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$\boldsymbol{k}\cdot\boldsymbol{p}$ Zincblende Hamiltonian and Optical Matrix with Bulk Inversion Asymmetry

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A conventional 8 × 8 $\boldsymbol{k}\cdot\boldsymbol{p}$ zincblende Hamiltonian is corrected to include the bulk (or intracell) inversion asymmetry. Meanwhile, a conventional 8 × 8 $\boldsymbol{k}\cdot\boldsymbol{p}$ zincblende optical matrix is also corrected to include this intracell asymmetry.

1. Introduction

In zincblende semiconductors, the odd-in-k terms exist in both bulk and quantum well expressions due to the bulk inversion asymmetry (i.e., tetrahedral symmetry) effect. The presence of these terms is shown to induce the spin-splitting phenomena, which have been extensively studied both experimentally[1,2] and theoretically.[3–7]

In our previous article,[8] we had demonstrated the effect of the bulk inversion asymmetry on the optical transitions in zincblende semiconductor quantum wells. The results have shown that asymmetry effects cause a clear difference in the optical transition strength.[8]

In semiconductor physics, the conventional $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism does not take into account the tetrahedral symmetry within a unit cell.[9–17] However, this symmetry property can be accounted for by inserting the Kane B_0 parameter terms (i.e., $B_0k_xk_y$, $B_0k_yk_z$, and $B_0k_xk_z$) into the conventional sp^3 $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian matrix.[8,9,17] Accordingly, the aim of this study is to incorporate bulk (or intracell) inversion asymmetry into the matrix elements of the conventional 8×8 $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian and optical matrix.

Although the effects of inversion asymmetry within the unit cell are not accounted for in the conventional $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism, these effects are though to play a key role in determining the electronic and optical properties of semiconductors.[8,17]

2. Theoretical Method

The resulting $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian with bulk inversion asymmetry (in the sp^3 basis ordering as $|S\rangle$, $|X\rangle$, $|Y\rangle$, $|Z\rangle$) has the form[9]

$$H = \begin{bmatrix} E_c + \hbar^2k^2/2m_c & B_0(\boldsymbol{q}\cdot\hat{x}) + iP_0(\boldsymbol{k}\cdot\hat{x}) & B_0(\boldsymbol{q}\cdot\hat{y}) + iP_0(\boldsymbol{k}\cdot\hat{y}) & B_0(\boldsymbol{q}\cdot\hat{z}) + iP_0(\boldsymbol{k}\cdot\hat{z}) \\ B_0(\boldsymbol{q}\cdot\hat{x}) - iP_0(\boldsymbol{k}\cdot\hat{x}) & E_v + Lk_x^2 + M(k_y^2+k_z^2) & Nk_xk_y & Nk_xk_z \\ B_0(\boldsymbol{q}\cdot\hat{y}) - iP_0(\boldsymbol{k}\cdot\hat{y}) & Nk_xk_y & E_v + Lk_y^2 + M(k_z^2+k_x^2) & Nk_yk_z \\ B_0(\boldsymbol{q}\cdot\hat{z}) - iP_0(\boldsymbol{k}\cdot\hat{z}) & Nk_xk_z & Nk_yk_z & E_v + Lk_z^2 + M(k_x^2+k_y^2) \end{bmatrix}, \tag{1}$$

where $\boldsymbol{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$, $\boldsymbol{q} = k_yk_z\hat{x} + k_zk_x\hat{y} + k_xk_y\hat{z}$, P_0 (in units of eV Å) is the Kane parameter, i.e., $P_0 = (\hbar/m_0)\langle s|p_x|x\rangle$, and B_0 (in units of eV Å^2) is given by

$$B_0 = 2\frac{\hbar^2}{m^2}\sum_j^{\Gamma_{15}} \frac{\langle s|p_x|u_j\rangle\langle u_j|p_y|z\rangle}{[(E_c+E_v)/2 - E_j]}. \tag{2}$$

It is noted that in eq. (1), the B_0 terms are the only matrix elements that are incompatible with inversion symmetry.

