黎明學報　第二十四卷　第一期　中華民國一〇二年一月三十一日
JOURNAL OF LEE-MING INSTITUTE OF TECHNOLOGY
VOL. 24, NO.1, JAN. 2013

Mathematical Expressions of Optical Transition Strength in Zinc-Blende Semiconductor Quantum Wells Grown on (11N) Orientation
(11N)方向上生長閃鋅礦半導體量子阱光耀遷強度的數學表達式

Wei-Long Su
蘇惟隆
Department of Digital Mulitimedia Technology, Lee-Ming Institute of Technology
黎明技術學院數媒系

Chun-Nan Chen
陳俊男
Quantum Engineering Lab., Department of Physics, Tamkang University
淡江大學物理系

Abstract

An analytical **k • p** method is applied to calculate the optical transition strength of zinc-blende semiconductor quantum wells. Optical matrix elements and hole effective masses in quantum wells are presented in explicit mathematical forms. Calculations are performed for $In_{0.53}Ga_{0.47}As/InP$ quantum wells.

Key Words: anisotropy, optical matrix element, substrate orientation, quantum well

摘　要

一個解析式 **k • p** 方法，其被用來計算閃鋅半導體量子阱結構之光躍遷強度。文中，光矩陣元與電洞有效質量以數學表示式清析呈現。並以 $In_{0.53}Ga_{0.47}As/InP$ 量子阱為本文計算例子。

關鍵詞：各向異性、光矩陣元素、基板方向、量子阱

1. INTRODUCTION

Recent advances in growth technologies now enable the growth of high-quality semiconductor heterostructures on substrates with orientations other than the conventional (001) [1-3]. The general non-(001)-oriented planes have the potential as another crucial degree of freedom to offer device designers more flexibility in the tailoring of the band structure of the semiconductor heterostructures used in advanced optical devices [4-7].

These processes yield a consequence of the alteration of the crystal symmetry in the different growth directions and also of the modification of the valence band structure. Moreover, the low-symmetry planes will result in the optical anisotropy on the growth surface [1,3,8,9]. Specifically, the in-plane anisotropy has been confirmed experimentally for epitaxial layers grown on differently oriented substrates, such as (110), (113), and (112) substrates [3,10-13].

As an alternative to the conventional **k**・**p** method, an analytic expression for the **k**・**p** Hamiltonian [14-16] can be obtained by expanding the Hamiltonian of the bond orbital model [15-17] in a Taylor series with respect to the wave vector **k** and then omitting the series terms higher than the second order in **k**.

2. THEORETICAL METHODS

Truncating the **k**・**p** Hamiltonian in a matrix form and preserving only the Γ_8 band, gives the 4×4 Luttinger-Kohn Hamiltonian. At the Brillouin-zone center $(k_{x'}=k_{y'}=0)$, this 4×4 **k**・**p** Hamiltonian for holes in a (11N)-oriented quantum well (QW) [in the basis ordering $|3/2,3/2\rangle$, $|3/2,1/2\rangle$, $|3/2,-1/2\rangle$, $|3/2,-3/2\rangle$] can be written as [14,18]

$$\mathbf{H}_{\mathbf{k}\cdot\mathbf{p}}(k_{x'}=k_{y'}=0)=$$

$$(E_p+8E_{xx}+4E_{zz})-\frac{a^2}{4}k_{z'}^2\times\left\{\frac{4}{3}(2E_{xx}+E_{zz})\times\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}\right.$$

$$+\begin{bmatrix}(E_{xx}-E_{zz})(2\sin^2\theta-\frac{3}{2}\sin^4\theta-\frac{2}{3})\\+4E_{xy}\sin^2\theta(\frac{3}{4}\sin^2\theta-1)\end{bmatrix}\times\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{bmatrix}$$

