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Yoshinobu Aoyagi · Kotaro Kajikawa
Editors

Optical Properties of Advanced Materials

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Optical Properties of Advanced Materials

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Preface

This book is designed to explain fundamental optical properties of advanced materials, which are recently being paid much attention as topics of basic research and application. This book covers various optical and electrical materials: quantum structures of semiconductors, spintronics, photonic crystals, surface plasmons in metallic nanostructures, photonic metamaterials, organic materials, and magnet-optics. So far, there have been few books that summarize these materials and methods from the viewpoint of optical properties of advanced materials. These materials have their own peculiarities, which are very interesting in modern optical physics and also in applications, because the concepts appeared in the optical properties are quite different from those in conventional optical materials.

This book is designed for graduate students, researchers, and/or engineers who are interested in fundamental optical properties in such advanced materials. Chapter 1 deals with quantum structures. First, the basic theory of quantum structure is explained. After that, the fundamental optical properties of low-dimensional semiconductor materials are explained from analytical points of view, in addition to real application of those low-dimensional materials to devices. In Chap. 2, the basic theory and research topics on photonic crystals are summarized. Many new physical phenomena are discovered in the field of photonic crystals, in the last two decades. The photonic crystal materials will be more important in the field of optical advanced materials. The chapter focuses on the nonlinear optical properties of photonic crystals. Chapter 3 deals with surface plasmon photonics, which is a hot research field in nanophotonics. The surface plasmons give attractive optical properties that cannot be realized in dielectrics and semiconductors. It is used in wide range of research fields, such as optics, physics, chemistry, and biology. Chapter 4 describes optical metamaterials that show interesting optical properties originating from their higher order metallic nanostructures. We can obtain an optical medium with a wide range of refractive indexes: from negative to large positive. This allows us to realize special optical applications, such as super high-resolution microscopy and optical croaking. Chapter 5 reviews spintronics, which is a new type of electronics that uses the mutual control between magnetic and other physical signals such as electrical and optical signals. It is one of the most important research fields of advanced materials. Chapter 6 provides a review on liquid crystal optics. Liquid crystals are the most successful functional organic materials, and are widely used for the flat panel displays. The liquid crystals with chiral part spontaneously form periodic structures, which are useful for modern photonic applications. This chapter focuses on the photonic effects in the chiral liquid crystals. Chapter 7 describes a review on organic light emitting devices (OLED). OLEDs are promising optical devices for high-contrast display and illumination. This chapter mainly focuses on the OLED materials. In Chap. 8, the effect of magnetic field on optical properties, i.e., magneto-optical (MO) effects, is described. The dynamical MO properties are becoming more important, since the change in MO property is deeply relating with the dynamical behavior of spin in advanced materials, and therefore it plays the key role in the growing field of spintronics.

Authors will be very pleased if this book proves to be helpful for students, engineers, and scientists who would like to understand the fundamental optical properties of the advanced materials. Finally, we wish to express our appreciation to Dr. Claus E. Ascheron for his encouragement.

Shiga Yoshinobu Aoyagi
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Contents

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Chapter 1
Quantum Structures of Advanced Materials

Yoshinobu Aoyagi

Abstract In this chapter the fundamental optical properties of low dimensional semiconductor materials like quantum well, wire and dot will be explained from analytical points of view in addition to real application of those low dimensional materials to devices. At the beginning the analytical method of hetero junction will be explained which is a base of quantum structures. After that the density of states of low dimensional material will be calculated for free electron in materials which is important to understand the optical properties of real devices. The optical properties of each low dimensional material will be explained and readers can understand what the specific optical nature of each low dimensional material is. Finally in this section the real application of low dimensional material to laser will be introduced and advantage of the low dimensionality will be explained. Since many references are cited, readers can understand deeply the parts which are interested in through the references.

