Takahiro Numai

Fundamentals of Semiconductor Lasers

With 166 Figures



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Preface

Semiconductor lasers have been actively studied since the first laser oscillation in 1962. Through continuing efforts based on physics, characteristics of semiconductor lasers have been extensively improved. As a result, they are now widely used. For example, they are used as the light sources for bar-code readers, compact discs (CDs), CD-ROMs, magneto-optical discs (MOs), digital video discs (DVDs), DVD-ROMs, laser printers, lightwave communication systems, and pumping sources of solid-state lasers. From these facts, it may be said that semiconductor lasers are indispensable for our contemporary life.

This textbook explains the physics and fundamental characteristics of semiconductor lasers with regard to system applications. It is aimed at senior undergraduates, graduate students, engineers, and researchers. The features of this book are as follows:

- 1. The required knowledge to read this book is electromagnetism and introductory quantum mechanics taught in undergraduate courses. After reading this book, students will be able to understand journal papers on semiconductor lasers without difficulty.
- 2. To solve problems in semiconductor lasers, sometimes opposite approaches are adopted according to system applications. These approaches are compared and explained.
- 3. In the research of semiconductor lasers, many ideas have been proposed and tested. Some ideas persist, and others have faded out. These ideas are compared and the key points of the persisting technologies will be revealed.
- 4. The operating principles are often the same, although the structures seem to be different. These common concepts are essential and important; they allow us to deeply understand the physics of semiconductor lasers. Therefore, common concepts are emphasized in several examples, which will lead to both a qualitative and a quantitative understanding of semiconductor lasers.

This book consists of two parts. The first part, Chapters 1–4, reviews fundamental subjects such as the band structures of semiconductors, optical transitions, optical waveguides, and optical resonators. Based on these fundamentals, the second part, Chapters 5–8, explains semiconductor lasers.

The operating principles and basic characteristics of semiconductor lasers are discussed in Chapter 5. More advanced topics, such as dynamic single-mode lasers, quantum well lasers, and control of the spontaneous emission, are described in Chapters 6–8.

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1 Band Structures

1.1 Introduction

Optical transitions, such as the emission and absorption of light, are closely related to the energies of electrons, as shown in Table 1.1. When electrons transit from high energy states to lower ones, lights are emitted, and in the reverse process, lights are absorbed. Note that nonradiative transitions, which do not emit lights, also exist when electrons transit from high energy states to lower ones. Light emissions, however, always accompany the transitions of electrons from high energy states to lower ones, which are referred to as radiative transitions.

Table 1.1. Relationship between electron energies and optical transitions

Energy of the Electrons	Optical Transition
$High \rightarrow low$	Emission
$Low \rightarrow high$	Absorption

Let us consider electron energies, which are the bases of the optical transitions. Figure 1.1 shows a relationship between atomic spacing and electron energies. When the atomic spacing is large, such as in gases, the electron energies are discrete and the energy levels are formed. With a decrease in the atomic spacing, the wave functions of the electrons start to overlap. Therefore, the energy levels begin to split so as to satisfy the Pauli exclusion principle. With an increase in the number of neighboring atoms, the number of split energy levels is enhanced, and the energy differences in the adjacent energy levels are reduced. In the semiconductor crystals, the number of atoms per cubic centimeter is on the order of 10^{22} , where the lattice constant is approximately 0.5 nm and the atomic spacing is about 0.2 nm. As a result, the spacing of energy levels is on the order of 10^{-18} eV. This energy spacing is much smaller than the bandgap, which is on the order of electron volts. Therefore, the constituent energy levels, which are known as the energy bands, are considered to be almost continuous.

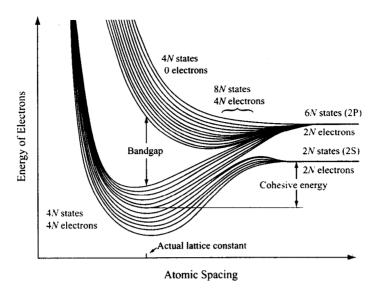


Fig. 1.1. Relationship between atomic spacing and electron energies for the diamond structure with N atoms

1.2 Bulk Structures

1.2.1 $k \cdot p$ Perturbation Theory

We study the band structures of the *bulk* semiconductors, in which constituent atoms are periodically placed in a sufficiently long range compared with the lattice spacing.