$$+(E_{xx}-E_{zz}-2E_{xy})(\frac{1}{\sqrt{3}}\sin\theta)(1-\frac{3}{2}\sin^2\theta)\times\left.\begin{bmatrix}\mathbf{0}&\mathbf{2\cos}\theta&-\sin\theta&\mathbf{0}\\\mathbf{2\cos}\theta&\mathbf{0}&\mathbf{0}&-\sin\theta\\-\sin\theta&\mathbf{0}&\mathbf{0}&-2\cos\theta\\\mathbf{0}&-\sin\theta&-2\cos\theta&\mathbf{0}\end{bmatrix}\right\}\quad(1)$$

where 'a' is the lattice constant, $k_{z'}$ is the wave vector along the growth direction[11N], θ ($=\sin^{-1}\sqrt{2}/\sqrt{\mathbf{N}^2+2}$) denotes the polar angle of the growth direction (z') relative to the (x, y, z) crystallographic coordinate system, a total of four interaction parameters exist, namely E_p, E_{xx}, E_{xy}, and E_{zz}, the first parameter relates to the on-site orbital energy, while the remaining parameters represent the nearest neighbor interactions [15]. Note that the 4×4 real symmetric matrix is along the directions of $x'//[\mathbf{NN}\bar{2}]$, $y'//[\bar{1}10]$, and $z'//[11\mathbf{N}]$. The matrix of this (11N)-oriented Hamiltonian becomes diagonal while the polar angle θ is equal to 0° (when $\mathrm{N}=\infty$) or $\sin^{-1}\sqrt{2}/\sqrt{3}\approx 54.7^\circ$ (when $\mathrm{N}=1$), corresponding to situations in which the QWs are oriented to (001) or (111) surface, respectively. Except for (001) and (111), the (11N) surfaces own the non-diagonal matrix elements at zone-center and hence result in the zone-center mixing among the valence bands.

3. CALCULATED RESULTS

According to the secular equation in Eq. (1), the explicit form of the eigenvalues and eigenvectors can be expressed as

$$E_\pm=(E_p+8E_{xx}+4E_{zz}) -\frac{a^2}{4}k_{z'}^2\{\frac{4}{3}(2E_{xx}+E_{zz}) \pm\frac{1}{\sqrt{3}}(E_{xx}-E_{zz}-2E_{xy})\Delta\sin\theta\} \quad (2)$$

for the doubly degenerate eigenvalues and

$$|v_\pm\rangle=\frac{1}{\mathbf{N}}\begin{bmatrix}(\mathbf{G}\pm\Delta)\\(\mathbf{S}+\mathbf{T})\\(-\mathbf{S}+\mathbf{T})\\(\mathbf{G}\pm\Delta)\end{bmatrix} \quad (3)$$

for the corresponding eigenvectors, where

$$\mathbf{S}=2\cos\theta(1-\frac{3}{2}\sin^2\theta), \quad (4a)$$

$$\mathbf{T}=-\sin\theta(1-\frac{3}{2}\sin^2\theta), \quad (4b)$$

$$\mathbf{G}=\{(E_{xx}-E_{zz}-2E_{xy})\sin^2\theta(2 -\frac{3}{2}\sin^2\theta)-\frac{2}{3}(E_{xx}-E_{zz})\} /(E_{xx}-E_{zz}-2E_{xy})(\sin\theta/\sqrt{3}) \quad (4c)$$

$$\Delta=\sqrt{\mathbf{G}^2+\mathbf{S}^2+\mathbf{T}^2}, \quad (4d)$$

$$\mathbf{N}^2=2(\mathbf{G}\pm\Delta)^2+(\mathbf{S}+\mathbf{T})^2 +(-\mathbf{S}+\mathbf{T})^2. \quad (4e)$$

Through out this paper, it should be noted that the upper sign $(+)$ refers to heavy hole (hh), the lower sign $(-)$ to light hole (lh).