1.1 Quantum Structures of Advanced Materials

1.1.1 Introduction

When a super-lattice was proposed by Prof. L. Ezaki for the first time, we learnt that artificial nano structure material like the super-lattice showed various interesting properties explained only by quantum mechanics. Some parts of properties were not obtained in natural world. We obtained wisdom not only that the band structure of the semiconductor and the metal was given in nature, but also that was able to control freely. Now the understanding of optical properties of the artificial new materials

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like the super-lattice, the quantum wire, and the quantum dot is very important. This chapter treats the event related to optical properties of the artificial nano-structured materials.

1.1.2 Heterostructure

For easy understanding the hetero-structure of p-GaAs and n-Ge will be discussed. The band diagram of each material is shown in Fig. 1.1.

For the calculation going underneath, parameters shown in Table 1.1 are used. In this figure the Fermi level, and energy of valence band and conduction band for p-GaAs and n-Ge are shown E_{fp}, E_{fn}, E_{vp}, E_{vn}, E_{cp}, E_{cn}, respectively. When forming the hetero-structure the Fermi level of each material should be coincident. So, the band should bend and notch and/or jump of band structure at the interface should appear. First of all these values are calculated (Table 1.1).

$$E_{\mathrm{fp}} = (\chi_{\mathrm{GaAs}} + E_{\mathrm{g}}(\mathrm{GaAs})) - \delta_{\mathrm{GaAs}}) = 5.72\,\mathrm{eV} \tag{1.1}$$

$$E_{\mathrm{fn}} = \chi_{\mathrm{Ge}} + \delta_{\mathrm{Ge}} = 4.23\,\mathrm{eV} \tag{1.2}$$

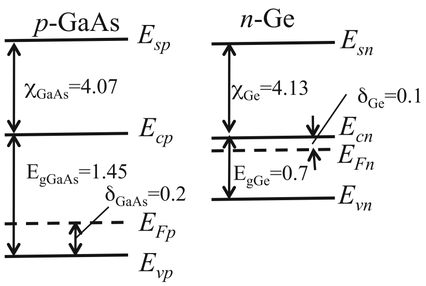


Fig. 1.1 Band structure of p-GaAs and n-Ge before formation of the hetero structure

Table 1.1 Fundamental parameters for the calculation of band diagram of p-GaAs/n-Ge hetero structure

	p-GaAs	n-Ge
Band gap (E_g)	1.45 eV	0.7 eV
Electron affinity χ	4.07 eV	4.13 eV
Donor density N_{d}		$1 \times 10^{16}\,\mathrm{cm}^{-3}$
Acceptor density N_{a}	$3 \times 10^{16}\,\mathrm{cm}^{-3}$	
$E_{\mathrm{f}} - E_{\mathrm{v}} = \delta_{\mathrm{GaAs}}$	0.2 eV	
$\mathrm{E_f} - \mathrm{E_v} = \delta_{\mathrm{Ge}}$		0.1 eV
Relative dielectric constant ϵ	11.5	16

As mentioned above, since the Fermi level of each material after forming the hetero-structure should be coincident, the a voltage appears at both sides of hetero-structure due to the charge transfer and the vacuum level should be bended with a value of V_{Dn} and V_{Dp} due to this voltage. The sum of the band $V_{Dn}+V_{Dp}$ is calculated to be

$$E_{fp}-E_{fn} = (\chi_{Ge}+E_g(Ge)-\delta_{Ge})-(\chi_{GaAs}+\delta_{GaAs}) = V_{Dn}+V_{Dp} = 1.45\,eV \quad (1.3)$$

If we assume the charge appears only in the region of X_n and X_p near the interface for simple calculation,

$$X_n/X_p = N_A/N_D = 3 \quad (1.4)$$

from charge conservation low. From Poisson's equation

$$d^2V/dx^2 = -\rho/\epsilon \quad (1.5)$$

V_{Dn} and V_{Dp} can be easily calculated as follows;

$$V_{Dn} = N_D X_n^2/(2\epsilon_{Ge}) \quad (1.6)$$

$$V_{Dp} = N_A X_p^2/(2\epsilon_{GaAs}) \quad (1.7)$$

$$V_{Dn}/V_{Dp} = (N_{GaAs}/N_{Ge}) \cdot (\epsilon_{GaAs}/\epsilon_{Ge}) = 2.16 \quad (1.8)$$