The resulting 8×8 $\boldsymbol{k}\cdot\boldsymbol{p}$ Hamiltonian with bulk inversion asymmetry (in the spin–orbit coupling basis ordering as $|iS\uparrow\rangle$, $|iS\downarrow\rangle$, $|3/2,3/2\rangle$, $|3/2,1/2\rangle$, $|3/2,-1/2\rangle$, $|3/2,-3/2\rangle$, $|1/2,1/2\rangle$, $|1/2,-1/2\rangle$) can be expressed as

$$H_{8\times8} = \begin{bmatrix} A & 0 & S & T & \frac{R}{\sqrt{3}} & 0 & \frac{T}{\sqrt{2}} & \frac{\sqrt{2}}{\sqrt{3}}R \\ 0 & A & 0 & \frac{S}{\sqrt{3}} & T & R & -\frac{\sqrt{2}}{\sqrt{3}}S & -\frac{T}{\sqrt{2}} \\ S^* & 0 & P+Q & D & C & 0 & \frac{D}{\sqrt{2}} & \sqrt{2}C \\ T^* & \frac{S^*}{\sqrt{3}} & D^* & P-Q & 0 & C & -\sqrt{2}Q & -\frac{\sqrt{3}}{\sqrt{2}}D \\ \frac{R^*}{\sqrt{3}} & T^* & C^* & 0 & P-Q & -D & -\frac{\sqrt{3}}{\sqrt{2}}D^* & \sqrt{2}Q \\ 0 & R^* & 0 & C^* & -D^* & P+Q & -\sqrt{2}C^* & \frac{D^*}{\sqrt{2}} \\ \frac{T^*}{\sqrt{2}} & -\frac{\sqrt{2}}{\sqrt{3}}S^* & \frac{D^*}{\sqrt{2}} & -\sqrt{2}Q & -\frac{\sqrt{3}}{\sqrt{2}}D & -\sqrt{2}C & P-\Delta & 0 \\ \frac{\sqrt{2}}{\sqrt{3}}R^* & -\frac{T^*}{\sqrt{2}} & \sqrt{2}C^* & -\frac{\sqrt{3}}{\sqrt{2}}D^* & \sqrt{2}Q & \frac{D}{\sqrt{2}} & 0 & P-\Delta \end{bmatrix}, \tag{3}$$

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where $*$ denotes the Hermitian conjugate, and the matrix elements can be written as

$$A = E_c + \frac{\hbar^2 k^2}{2m_c},$$
$$S = -\frac{1}{\sqrt{2}}\langle iS|H|X+iY\rangle = i\frac{B_0}{\sqrt{2}}\boldsymbol{q}\cdot(\hat{x}+i\hat{y}) - \frac{P_0}{\sqrt{2}}\boldsymbol{k}\cdot(\hat{x}+i\hat{y}),$$
$$R = \frac{1}{\sqrt{2}}\langle iS|H|X-iY\rangle = -i\frac{B_0}{\sqrt{2}}\boldsymbol{q}\cdot(\hat{x}-i\hat{y}) + \frac{P_0}{\sqrt{2}}\boldsymbol{k}\cdot(\hat{x}-i\hat{y}),$$
$$T = \frac{\sqrt{2}}{\sqrt{3}}\langle iS|H|Z\rangle = -i\frac{\sqrt{2}}{\sqrt{3}}B_0\boldsymbol{q}\cdot\hat{z} + \frac{\sqrt{2}}{\sqrt{3}}P_0\boldsymbol{k}\cdot\hat{z},$$
$$C = -\frac{1}{2\sqrt{3}}\langle X+iY|H|X-iY\rangle,$$
$$D = -\frac{1}{\sqrt{3}}\langle X+iY|H|Z\rangle,$$
$$P = \frac{1}{3}\langle X+iY|H|X+iY\rangle + \frac{1}{3}\langle Z|H|Z\rangle,$$
$$Q = \frac{1}{6}\langle X+iY|H|X+iY\rangle - \frac{1}{3}\langle Z|H|Z\rangle.$$

Other than the matrix elements (S, R, and T) described above, all other elements are the same as those of the conventional 8×8 $\boldsymbol{k}{\cdot}\boldsymbol{p}$ Hamiltonian.