Using Eq. (2), we can arrive with the following analytical formula of effective hole-masses $(m'_\pm)$ along the growth direction. Expressed in terms of interaction parameters, the effective masses, $(m'_\pm)$ in units of free electron mass $(m_\circ)$, both for hh $(+)$ and lh $(-)$ in vicinity of the zone center can be written as

$$\frac{1}{m'_\pm}=\frac{a^2}{2\hbar^2}\left\{\begin{matrix}\frac{4}{3}(2E_{xx}+E_{zz})\\ \pm\frac{1}{\sqrt{3}}(E_{xx}-E_{zz}-2E_{xy})\Delta\sin\theta\end{matrix}\right\}. \quad (5)$$

h is Planck's constant

h takes the value of 6.6x10^-34 J.s

The calculated results of hh and lh effective masses as a function of the growth direction are shown in Fig. 1 for $In_{0.53}Ga_{0.47}As$ QWs.

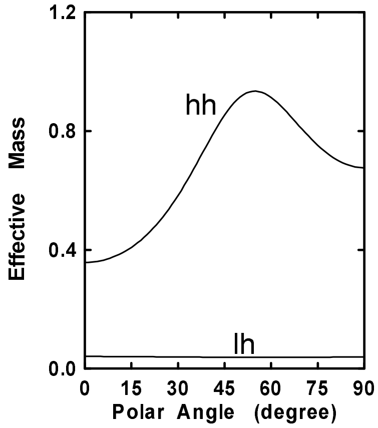

Fig.1. Effective masses (in units of $m_\circ$) of the heavy hole (hh) and light hole (lh) as a function of polar angles.

The hh effective mass is found to have a strong dependence on the substrate orientation, but not the lh effective mass. It is shown that the hh effective mass exhibits its maximum value on the samples grown along the [111] direction, and its minimum value along the [001] direction.

For simplicity, a QW within infinite barrier height approximation is now adopted. Hence, the squared interband momentum matrices at the zone center for $x'-$, $y'-$, and $z'-$polarizations can be calculated as [8,19,20]

$$|\mathbf{M}_{x'}|^2 = \frac{\mathbf{P}_{cv}^2}{\mathbf{N}^2}\left|-\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}(\mathbf{G}\pm\Delta)+\frac{\mathbf{1}}{\sqrt{\mathbf{6}}}(-\mathbf{S}+\mathbf{T})\right|^2 + \frac{\mathbf{P}_{cv}^2}{\mathbf{N}^2}\left|\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}(\mathbf{G}\pm\Delta)-\frac{\mathbf{1}}{\sqrt{\mathbf{6}}}(\mathbf{S}+\mathbf{T})\right|^2, \qquad (6a)$$

$$|\mathbf{M}_{y'}|^2 = \frac{\mathbf{P}_{cv}^2}{\mathbf{N}^2}\left|-\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}(\mathbf{G}\pm\Delta)-\frac{\mathbf{1}}{\sqrt{\mathbf{6}}}(-\mathbf{S}+\mathbf{T})\right|^2 + \frac{\mathbf{P}_{cv}^2}{\mathbf{N}^2}\left|-\frac{\mathbf{1}}{\sqrt{\mathbf{2}}}(\mathbf{G}\pm\Delta)-\frac{\mathbf{1}}{\sqrt{\mathbf{6}}}(\mathbf{S}+\mathbf{T})\right|^2, \qquad (6b)$$

$$|\mathbf{M}_{z'}|^2 = \frac{\mathbf{2}}{\mathbf{3N}^2}\left|(-\mathbf{S}+\mathbf{T})\right|^2\mathbf{P}_{cv}^2 + \frac{\mathbf{2}}{\mathbf{3N}^2}\left|(\mathbf{S}+\mathbf{T})\right|^2\mathbf{P}_{cv}^2, \qquad (6c)$$

respectively, where $\mathbf{P}_{cv}$ is a momentum matrix parameter between orbital $'s'$ and $'p'$ states. $\mathbf{M}_b^2 = \mathbf{1/3}\,\mathbf{P}_{cv}^2$ is the bulk momentum matrix element.

