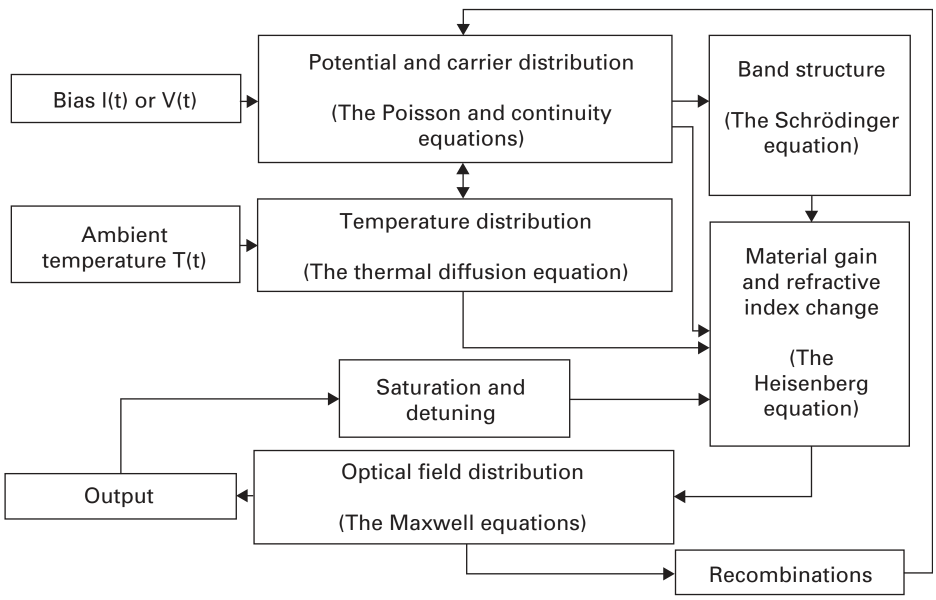

Fig. 1.1. The physical processes and their linkages in the operation of optoelectronic devices. Noted in brackets are the first principle equations that govern these processes.

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.

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More Information

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 ρ 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 ε and μ_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 ε_0 denoting the permittivity in a vacuum in F/m and χ the dimensionless time-domain susceptibility of the host medium, equation (2.5) can also be written as

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

where the induced polarization of the host medium in $\mathrm{C/m^2}$ is defined as

$$\vec{P}(\vec{r},t) \equiv \varepsilon_0 \int_{-\infty}^{t} \chi(\vec{r},t-\tau)\vec{E}(\vec{r},\tau)\mathrm{d}\tau. \tag{2.9}$$

For an electromagnetic field at optical frequencies

$$\rho = 0. \tag{2.10}$$

In a passive area without any radiative recombination process

$$\vec{J} = 0. \tag{2.11}$$

In an active area with a spontaneous emission process

$$\vec{J} = \vec{J}_{\mathrm{sp}}. \tag{2.12}$$

It is worth mentioning that, in an active area, the stimulated emission process will be included in the susceptibility, as it is a purely homogeneous process induced by a given electric field. Therefore, the stimulated emission process is excluded from equation (2.12), as the driven current must be a purely inhomogeneous source.

By using equations (2.5) and (2.6), the electrical and magnetic flux densities $\vec{D}$ and $\vec{B}$ can be eliminated from equations (2.1) and (2.2); hence we obtain

$$\nabla \times \vec{E} = -\mu_0 \frac{\partial}{\partial t}\vec{H}, \tag{2.13}$$

$$\nabla \times \vec{H} = \varepsilon_0 \frac{\partial}{\partial t}\vec{E} + \frac{\partial}{\partial t}\vec{P} + \vec{J}_{\mathrm{sp}}. \tag{2.14}$$

At least in principle, equations (2.13), (2.14) and (2.9) can be solved directly under the given semiconductor material property described by the susceptibility χ over the entire device structure and the spontaneous emission source $\vec{J}_{\mathrm{sp}}$ in the active area. For example, a finite difference time domain (FDTD) approach can be used to discretize equations (2.13) and (2.14) on Yee's unit cells [1]. Each electrical and magnetic field component can therefore be solved through the resulted recursion in the time domain on those cells that fill out the whole device domain. However, although FDTD based numerical solvers have been very successful in dealing with passive structures, they have seldom been employed for solving active structures because of the highly dispersive material property with embedded non-linearity and distributed inhomogeneous driving source. Moreover, every component of the electrical and magnetic fields must be handled as an unknown variable, which exhausts memory capacity and hence makes the computation impossible for devices with sizeable domains. For this reason, a wave equation model with a reduced number of unknown variables is usually more convenient in dealing with active devices.