The present study applies a conceptually straightforward approach to derive an analytical expression for the momentum (or optical) matrix elements, $\mathbf{M}_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k})_{i,j}$ with the spin–orbit coupling basis $i,j = 1$–8. The first-order derivative of the $\boldsymbol{k}{\cdot}\boldsymbol{p}$ Hamiltonian with respective to the wave vector $\mathbf{k}$ is given by[12,13,15,16)]

$$\boldsymbol{\varepsilon}_\xi\cdot\mathbf{M}_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k})_{i,j} = \boldsymbol{\varepsilon}_\xi\cdot\left[\frac{\partial\mathbf{H}_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k})_{i,j}}{\partial\mathbf{k}}\right], \tag{4}$$

where $\boldsymbol{\varepsilon}_\xi$ is the unit vector of the ξ-polarization optical field, and ξ ($= x$, y, or z) is the polarization direction of the optical field.

The expansion for the quantum-well state $|n,\mathbf{k}_\parallel\rangle$ is written as

$$|n,\mathbf{k}_\parallel\rangle = \sum_{j,k_z} F_j(n,\mathbf{k}_\parallel,k_z)|j,\mathbf{k}\rangle, \tag{5}$$

where j is the spin–orbit coupling basis, n is a label for the subband index of the quantum well, $\mathbf{k} = \mathbf{k}_\parallel + k_z\hat{z}$, and $F_j(n,\mathbf{k}_\parallel,z)$ is the so-called envelope function of the quantum-well state and is given by the following Fourier transform:

$$F_j(n,\mathbf{k}_\parallel,z) \equiv \sum_{k_z} F_j(n,\mathbf{k}_\parallel,k_z)e^{ik_z z}. \tag{6}$$

The momentum matrix element between subband states $|n',\mathbf{k}_\parallel\rangle$ and $|n,\mathbf{k}_\parallel\rangle$ is given by[12,13,15,16)]

$$\begin{aligned}
&\boldsymbol{\varepsilon}_\xi\cdot\mathbf{M}_{n',n}(\mathbf{k}_\parallel)\\
&\quad= \sum_{i,j,k_z} F_i(n',\mathbf{k}_\parallel,k_z) * [\boldsymbol{\varepsilon}_\xi\cdot\mathbf{M}_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k})_{i,j}]F_j(n,\mathbf{k}_\parallel,k_z)\\
&\quad= \boldsymbol{\varepsilon}_\xi\cdot\sum_{i,j}\int dz F_i(n',\mathbf{k}_\parallel,z) * \mathbf{O}_{i,j}(\mathbf{k}_\parallel,z)F_j(n,\mathbf{k}_\parallel,z)\\
&\quad\quad+\frac{1}{2}\boldsymbol{\varepsilon}_\xi\cdot\sum_{i,j}\int dz\left[-i\frac{d}{dz}F_i(n',\mathbf{k}_\parallel,z)\right]\\
&\quad\quad* \mathbf{Q}_{i,j}(\mathbf{k}_\parallel,z)F_j(n,\mathbf{k}_\parallel,z)\\
&\quad\quad+\frac{1}{2}\boldsymbol{\varepsilon}_\xi\cdot\sum_{i,j}\int dz F_i(n',\mathbf{k}_\parallel,z)\\
&\quad\quad* \mathbf{Q}_{i,j}(\mathbf{k}_\parallel,z)\left[-i\frac{d}{dz}F_j(n,\mathbf{k}_\parallel,z)\right],
\end{aligned} \tag{7}$$

where $\boldsymbol{\varepsilon}_\xi\cdot\mathbf{O}_{i,j}(\mathbf{k}_\parallel,z)$ and $\boldsymbol{\varepsilon}_\xi\cdot\mathbf{Q}_{i,j}(\mathbf{k}_\parallel,z)$ are the ξ-polarization momentum (or optical) matrix elements in the finite-difference scheme.