As a function of the substrate orientation, Figs.2(a)(b) and Figs.3(a)(b) show the calculated results (in units of $\mathbf{P}_{cv}^2$) of the squared optical matrix elements for the $c-hh$ and $c-lh$ transition, respectively, where $'c'$ denotes the conduction band.

From these figures, it became clear that the optical properties of these QWs should be sensitive to the crystallographic directions of the epitaxial growth.

Generally, the in-plane optical anisotropy ρ is defined as

$$\rho = \frac{|\mathbf{M}_{x'}|^2 - |\mathbf{M}_{y'}|^2}{|\mathbf{M}_{x'}|^2 + |\mathbf{M}_{y'}|^2}, \qquad (7)$$

where $|\mathbf{M}_{x'}|^2$ and $|\mathbf{M}_{y'}|^2$ are the squared momentum matrix elements for the polarization parallel to the in-plane $x'-$direction and $y'-$direction, respectively. So, the in-plane optical anisotropy ρ can be written as

$$\rho = \frac{2\sqrt{3}\sin\theta(1-\frac{3}{2}\sin^2\theta)(\mathbf{G}\pm\Delta)}{(4-3\sin^2\theta)(1-\frac{3}{2}\sin^2\theta)^2+3(\mathbf{G}\pm\Delta)^2}. \qquad (8)$$

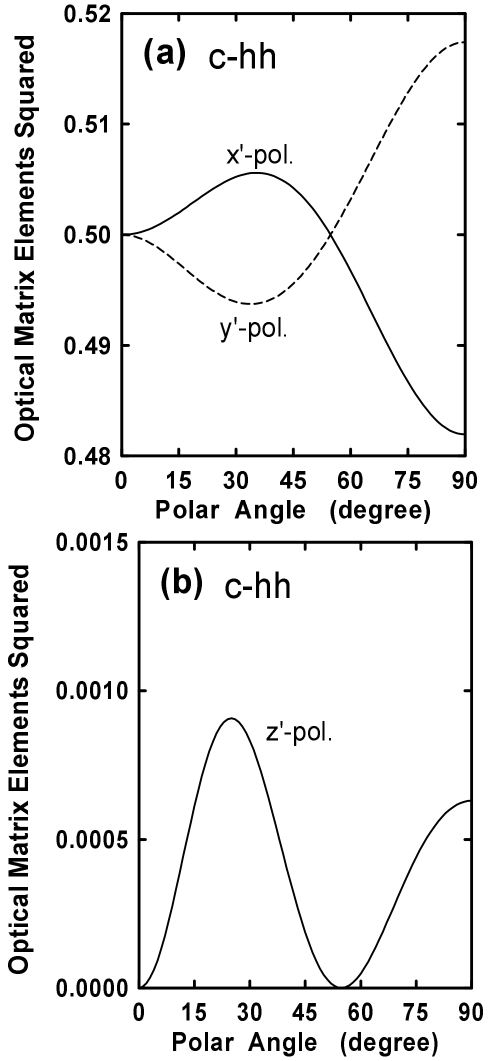

Fig.2. The squared optical matrix elements (in units of P_{cv}^{2}) of the $c-hh$ interband transition for (a) $x'-$ as well as $y'-$ polarization light and (b) $z'-$polarization light as a function of polar angles.