Semiconductors have carriers, such as free electrons and holes, only in the vicinity of the band edges. As a result, we would like to know the band shapes and the effective masses of the carriers near the band edges, and they often give us enough information to understand fundamental characteristics of the optical transitions. When we focus on the neighbor of the band edges, it is useful to employ the $\mathbf{k} \cdot \mathbf{p}$ perturbation theory [1-4] whose wave vectors \mathbf{k} s are near the band edge wave vector \mathbf{k}_0 inside the Brillouin zone. The wave functions and energies of the bands are calculated with $\Delta \mathbf{k} = \mathbf{k} - \mathbf{k}_0$ as a perturbation parameter. For brevity, we put $\mathbf{k}_0 = 0$ in the following.

The Schrödinger equation in the steady state is written as [5,6]

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) \psi_{n\mathbf{k}}(\mathbf{r}), \tag{1.1}$$

where $\hbar = h/2\pi = 1.0546 \times 10^{-34} \, \mathrm{J} \, \mathrm{s}$ is Dirac's constant, $h = 6.6261 \times 10^{-34} \, \mathrm{J} \, \mathrm{s}$ is Planck's constant, $m = 9.1094 \times 10^{-31} \, \mathrm{kg}$ is the electron mass in a vacuum, V(r) is a potential, $\psi_{n\mathbf{k}}(r)$ is a wave function, $E_n(\mathbf{k})$ is an energy eigenvalue, n is a quantum number, and \mathbf{k} is a wave vector. In the single crystals where the atoms are placed periodically, the potential V(r) is

spatially periodic. Therefore, as a solution of (1.1), we can consider the *Bloch* function given by

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r}), \tag{1.2}$$

$$u_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r} + \mathbf{R}), \tag{1.3}$$

where \mathbf{R} is a vector indicating the periodicity of the crystal. Equations (1.2) and (1.3) are called the *Bloch theorem*, which indicates that the wave function $u_{n\mathbf{k}}(\mathbf{r})$ depends on the wave vector \mathbf{k} and has the same periodicity as that of the crystal. Substituting (1.2) into (1.1) results in

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + \mathcal{H}' \right] u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) u_{n\mathbf{k}}(\mathbf{r}), \tag{1.4}$$

where

$$\mathcal{H}' = \frac{\hbar^2 \mathbf{k}^2}{2m} + \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p},\tag{1.5}$$

$$\boldsymbol{p} = -\mathrm{i}\,\hbar\nabla.\tag{1.6}$$

In the $k \cdot p$ perturbation theory, which is only valid for small k, we solve (1.4) by regarding (1.5) as the *perturbation*. Note that the name of the $k \cdot p$ perturbation stems from the second term on the right-hand side of (1.5).

When we consider the energy band with n = 0, the wave equation for the unperturbed state with k = 0 is expressed as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] u_{00}(\mathbf{r}) = E_0(0) u_{00}(\mathbf{r}). \tag{1.7}$$

In the following, for simplicity, the wave function $u_{nk}(r)$ and the energy $E_0(0)$ are represented as $u_n(k,r)$ and E_0 , respectively.

At first, we consider a nondegenerate case, in which the energy of the state n is always different from that of the other state $n' \ (\neq n)$. From the first-order perturbation theory (see Appendix B), the wave function $u_0(k, r)$ is given by

$$u_0(\mathbf{k}, \mathbf{r}) = u_0(0, \mathbf{r}) + \sum_{\alpha \neq 0} \frac{-i \left(\hbar^2 / m\right) \mathbf{k} \cdot \langle \alpha | \nabla | 0 \rangle}{E_0 - E_\alpha} u_\alpha(0, \mathbf{r}), \tag{1.8}$$

$$\langle \alpha | \nabla | 0 \rangle = \int u_{\alpha}^*(0, \mathbf{r}) \nabla u_0(0, \mathbf{r}) d^3 \mathbf{r},$$
 (1.9)