2.1.2 The wave equation

The duality principle implies that it is not necessary to use both electrical and magnetic fields to describe optical wave propagation: either an electrical or magnetic field will be sufficient. To reduce the number of variables involved, we perform $\nabla\times$ on both sides of equation (2.13) and replace the right hand side (RHS) $\nabla \times \vec{H}$ with equation (2.14) to obtain

$$\nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = -\mu_0 \left(\varepsilon_0 \frac{\partial^2}{\partial t^2} \vec{E} + \frac{\partial^2}{\partial t^2} \vec{P} + \frac{\partial}{\partial t} \vec{J}_{\mathrm{sp}} \right). \tag{2.15}$$

From equations (2.3), (2.8), (2.10) and (2.9), we also have

$$\begin{aligned} \nabla \cdot \vec{E} &= -\frac{1}{\varepsilon_0} \nabla \cdot \vec{P} = -\int_{-\infty}^{t} \nabla \cdot \left[\chi(\vec{r}, t-\tau) \vec{E}(\vec{r}, \tau) \right] \mathrm{d}\tau \\ &= -\int_{-\infty}^{t} \chi(\vec{r}, t-\tau) \left[\nabla \cdot \vec{E}(\vec{r}, \tau) \right] \mathrm{d}\tau - \int_{-\infty}^{t} \left[\nabla \chi(\vec{r}, t-\tau) \cdot \vec{E}(\vec{r}, \tau) \right] \mathrm{d}\tau. \end{aligned} \tag{2.16}$$

If we restrict our model to those structures with

$$\nabla \chi(\vec{r}, t) \cdot \vec{E}(\vec{r}, t) \approx 0, \tag{2.17}$$

we find

$$\nabla \cdot \vec{E} = 0. \tag{2.18}$$

Hence equation (2.15) becomes

$$\nabla^2 \vec{E} = \frac{1}{\mathrm{c}^2} \frac{\partial^2}{\partial t^2} \vec{E} + \frac{1}{\mathrm{c}^2 \varepsilon_0} \frac{\partial^2}{\partial t^2} \vec{P} + \mu_0 \frac{\partial}{\partial t} \vec{J}_{\mathrm{sp}}, \tag{2.19}$$

with

$$\mathrm{c} \equiv 1/\sqrt{(\mu_0 \varepsilon_0)}, \tag{2.20}$$

defined as the speed of light in a vacuum in m/s.

Condition (2.17) holds for those structures with weak optical guidance, i.e., χ only changes slightly in the plane perpendicular to the wave propagation direction, as such $\nabla_{\mathrm{T}} \chi(\vec{r}, t) \cdot \vec{E}_{\mathrm{T}}(\vec{r}, t) \approx 0$. Along the wave propagation direction (assumed to be z), however, $\partial\chi/\partial z$ does not need to be small since $E_z \approx 0$ anyway. Therefore, wave equation (2.19) holds even for devices with non-uniform structures along the wave propagation direction, e.g., distributed feedback (DFB) or distributed Bragg reflector (DBR) lasers, as long as the wave is weakly guided in the cross-section.

Expressions (2.19) and (2.9) form the wave equation model that describes optical wave propagation in a weakly guided device structure. In the wave equation (2.19), the only term on the left hand side (LHS) gives the spatial diffraction of the electrical field, while the first term on the RHS gives the time dispersion of the electrical field. The balance of these two terms gives the inherent property of the optical wave, i.e., the propagation in space. The second term on the RHS denotes the contribution from the wave–media interaction where the convolution reveals that the wave at a certain time t will be affected by the whole past "history" of the media response. This is simply because the media cannot instantaneously respond to the incident wave. The last term on the RHS represents the contribution of the spontaneous emission known as a noise current source. As the only inhomogeneous term, it plays a crucial role as the "seed" in light-emitting devices. Without the inclusion of this inhomogeneous contribution in equation (2.19), a laser will never lase as equation (2.19) would have only zero solution because of its homogeneity.

In comparison with the Maxwell equations in their original form, the wave equation model is physically straightforward and has minimum required unknown variables involved. However, equation (2.19) contains the second order derivatives with respect to time and is in the form of a hyperbolic partial differential equation (PDE). Unlike an elliptical PDE with only static solutions, or a parabolic PDE with solutions exponentially approaching its steady state, a hyperbolic PDE takes harmonic oscillations as its inherent solution and bears no time-invariant steady state. Therefore, stability will always be an issue in looking for its solutions if the initial value is not well posed or not sufficiently smooth.

Knowing that a hyperbolic PDE takes the harmonic wave as its "static" solution, we can therefore write the general solution of the wave equation (2.19) in the form of a "modulated" wave, i.e., a harmonic wave with "slow-varying" envelope. By doing so, we should be able to extract a governing equation for this envelope from equation (2.19). As the envelope changes more slowly, the new equation will take a reduced time derivative and hence become more stable.