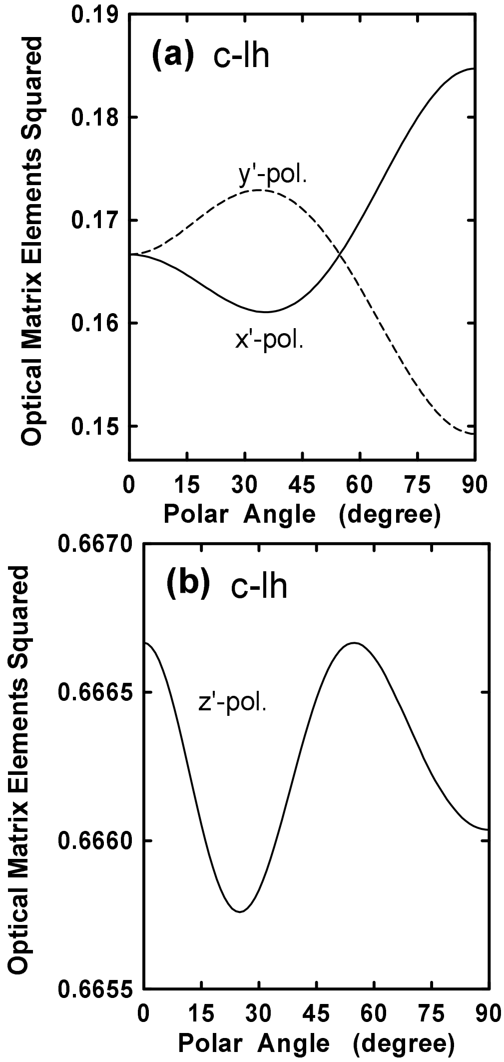

Fig.3. The squared optical matrix elements (in units of P_{cv}^{2}) of the $c-lh$ interband transition for (a) $x'-$ as well as $y'-$ polarization light and (b) $z'-$polarization light as a function of polar angles.

Figure 4 illustrates the optical anisotropy ρ of the $c-hh$ and $c-lh$ interband transition. The result of this calculation shows that no in-plane anisotropy is induced for structures grown on (001) and (111) QW planes. The anisotropy reaches its peak value on (110) well plane. Since (001) and (111)-oriented QWs belong to D_{4h} and D_{3d} high-symmetry point groups, respectively, their polarization properties are isotropic in the layer plane. Furthermore, other QW orientations have only low two-fold symmetry such as D_{2h} for (110), and hence their polarization properties are presented in anisotropy. A fundamental consequence of symmetry reduction is that the interplay of the zone-center mixing leads to anisotropy.

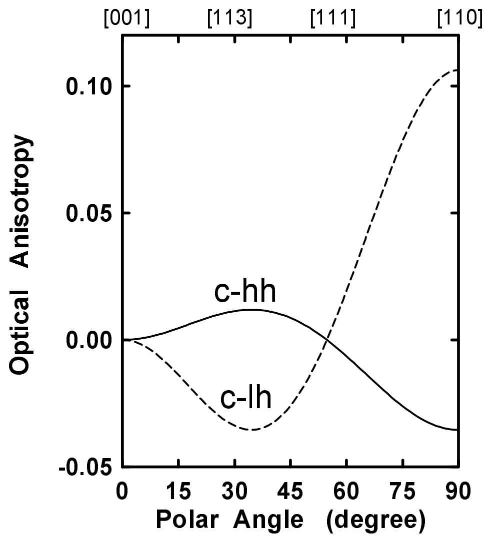

Fig.4. The degree of in-plane optical anisotropy of the $c-hh$ and $c-lh$ transition as a function of polar angle.

4. CONCLUSION

In conclusion, we have presented the explicit mathematical expressions of the optical transition matrix elements and hole effective masses. It has been shown that the (110) well plane exhibits the largest anisotropy among the various QW planes, but the (001) and (111) well plane are found to be completely polarization independent. The effective mass of heavy hole has been found to have a strong dependence on the substrate orientation, and it exhibits its maximum value on the samples grown along the [111] direction. Therefore, our investigation can offer useful guideline for the design of the polarization control devices.