where $u_n(\mathbf{k}, \mathbf{r})$ is assumed to be an orthonormal function. Here, $\langle \alpha |$ and $|0\rangle$ are the *bra vector* and the *ket vector*, respectively, which were introduced by Dirac. In the *second-order perturbation theory*, an energy eigenvalue is obtained as

$$E(\mathbf{k}) = E_0 + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{i,j} k_i k_j \sum_{\alpha \neq 0} \frac{\langle 0 | p_i | \alpha \rangle \langle \alpha | p_j | 0 \rangle}{E_0 - E_\alpha}.$$
 (1.10)

From (1.10), the reciprocal effective mass tensor is defined as

$$\left(\frac{1}{m}\right)_{ij} \equiv \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j} = \frac{1}{m} \left(\delta_{ij} + \frac{2}{m} \sum_{\alpha \neq 0} \frac{\langle 0|p_i|\alpha\rangle\langle\alpha|p_j|0\rangle}{E_0 - E_\alpha}\right). \tag{1.11}$$

With the help of (1.11), (1.10) reduces to

$$E(\mathbf{k}) = E_0 + \frac{\hbar^2}{2} \sum_{i,j} \left(\frac{1}{m}\right)_{ij} \mathbf{k}_i \mathbf{k}_j. \tag{1.12}$$

This equation includes the periodicity of the crystal (potential) in the mass of the electron as the effective mass. This effective mass is useful to make analysis easier. For example, in the quantum well (QW) structures, the electrons see both the periodic potential of the crystal and the quantum well potential. If we express equations using the effective mass, we have only to consider the quantum well potential, because the periodic potential of the crystal is already included in the effective mass. This approximation is referred to as the effective mass approximation.

In the following, we will consider the band structures of semiconductor crystals. Most semiconductor crystals for semiconductor lasers have a zinc-blende structure, in which the bottom of the conduction bands is s-orbital-like and the tops of the valence bands are p-orbital-like. In zinc-blende or diamond structures, the atomic bonds are formed via sp^3 hybrid orbitals as follows:

$$\begin{array}{c} \mathrm{C}: (2s)^2 (2p)^2 \to (2s)^1 (2p)^3 \\ \mathrm{Si}: (3s)^2 (3p)^2 \to (3s)^1 (3p)^3 \\ \mathrm{ZnS}: \mathrm{Zn}: (3d)^{10} (4s)^2 \to \mathrm{Zn}^{2-}: (3d)^{10} (4s)^1 (4p)^3 \\ \mathrm{S}: (3s)^2 (3p)^4 \to \mathrm{S}^{2+}: (3s)^1 (3p)^3 \end{array}$$

Therefore, the wave functions for the electrons in the zinc-blende or diamond structures are expressed as superpositions of the s-orbital function and p-orbital functions.

Let us calculate the wave functions and energies of the bands in the zincblende structures. We assume that both the bottom of the conduction band and the tops of the valence bands are placed at k=0, as in the direct transition semiconductors, which will be elucidated in Section 2.1. When the spin-orbit interaction is neglected, the tops of the valence bands are threefold degenerate corresponding to the three p-orbitals (p_x, p_y, p_z) . Here, the wave functions are written as

the s-orbital function for the bottom of the conduction band: $u_s(r)$, the p-orbital functions for the tops of the valence bands:

$$u_x = xf(r)$$
, $u_y = yf(r)$, $u_z = zf(r)$, $f(r)$: a spherical function.

When the energy bands are degenerate, a perturbed wave equation is given by a linear superposition of $u_s(\mathbf{r})$ and $u_j(\mathbf{r})$ (j=x,y,z) as

$$u_n(\mathbf{k}, \mathbf{r}) = Au_s(\mathbf{r}) + Bu_x(\mathbf{r}) + Cu_y(\mathbf{r}) + Du_z(\mathbf{r}), \tag{1.13}$$

where A, B, C, and D are coefficients.