3. Results and Discussion

Owing to the adopted bulk inversion asymmetry effect, some of the conventional Hamiltonian matrix elements in the 8×8 $\boldsymbol{k}{\cdot}\boldsymbol{p}$ framework should be corrected as

$$\begin{aligned}
H_{13} &= \sqrt{3}H_{24} = -\frac{\sqrt{3}}{\sqrt{2}}H_{27}\\
&= -\frac{B_0}{\sqrt{2}}(k_x - ik_y)k_z - \frac{P_0}{\sqrt{2}}(k_x+ik_y),\\
H_{26} &= \sqrt{3}H_{15} = \frac{\sqrt{3}}{\sqrt{2}}H_{18}\\
&= -\frac{B_0}{\sqrt{2}}(k_x + ik_y)k_z + \frac{P_0}{\sqrt{2}}(k_x-ik_y),\\
H_{14} &= \sqrt{2}H_{17} = H_{25} = -\sqrt{2}H_{28}\\
&= -i\frac{\sqrt{2}}{\sqrt{3}}B_0k_xk_y + \frac{\sqrt{2}}{\sqrt{3}}P_0k_z.
\end{aligned}$$

Note that the 8×8 $\boldsymbol{k}{\cdot}\boldsymbol{p}$ Hamiltonian is Hermitian, which results in $H_{ij} = H_{ji}^*$ with $i,j = 1$–8. Other than the matrix elements described above, all other elements are the same as those of the conventional 8×8 $\boldsymbol{k}{\cdot}\boldsymbol{p}$ Hamiltonian.

Owing to the adopted bulk inversion asymmetry effect, some of the conventional 8×8 optical matrix elements (in the finite-difference scheme) should be corrected as follws.

(1) The corrected x-polarization matrixes $\boldsymbol{\varepsilon}_x\cdot\mathbf{O}_{i,j}(\mathbf{k}_\parallel,z)$ and $\boldsymbol{\varepsilon}_x\cdot\mathbf{Q}_{i,j}(\mathbf{k}_\parallel,z)$ in the same basis ordering as the Hamiltonian are given by

$$O_{14} = \sqrt{2}O_{17} = O_{25} = -\sqrt{2}O_{28} = -i\frac{\sqrt{2}}{\sqrt{3}}B_0k_y,$$
$$Q_{13} = \sqrt{3}Q_{24} = -\frac{\sqrt{3}}{\sqrt{2}}Q_{27} = -\frac{B_0}{\sqrt{2}},$$
$$Q_{26} = \sqrt{3}Q_{15} = \frac{\sqrt{3}}{\sqrt{2}}Q_{18} = -\frac{B_0}{\sqrt{2}}.$$

(2) The corrected y-polarization matrixes $\boldsymbol{\varepsilon}_y\cdot\mathbf{O}_{i,j}(\mathbf{k}_\parallel,z)$ and $\boldsymbol{\varepsilon}_y\cdot\mathbf{Q}_{i,j}(\mathbf{k}_\parallel,z)$ in the same basis ordering as the Hamiltonian are given by

$$O_{14} = \sqrt{2}O_{17} = O_{25} = -\sqrt{2}O_{28} = -i\frac{\sqrt{2}}{\sqrt{3}}B_0k_x,$$
$$Q_{13} = \sqrt{3}Q_{24} = -\frac{\sqrt{3}}{\sqrt{2}}Q_{27} = i\frac{B_0}{\sqrt{2}},$$
$$Q_{26} = \sqrt{3}Q_{15} = \frac{\sqrt{3}}{\sqrt{2}}Q_{18} = -i\frac{B_0}{\sqrt{2}}.$$