5. REFERENCES

1. R. H. Henderson and E. Towe, ” Effective mass theory for Ⅲ - V semiconductors on arbitrary (hkl) surfaces,” J. Appl. Phys., Vol. 79, 1996, pp. 2029.
2. Y. Kajikawa, M. Hata, N. Sugiyama, and Y. Katayama,“Anisotropic optical matrix elements in (11N)-oriented Analytical k · p method: quantum wells” ,Phys. Rev. B, Vol. 42, 1990, pp. 9540.
3. Y. Kajikawa, O. Brandt, K. Kanamoto, and N. Tsukada,“Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band” , J. Cryst. Gowth, Vol. 150, 1995, pp. 431.
4. H. Dhrvhyrt, L. D. Shvartsman, and J. E. Golub, “Analytical k · p Anisotropic optical matrix elements in (11N)-oriented quantum wells method”:Phys. Rev. B, Vol. 51, 1995, pp. 10857.
5. R. A. Abram and M. Jaros, “Band Structure Engineering in Semiconductor Microstructures”, Plenum, New York, 1989.
6. A. Niwa, T. Ohtoshi, and T. Kuroda,“Optical anisotropy in [hkil]-oriented wurtzite semiconductor quantum wells” ,IEEE J. Sel. Top. Quantum Electron, Vol. 1, 1995, pp. 211.
7. J. B. Xia, Phys.Rev. B, “Growth of p-type GaAs/AlGaAs(111) quantum

well infrared photodetector using solid source molecular-beam epitaxy" ,Vol. 43, 1991, pp. 9856.

8. Y. Kajikawa,"Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" ,J. Appl. Phys., Vol. 86, 1999, pp. 5663.
9. R. H. Henderson and E. Towe, "Effective mass theory for Ⅲ-Ⅴband gaps of [11N]-oriented Ⅲ - Ⅴ epliayers " ,J. Appl. Phys., Vol. 78, 1995, pp. 2447.
10. Y. Kajikawa, M. Hata, T. Isu, and Y. Katayama, "Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band", Surf. Sci., Vol. 267, 1992, pp. 501.
11. D. S. McCallum, X. R. Huang, and Arthur L. Smirl, " Effects of Crystaiiographic Grientation and Strain on Quantum Confined Structures and Devices," , Appl. Phys. Lett., Vol. 66, 1995, pp. 2885.
12. G. Armelles, P. Castrillo, P. S. Dominguez, L. Gonzales, A. Ruiz, D. A. Contreras-Solorio, V. R. Velasco, and F. Garcia-Moliner, "Optical anisotropy of (113)-oriented GaAs/AlAs superiattices" ,Phys. Rev. B, Vol. 49, 1994, pp. 14020.
13. R. H. Henderson, D. Sun, and E. Towe, "Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" , Surf. Sci., Vol. 327, 1995, pp. L521.
14. C. N. Chen, " Fabrication and Study of ZnO-Based MIS Photodetectors and Heterostructure Devices" , J. Appl. Phys., Vol. 96, 2004, pp. 7473.
15. Y. C. Chang, " Band parameters for III–V compound semiconductors and their alloys" ,Phys. Rev. B, Vol. 37, 1988, pp. 8215.
16. S. F. Tsay, J. C. Chiang, Z. M. Chau, and I. Lo, " Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" , Phys. Rev. B, Vol. 56, 1997, pp. 13242.
17. C. N. Chen, Y. H. Wang, M. P. Houng, and J. C. Chiang, " Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" , Jap. J. Appl. Phys. Part 1, Vol. 41, 2002, pp. 36.
18. A. A. Yamaguchi, K. Nishi, and A. Usui, " In-plane anisotropic lasing characteristics of (110)-oriented GaInAsP quantum-well lasers" , Jpn. J. Appl. Phys. Part 2, Vol. 33, 1994, pp. L912.
19. Y. Kajikawa, "Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" , Phys. Rev. B, Vol. 47, 1993, pp. 3649.
20. Y. Kajikawa, " Optical anisotropy of (11l)-oriented strained quantum-wells calculated with the effect of the spin-orbit split-off band" , Phys. Rev. B, Vol. 51, 1995, pp. 16790.