To obtain the energy eigenvalues, we rewrite (1.4) as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + \mathcal{H}'_{d} \right] u_n(\mathbf{k}, \mathbf{r}) = \left[E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m} \right] u_n(\mathbf{k}, \mathbf{r}), \quad (1.14)$$

$$\mathcal{H}_{d}' = \frac{\hbar}{m} \mathbf{k} \cdot \mathbf{p} = -\frac{i \hbar^{2}}{m} \mathbf{k} \cdot \nabla.$$
 (1.15)

Note that the unperturbed equation is obtained by setting $\mathbf{k} = 0$ in (1.14), where $E_n(0) = E_c$ and $u_0(0, \mathbf{r}) = u_s(\mathbf{r})$ for the conduction band, while $E_n(0) = E_v$ and $u_0(0, \mathbf{r}) = u_j(\mathbf{r})$ (j = x, y, z) for the valence bands. Here, E_c is the energy of the bottom of the conduction band, and E_v is the energy of the tops of the valence bands.

Substituting (1.13) into (1.14); multiplying $u_s^*(\mathbf{r})$, $u_x^*(\mathbf{r})$, $u_y^*(\mathbf{r})$, and $u_z^*(\mathbf{r})$ from the left-hand side; and then integrating with respect to a volume over the space leads to

$$(\mathcal{H}'_{ss} + E_{c} - \lambda)A + \mathcal{H}'_{sx}B + \mathcal{H}'_{sy}C + \mathcal{H}'_{sz}D = 0, \mathcal{H}'_{xs}A + (\mathcal{H}'_{xx} + E_{v} - \lambda)B + \mathcal{H}'_{xy}C + \mathcal{H}'_{xz}D = 0, \mathcal{H}'_{ys}A + \mathcal{H}'_{yx}B + (\mathcal{H}'_{yy} + E_{v} - \lambda)C + \mathcal{H}'_{yz}D = 0, \mathcal{H}'_{zs}A + \mathcal{H}'_{zx}B + \mathcal{H}'_{zy}C + (\mathcal{H}'_{zz} + E_{v} - \lambda)D = 0,$$
 (1.16)

where

$$\mathcal{H}'_{ij} = \langle u_i | \mathcal{H}'_{d} | u_j \rangle = \int u_i^*(\mathbf{r}) \mathcal{H}'_{d} u_j(\mathbf{r}) d^3 \mathbf{r} \quad (i, j = s, x, y, z),$$

$$\lambda = E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m}.$$
(1.17)

Note that the orthonormality of $u_s(\mathbf{r})$ and $u_j(\mathbf{r})$ (j = x, y, z) were used to derive (1.16).

In (1.16), only when the determinant for the coefficients A, B, C, and D is zero, we have solutions A, B, C, and D other than A = B = C = D = 0. From (1.16) and (1.17), the determinant is given by

$$\begin{vmatrix} E_{c} - \lambda & Pk_{x} & Pk_{y} & Pk_{z} \\ P^{*}k_{x} & E_{v} - \lambda & 0 & 0 \\ P^{*}k_{y} & 0 & E_{v} - \lambda & 0 \\ P^{*}k_{z} & 0 & 0 & E_{v} - \lambda \end{vmatrix} = 0,$$
 (1.18)

$$P = -i \frac{\hbar^2}{m} \int u_s^* \frac{\partial u_j}{\partial r_j} d^3 \boldsymbol{r}, \quad P^* = -i \frac{\hbar^2}{m} \int u_j^* \frac{\partial u_s}{\partial r_j} d^3 \boldsymbol{r}$$

$$(j = x, y, z, \quad r_x = x, \quad r_y = y, \quad r_z = z).$$
(1.19)

The solutions of (1.18) are obtained as

$$E_{1,2}(\mathbf{k}) = \frac{E_{\rm c} + E_{\rm v}}{2} + \frac{\hbar^2 k^2}{2m} \pm \left[\left(\frac{E_{\rm c} - E_{\rm v}}{2} \right)^2 + k^2 |P|^2 \right]^{1/2}, \quad (1.20)$$

$$E_{3,4}(\mathbf{k}) = E_{\rm v} + \frac{\hbar^2 k^2}{2m},\tag{1.21}$$

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where (1.17) was used. Figure 1.2 shows the calculated results of (1.20) and (1.21). It should be noted that the spin-orbit interaction has been neglected and only the first-order perturbation has been included to derive these equations.