So,

$$V_{Dn} = 2.16 V_{Dp} \quad (1.9)$$

In this case the band discontinuity is named to be the energy spike ΔE_v. The energy kink or the notch and the jump of band structure ΔE_c also appear. The each value is calculated to be

$$\delta E_c = \chi_{GaAs} - \chi_{Ge} = -0.06\,eV \quad (1.10)$$

$$\delta E_v = (E_{gGe} - E_{gGaAs}) - (\chi_{GaAs} - \chi_{Ge}) = -0.69\,eV \quad (1.11)$$

So,

$$\delta E_c + \Delta E_v = E_{gGe} - E_{gGaAs}. \quad (1.12)$$

According to these calculations the band diagram of this p-GaAs and n-Ge is shown in Fig. 1.2. The details will be understood by referring the article [1].

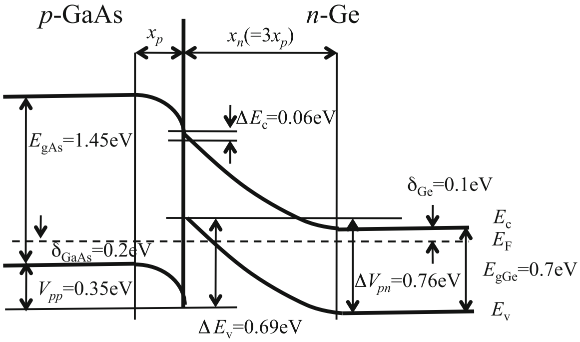


Fig. 1.2 Band structure of p-GaAs and n-Ge hetero-structure

1.2 Quantum Effects

1.2.1 Electron State in Semiconductor Quantum Well

We can make a hetero-structure of semiconductor by stacking different composite material of A and B like B/A/B, for example, AlGaAs/GaAs/AlGaAs as shown in Fig. 1.3. The band gap of material A and B is different. If the band gap of A is smalller than that of B we can construct quantum well structure shown in Fig. 1.3, and electron can be confined in the quantum well.

1.2.2 Energy State of Electron in Infinite Depth Quantum Well

Here, the rectangular well type potential problem shown in the semiconductor hetero-structure is taken up. First of all, let's evaluate the energy eigen-value of the well of infinite depth with an easy handling.

When the thickness of the well (the direction of x) is assumed to be L, and the starting point is taken at the center of the well, the potential structure is given as shown in Fig. 1.4. When width L is shorter than the de Broglie wavelength of the electron, the effect of quantum mechanics becomes strongly visible. Therefore, the well is especially called "Quantum well". Here, the center of the well was assumed to be a coordinate origin, and the energy of potential in the well was assumed to be 0. At this time, Schrödinger equation in the well is given by (1.13). As the boundary condition, because the electron cannot exist outside of the well, wave function given by Eq. 1.14 is used. Because the outside in this well is a barrier for the existence of electron, it is especially called barrier layer.

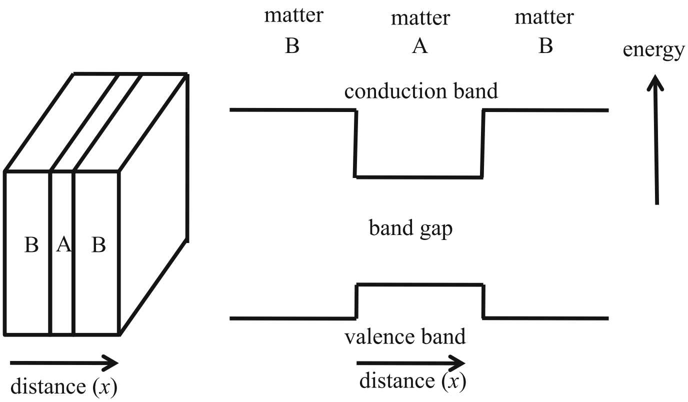
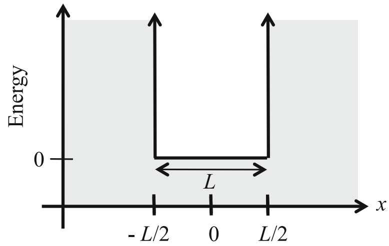