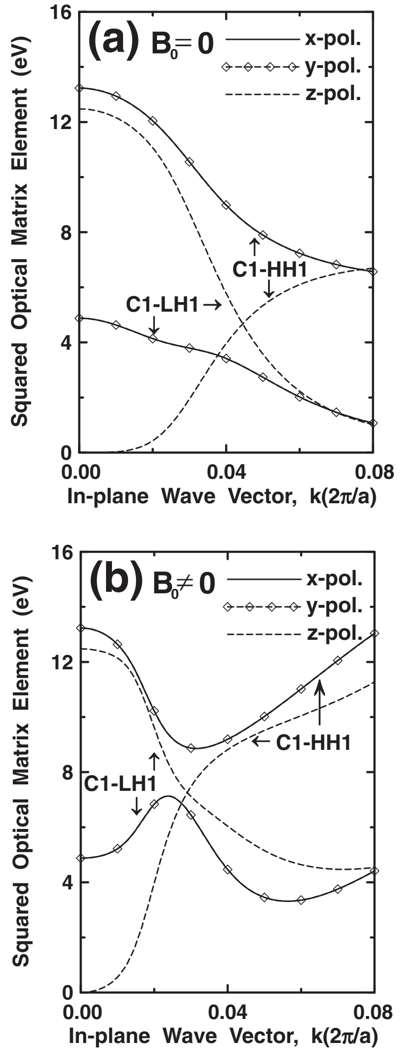

Fig. 1. Squared optical matrix elements of C1–HH1 and C1–LH1 transitions for 50 Å well-width GaSb/AlSb quantum wells for (a) $B_0 = 0$ and (b) $B_0 \neq 0$, respectively.

(3) The corrected z-polarization matrixes $\boldsymbol{\varepsilon}_z \cdot \mathbf{O}_{i,j}(\mathbf{k}_\parallel, z)$ and $\boldsymbol{\varepsilon}_z \cdot \mathbf{Q}_{i,j}(\mathbf{k}_\parallel, z)$ in the same basis ordering as the Hamiltonian are given by

$$O_{13} = \sqrt{3}O_{24} = -\frac{\sqrt{3}}{\sqrt{2}}O_{27} = -\frac{B_0}{\sqrt{2}}(k_x - ik_y),$$

$$O_{26} = \sqrt{3}O_{15} = \frac{\sqrt{3}}{\sqrt{2}}O_{18} = -\frac{B_0}{\sqrt{2}}(k_x + ik_y).$$

Note that $O_{ij} = O_{ji}^*$ and $Q_{ij} = Q_{ji}^*$ $(i,j = 1$–$8)$ in the above matrix elements. Other than the matrix elements described above, all other elements are the same as those of the conventional 8×8 optical matrix. All of the matrix elements presented above can be divided by a factor of $(\hbar^2/2m_0)$ to yield units of eV.

The value of B_0 can be obtained from [also see eq. (40a) in ref. 9]

$$\gamma = \frac{2}{3}P_0 B_0 \frac{\Delta}{E_g(E_g + \Delta)},$$

where γ is the conduction band spin-splitting parameter for the bulk semiconductor.[9,17–21] It has been shown experimentally that $\gamma = 186\,\text{eV}\,\text{Å}^3$ for GaSb.[20–22] Consequently, B_0 has a value of $43.1\,\text{eV}\,\text{Å}^2$ for the zincblende semiconductor quantum wells considered in the current analysis. Applying this value to calculate the optical transition strength of 50 Å well-width GaSb/AlSb quantum wells. As shown in Figs. 1(a) and 1(b), the results reveal that asymmetry effects (B_0 terms) can cause a clear difference in the optical transition strength.

4. Conclusions

We have corrected the conventional 8×8 $\boldsymbol{k}\cdot\boldsymbol{p}$ zincblende Hamiltonian and optical matrix to include the bulk (or intracell) inversion asymmetry. By comparing the conventional $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism, the enhanced 8×8 $\boldsymbol{k}\cdot\boldsymbol{p}$ zincblende Hamiltonian and optical matrix have shown some extra terms (B_0 terms).

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