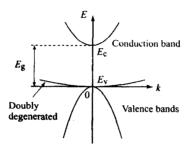


Fig. 1.2. Energy of the conduction and valence bands. Here, only the first-order perturbation is included; the spin-orbit interaction is neglected

1.2.2 Spin-Orbit Interaction

We consider the band structures by introducing the spin-orbit interaction and the second-order perturbation. First, let us treat the *spin-orbit interaction* semiclassically. As shown in Fig. 1.3, the electron with the electric charge $-e = -1.6022 \times 10^{-19}$ C rotates about the nucleus with the electric charge +Ze. The velocity of the electron is v, and the distance between the electron and the nucleus is |r|.



Fig. 1.3. Motions of the electron

If the origin of the reference system is placed at the electron, the nucleus seems to rotate about the electron with the velocity -v. As a result, due

to Biot-Savart's law, a magnetic flux density \boldsymbol{B} is produced at the electron, which is written as

$$\boldsymbol{B} = \frac{\mu_0}{4\pi} Z e \frac{\boldsymbol{r} \times \boldsymbol{v}}{r^3} = \frac{\mu_0}{4\pi} \frac{Z e}{m} \frac{1}{r^3} \boldsymbol{l}. \tag{1.22}$$

Here, μ_0 is magnetic permeability in a vacuum, and \boldsymbol{l} is the *orbital angular momentum* given by

$$\boldsymbol{l} = \boldsymbol{r} \times \boldsymbol{p} = \boldsymbol{r} \times m\boldsymbol{v}. \tag{1.23}$$

The spin magnetic moment μ_s is expressed as

$$\mu_{\rm s} = -\frac{e}{m}s = -\frac{2\mu_{\rm B}}{\hbar}s,\tag{1.24}$$

where \boldsymbol{s} is the spin angular momentum and μ_{B} is the Bohr magneton defined as

$$\mu_{\rm B} \equiv \frac{e\hbar}{2m} = 9.2732 \times 10^{-24} \,\mathrm{A}\,\mathrm{m}^2.$$
 (1.25)

As a result, the interaction energy \mathcal{H}_{SO} between the spin magnetic moment μ_s and the magnetic flux density \boldsymbol{B} is obtained as

$$\mathcal{H}_{SO} = -\boldsymbol{\mu}_{s} \cdot \boldsymbol{B} = \frac{\mu_{0}}{4\pi} \frac{Ze^{2}}{m^{2}} \frac{1}{r^{3}} \boldsymbol{l} \cdot \boldsymbol{s}. \tag{1.26}$$

From Dirac's relativistic quantum mechanics, the interaction energy \mathcal{H}_{SO} is given by

$$\mathcal{H}_{SO} = \frac{\mu_0}{4\pi} \frac{Ze^2}{2m^2} \frac{1}{r^3} \boldsymbol{l} \cdot \boldsymbol{s}, \tag{1.27}$$

which is half of (1.26). As explained earlier, the spin-orbit interaction generates a magnetic field at the electron due to the orbital motions of the nucleus, and this field interacts with the electron's spin magnetic moment.

Introducing Pauli's spin matrices σ such as

$$s = \frac{\hbar}{2} \sigma, \tag{1.28}$$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix},$$
 (1.29)

we can write the spin-orbit interaction Hamiltonian \mathcal{H}_{SO} as

$$\mathcal{H}_{SO} = \frac{\mu_0}{4\pi} \frac{Ze^2}{2m^2} \frac{1}{r^3} \frac{\hbar}{2} \mathbf{l} \cdot \boldsymbol{\sigma}. \tag{1.30}$$

If we express the up- $spin \uparrow (s_z = \hbar/2)$ as α and the down- $spin \downarrow (s_z = -\hbar/2)$ as β , they are written in matrix form as