Fig. 1.3 Typical hetero-structure and the band structure

Fig. 1.4 Potential structure of quantum well with barrier of infinity of depth



$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad (|x| < \frac{L}{2}) \tag{1.13}$$

$$\psi(x) = 0 \qquad (|x| \geq \frac{L}{2}) \tag{1.14}$$

Energy related team in Eq. 1.13 is expressed as

$$k = \sqrt{\frac{2mE}{\hbar^2}} \tag{1.15}$$

It is possible to show by putting it into Eq. 1.13 as follows.

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \tag{1.16}$$

It is understood that Schrödinger equation shown above has the shape of an easy second order differential equation. The solution of Eq. 1.16 is given as,

$$\psi(x) = C_1\cos(kx) \tag{1.17}$$

$$\psi(x) = C_2\sin(kx) \tag{1.18}$$

Here, C_1 and C_2 are the integration constants, respectively.

For satisfying a boundary condition of Eq. 1.17, an equation $\cos(kL/2) = 0$ should be satisfied. So as to fill this equation

$$k\frac{L}{2} = \frac{\pi}{2}(2q - 1) \qquad (q = 1, 2, 3, \ldots) \tag{1.19}$$

should be satisfied. For the boundary condition of the Eq. 1.18, it is necessary to fill the equation

$$k\frac{L}{2} = \frac{\pi}{2}2q \qquad (q = 1, 2, 3, \ldots) \tag{1.20}$$

when the expression 1.19 and the expression 1.20 are brought together, it becomes

$$k = \frac{\pi}{L}n \qquad (q = 1, 2, 3, \ldots) \tag{1.21}$$

From Eqs. 1.15 and 1.21, energy state E in the quantum well corresponding to each eigenstate n is obtained as follows;

$$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2 \tag{1.22}$$

When n is odd number, the wave function in the quantum well has even symmetry as shown in Eq. 1.17 and when n is even number, the wave function has odd symmetry shown in Eq. 1.18, that is,

$$\psi(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}x\right) \qquad n = \text{odd number} \tag{1.23}$$

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \qquad n = \text{even number} \tag{1.24}$$

Integration constant C of the expression 1.23 and 1.24 is a normalized constant. The integrated value of the second power of the wave function in whole space must become one, because the total probability of finding electron in the whole space should be one.

1.2.3 Energy State in a Limited Depth Quantum Well

Next, let's take up the problem when the depth of a rectangular square well potential has a limited value of V. The thickness of the well is assumed to be L as shown in Fig. 1.5 and the starting point is taken at the center of the well. Electron energy E in the well is computed as follows. The effective mass of the electron in the barrier layer and the well layer is assumed to be m_B and m_w respectively now.

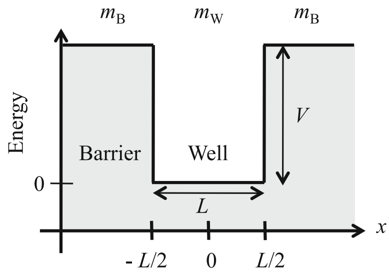


Fig. 1.5 Potential structure of quantum well

Because the potential energy is 0 in the well, the Schrödinger equation is similar as Eq. 1.13 and the solution in the well is also similar. That is, Schrödinger equation is given by

$$-\frac{\hbar^2}{2m_W}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad (|x| < \frac{L}{2}) \tag{1.25}$$

The solution is

$$\psi(x) = C_3 \cos(k_0 x) \tag{1.26}$$

$$\psi(x) = C_4 \sin(k_0 x) \tag{1.27}$$

Here,

$$k_0 = \sqrt{\frac{2m_W E}{\hbar^2}} \tag{1.28}$$

Here, C_3, and C_4 are the integration constants, respectively. It becomes from the shape of the solution that in case of quantum number is odd, the wave function is shown by a symmetric expression shown in Eq. 1.17 and the case of even, the function is asymmetric expression 1.18.