2.2 The reduced wave equation in the time domain

We assume that the optical wave is composed of harmonic waves with discrete frequencies and relatively slow-varying envelopes

$$\vec{E}(\vec{r}, t) = \frac{1}{2} \sum_k \vec{u}_k(\vec{r}, t) \mathrm{e}^{-\mathrm{j}\omega_k t} + \mathrm{c.c.}, \tag{2.21}$$

with $\vec{u}_k$ and ω_k indicating the kth harmonic wave envelope function in V/m and angular frequency in rad/s, respectively, and where c.c. means complex conjugate. By further assuming the linearity of equation (2.19) (i.e., χ has no explicit dependence on $\vec{E}$), we take only a single frequency ($k = 0$) in the following derivations without losing generality: when multiple frequencies are involved, it is trivial to consider a summation in a linear system because of the superposition principle. For the same reason, we can drop the complex conjugate part by considering

$$\vec{E}(\vec{r}, t) = \vec{u}(\vec{r}, t) \mathrm{e}^{-\mathrm{j}\omega_0 t}, \tag{2.22}$$

only, with ω_0 as the harmonic wave frequency (or reference frequency) and with the subscript of the envelope function omitted. Since equations (2.19) and (2.9) are all real, if we take our real-world optical wave as the real (or imaginary) part of equation (2.22), our real-world result will then be the real (or imaginary) part of the solution obtained from equations (2.19) and (2.9). The reason that we use a complex exponential function to replace the sinusoidal function is that the former is the eigenfunction of any linear and time-invariant system, whereas the latter is not, unless it forms a proper linear combination, i.e., a complex exponential function.

Replacing the optical field in equation (2.9) with equation (2.22) yields

$$\begin{aligned}\vec{P}(\vec{r},t) &= \varepsilon_0 \int_{-\infty}^{t} \chi(\vec{r},t-\tau)\vec{u}(\vec{r},\tau)\mathrm{e}^{-\mathrm{j}\omega_0\tau}\,\mathrm{d}\tau = \varepsilon_0 F^{-1}\left[\widetilde{\chi}(\vec{r},\omega)\widetilde{\vec{u}}(\vec{r},\omega-\omega_0)\right] \\ &\approx \varepsilon_0\widetilde{\chi}(\vec{r},\omega_0)F^{-1}\left[\widetilde{\vec{u}}(\vec{r},\omega-\omega_0)\right] = \varepsilon_0\widetilde{\chi}(\vec{r},\omega_0)\vec{u}(\vec{r},t)\mathrm{e}^{-\mathrm{j}\omega_0 t},\end{aligned} \tag{2.23}$$

with $\widetilde{\vec{u}}$ and $\widetilde{\chi}$ indicating the frequency domain responses of the slow-varying harmonic wave envelope function and susceptibility, respectively, and $F^{-1}[\ldots]$ the inverse Fourier transform. Equation (2.23) holds only when the susceptibility varies much faster than the slow-varying envelope in the time domain; or equivalently, the bandwidth of $\widetilde{\chi}$ is much larger than that of $\widetilde{\vec{u}}$ in the frequency domain. In optoelectronic devices, this is usually true as long as the base-band signal (hence the slow-varying envelope) does not consist of very short pulses. Since the full width half maximum (FWHM) bandwidth of $\widetilde{\chi}$ is usually as broad as 5–10 THz (i.e., around 50–100 nm in a C-band centered at 1550 nm), i.e., χ can respond to any time change slower than sub-picosecond, any base-band signal that varies slower than 10 ps would make equation (2.23) a valid approximation.

We now plug both equations (2.22) and (2.23) into equation (2.19) to obtain

$$\mathrm{j}\frac{2\omega_0}{\mathrm{c}^2}\left[1+\widetilde{\chi}(\vec{r},\omega_0)\right]\frac{\partial\vec{u}}{\partial t} = -\nabla^2\vec{u} - \frac{\omega_0^2}{\mathrm{c}^2}\left[1+\widetilde{\chi}(\vec{r},\omega_0)\right]\vec{u} + \mu_0\mathrm{e}^{\mathrm{j}\omega_0 t}\frac{\partial}{\partial t}\vec{J}_{\mathrm{sp}}, \tag{2.24}$$

where under the slow-varying envelope assumption ($|\partial^2\vec{u}/\partial t^2| \ll \omega_0^2|\vec{u}|$), $\partial^2\vec{u}/\partial t^2$ is dropped.

Equation (2.24) is the reduced wave equation in the time domain. It governs the slow-varying envelope of an optical field that is assumed in a harmonic wave form with optical frequency ω_0. Compared with equation (2.19), equation (2.24) has the fast-varying harmonic factor ($\mathrm{e}^{-\mathrm{j}\omega_0 t}$) excluded, hence has a reduced time derivative order. Numerically, stable solutions can be obtained through time domain discretization by following the envelope change ($\partial\vec{u}/\partial t$), rather than by following the optical wave change ($\partial\vec{E}/\partial t$) itself. This normally results in a great saving of progressive steps as the former changes much slower than the latter in the time domain.

Actually, equation (2.24) is solved directly only when the device structure does not have any dominant feature in space and hence the wave does not form any time-invariant spatial pattern known as a "mode." In waveguide based optoelectronic and photonic devices, however, the wave is confined at least along one dimension. Therefore, an optical mode can be introduced at least along this dimension and the wave will travel in the reduced spatial dimensions. For this reason, equation (2.24) can be further simplified for waveguide based optoelectronic and photonic devices as shown in Section 2.4.