On the other hand, outside the well ($|x| \geq L/2$), the Schrödinger equation is given by

$$-\frac{\hbar^2}{2m_W}\frac{d^2\psi(x)}{dx^2} + V\psi(x) = E\psi(x) \tag{1.29}$$

In consideration of $E < V$,

$$k = \sqrt{\frac{2m_B(V-E)}{\hbar^2}} \tag{1.30}$$

The differential equation can be rewritten as

$$\frac{d^2\psi(x)}{d^2} = k^2\psi(x) \tag{1.31}$$

The solution becomes

$$\psi(x) = C_5 \exp(-kx) \qquad (x \geq \frac{L}{2}) \tag{1.32}$$

$$\psi(x) = C_6 \exp(kx) \qquad (x \leq -\frac{L}{2}) \tag{1.33}$$

Here, the wave function $\psi(x)$ should be zero at $x \rightarrow \pm\infty$ from the physics implication. So, Eqs. 1.32, 1.33 are obtained by excluding the solution which diverse at the infinite value of x. Here, C_5 and C_6 are the integration constants, respectively. Depending on the symmetry of the solution, the integration constant has a relation of $C_5 = C_6$ (symmetric case) and $C_5 = -C_6$ (asymmetric case).

From the continuous condition of existence probability and probability density flow of electron at any place, wave function $\psi(x)$ and $(1/m)(d\psi(x)/dx)$ should be continuous in any place. By putting the wave function inside the well and outside the well to be $\Psi_\mathrm{w}(x)$ and $\Psi_\mathrm{B}(x)$

$$(1/m_\mathrm{w})(d\Psi_\mathrm{w}/dx)(-L/2) = (1/m_\mathrm{B})(d\Psi_\mathrm{B}/dx)(-L/2) \tag{1.34}$$

$$(1/m_\mathrm{w})(d\Psi_\mathrm{w}/dx)(L/2) = (1/m_\mathrm{B})(d\Psi_\mathrm{B}/dx)(L/2) \tag{1.35}$$

By applying continuous condition at $x = L/2$ for symmetric wave function 1.26 in the well (same in case of $-L/2$) we obtain following equation.

$$C_3 \cos\left(\frac{kL}{2}\right) = C_5 \exp\left(-\frac{k_0 L}{2}\right) \tag{1.36}$$

$$-C_3\left(\frac{k}{m_\mathrm{w}}\right) \sin\left(\frac{kL}{2}\right) = -C_5\left(\frac{k_0}{m_\mathrm{B}}\right) \exp\left(-\frac{k_0 L}{2}\right) \tag{1.37}$$

By dividing Eq. 1.36 by Eq. 1.37, the integration constant C_3 and C_5 can be deleted, and the energy eigenvalue is obtained.

$$\left(\frac{k}{m_\mathrm{w}}\right) \tan\left(\frac{k_0 L}{2}\right) = \frac{k}{m_\mathrm{B}} \tag{1.38}$$

Because k_0 and k are functions of energy E, from the eigenvalue equation

$$\tan\left(\frac{k_0 L}{2}\right) = \frac{k}{k_0}\frac{m_\mathrm{w}}{m_\mathrm{B}} \tag{1.39}$$

the eigenvalue E can be numerically calculated. Similarly, for the asymmetric wave 1.27 the following eigen equation is obtained by applying the continuous condition at $x = L/2$.

$$\cot\left(\frac{kL}{2}\right) = -\frac{k_0}{k}\frac{m_\mathrm{w}}{m_\mathrm{B}} \tag{1.40}$$