Magneto-optical Transitions in Electron-Piezoelectric Phonon Scattering Materials Using Projected Liouville Equation

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ABSTRACT

Using the projected Liouville equation, we theoretically investigated the temperature dependence of the magneto-optical cyclotron transition of the quasi two-dimensional Landau splitting system in GaAs and CdS. Through the analysis, we found that the line-widths of GaAs and CdS increased with the increase in temperature. We also found that $\gamma_{\text{total}}(B)$ of GaAs < $\gamma_{\text{total}}(B)$ of CdS in the magnetic field region of $B > 4.2 \, \text{T}$ and we presented reasonable resonating pictures of the line-shapes.

Keywords: Electron-piezoelectric materials, Magneto-optical transition, Phonon scattering, Projected Liouville equation

1. Introduction

The electronic state in crystals is known to be quantized in the $x$–$y$ plane in the presence of a static magnetic field applied along the $z$–axis. When an electromagnetic wave is applied to a system, the electrons absorb the proper photon energies to make magneto-optical transitions, among which the cyclotron transition is the most typical one [1]. Several studies have used the conductivity formalism, which is based on the Liouville equation, to successfully handle the cyclotron transition phenomena [2–7]. We also used the projected Liouville equation method with the equilibrium average projection technique (EAPT) in a previous study [8]. The advantage of using the EAPT is that the quantum response function and the scattering factor formula can be obtained in a single-step by expanding the quantum transport theory. Furthermore, the optical power absorption spectrum of the measured transitions is directly related to both the electric conductivity tensor and the line-width of the spectrum with its line-shape function.

In our previous studies [8–14], we applied the EAPT theory to Ge and Si, because there are abundant experimental data on non-confining deformation potential systems. We also compared our numerical calculation results using the EAPT theory with the existing experimental data and found them to be in good agreement with each other. However, the EAPT theory was only applicable to non-confining deformation potential systems with an extremely weak coupling approximation. We therefore suggested a more precise procedure for the expansion and application of the EAPT theory to low-dimensional electron systems with a moderately weak coupling approximation (MWCA). Using the MWCA, the distribution components can provide an adequate explanation of the quantum transition processes [15–17].

In this study, through a numerical calculation of the theoretical result, we analyzed the magneto-optical cyclotron transition in electron-piezoelectric phonon scattering materials such as GaAs and CdS. In this paper, we first review a previously presented theory, and then, using the MWCA for piezoelectric materials, we modify the formula into one that is easily manageable. Next, we calculate the line-widths of GaAs and CdS for $\lambda = 220, 394, 513, 550$, and $720 \, \mu\text{m}$. Finally, we present the conclusions of the study.

2. Theory

When a static magnetic field $\vec{B} = B\hat{z}$ is applied to an electron system, the single electron energy state is quantized to the Landau levels. In this study, we consider a system of electrons confined in an infinite square well potential between $z = 0$ and $z = L_z$ in the $z$–direction. An oscillatory electric field $E(t) = E_0 \exp(i\omega t)$ is assumed to be applied along the $z$–axis, which delivers the absorption power to the system as $P_{\text{abs}}(\omega) = (E_0^2/2) \text{Re}(\sigma(\omega))$. In this equation, $\text{Re}$ refers to the real component and $\sigma(\omega)$ refers to the magneto-optical conductivity tensor, which is the coefficient of the aforementioned formula. Here, the absorption power represents the cyclotron transition line-shapes, and the scattering factor function represents the line-widths. We obtained the Hamiltonian of the aforementioned electron-piezoelectric phonon scattering system as follows:

$$H_{\text{total}} = H_{\text{e}} + H_{\text{ph}} + V$$

$$= \sum_\alpha \langle \alpha | \hat{p}_\alpha \hat{a}_\alpha^\dagger \rangle + \sum_\alpha \sum_\delta \sum_{\sigma_1} \sum_{\sigma_2} C_{\delta \sigma_1 \sigma_2} \langle \sigma_1 | \hat{a}_\alpha^\dagger \hat{a}_{\delta \sigma_2} \rangle \hat{b}_\alpha \hat{b}_\sigma \hat{b}_\delta.$$  \hspace{1cm} (1)

In Eq. (1), $H_{\text{e}}$ refers to the electron Hamiltonian, $H_{\text{ph}}$ to the phonon Hamiltonian, and $V$ to the electron-piezoelectric phonon interaction Hamiltonian. Furthermore, $\hat{b}_\sigma^\dagger(\hat{b}_\delta)$ refers to the creation operator (annihilation operator) of the boson particles and $\hat{q}$ to the...
phonon wave vector. The interaction Hamiltonian of the aforementioned system is represented by $V$, where the coupling matrix element of the electron-phonon interaction $C_{i,j}(q)$ is $C_{i,j}(q) = \frac{g^2}{\hbar^2} \left\{ \langle \phi| \exp(iq \cdot \vec{r})|\psi\rangle \right\}$, and $\vec{r}$ is the position vector of the electrons. For the magneto-optical quantum transition system under a circularly polarized external field, the operators $J^+\alpha$ are defined as $J^+\alpha = \sum_{\beta} J_{\alpha\beta} a^\dagger_{\beta} a_{\alpha}$, and $\sum_{\beta}$ are the two components of the single electron current operator $J$. Regarding the Landau gauge, the magnetic field $B$ is perpendicular to the barriers of the well, and the distance between the barriers is assumed to be infinite. From the eigenstate, we can obtain the matrix element of the current as $J_{\alpha\beta} = -i\hbar \langle 2(N_c + 1)\hbar c/m^* \rangle$, where $m^*$ is the effective mass of the electrons. In a previous study [8], we derived the current in the $\omega$ space as $\operatorname{Re} \langle \sigma_\alpha(\omega) \rangle \mathcal{E}_\alpha(\omega)$. Furthermore, by using the properties of the projection operator and the conventional series expansion of the propagator, we obtained the scattering factor where the conductivity tensor $\sigma_{\alpha\beta}$ is negligible in a real system owing to its small value; we define it as $\sigma_\alpha(\omega)$. We used the following relationship $\langle \sigma_\alpha(\omega) \rangle$ is the position vector of the electrons. For the magneto-optical electron-phonon interaction system, we approximated a weak interacting system as well as an interacting system, as follows:

$$\sigma_\alpha(\omega) = \frac{-i(\hbar/2)}{i\omega - \mathcal{A}_\alpha + \Xi_\alpha(\omega)},$$

$$\mathcal{A}_\alpha = -\left\{ \frac{i}{\hbar} \sum_{\beta} \int d\mathcal{F}_\alpha \mathcal{F}_\beta (f_{\alpha\beta} - f_\beta) \right\} = i\omega_\alpha,$$  (2)

where the diagonal propagator is denoted as $\mathcal{G}_\alpha = 1/(\hbar\omega - \mathcal{A}_\alpha)$, and $\omega_\alpha$ refers to the cyclotron frequency. We used the following relationship

$$\langle \operatorname{Tr} \{ Y^\dagger L^\dagger L^\prime L^\prime \} \rangle_{\mathcal{A}_\alpha} = \langle \operatorname{Tr} \{ Y Y^\dagger \} \rangle_{\mathcal{A}_\alpha},$$

$$\langle \operatorname{Tr} \{ \mathcal{R}_\alpha \mathcal{L}_\alpha \mathcal{R}_\alpha \cdots \mathcal{L}_\alpha \mathcal{L}_\alpha \mathcal{R}_\alpha \cdots \mathcal{R}_\alpha \} \rangle_{\mathcal{A}_\alpha} = (-1)^{\alpha} \langle \operatorname{Tr} \{ L^\dagger \cdots L^\dagger L^\dagger \cdots \mathcal{R}_\alpha \mathcal{L}_\alpha \mathcal{R}_\alpha \cdots \mathcal{R}_\alpha \} \rangle_{\mathcal{A}_\alpha},$$  (3)

here $\langle \cdots \rangle_{\mathcal{A}_\alpha}$ refers to the ensemble average of the background particle states and $\langle \cdots \rangle_{\mathcal{A}_\alpha}$ to the ensemble average of the electron states.

3. Line-shape function

3.1. Scattering factor function

The scattering factor function, $\Xi_\alpha(\omega)$, is expressed in the complex form as $\Xi_\alpha(\omega) = i\Delta_{\alpha\alpha} + \gamma_{\alpha\alpha}(\omega)$, where $\Delta_{\alpha\alpha} = \operatorname{Im} \Xi_\alpha(\omega)$ and $\gamma_{\alpha\alpha}(\omega) = \operatorname{Re} \Xi_\alpha(\omega)$ refer to the line-shift and half-width of the response-type formula, respectively. In most cases, the imaginary part of the scattering factor, $\Delta_{\alpha\alpha}$, is negligible in a real system owing to its small value; we define it as $\Xi_\alpha(\omega)$. The scattering factor function is schematically represented in Fig. 1, and its variation as a function of $\omega$ is illustrated in Fig. 2. By performing continuous approximation in a circularly polarized external field, the absorption power formula is obtained as follows:

$$\mathcal{P}_{\alpha\beta} = \left( \frac{e^2 c_0^2}{\pi \hbar c} \right) \gamma_{\alpha\beta}(\omega) \sum_{N_c} \int \frac{dk_q (N_c + 1)(f_q - f_{-q})}{(\omega - \omega_q)^2 + \gamma_{\alpha\beta}(\omega)},$$  (4)

$$\gamma_{\alpha\beta}(\omega) = \frac{\operatorname{Re} \Xi_\alpha(\omega)}{\sum_{N_c} \int \frac{dk_q (N_c + 1)(f_q - f_{-q})}{(\omega - \omega_q)^2 + \gamma_{\alpha\beta}(\omega)}}.$$

Here, the scattering factor function is expressed as follows:

$$\gamma_{\alpha\beta}(\omega) = \operatorname{Re} \Xi_\alpha(\omega) + \sum_{N_c} \int \frac{dk_q (N_c + 1)(f_q - f_{-q})}{(\omega - \omega_q)^2 + \gamma_{\alpha\beta}(\omega)},$$  (5)

In continuous approximation, the interaction matrix in an infinite square well potential system is expressed as follows:

$$C_{N_c, N_c}(\mathcal{E}_\alpha(\omega)) = \int_0^\infty K_{\alpha\beta}(t) F_{\alpha\beta}(\mathcal{E}_\alpha(\omega)) dt,$$

$$C_{N_c, N_c}(\mathcal{E}_\alpha(\omega)) = \int_0^\infty K_{\alpha\beta}(t) F_{\alpha\beta}(\mathcal{E}_\alpha(\omega)) dt,$$

where $N_c < N_{\beta}$ and $N_{\alpha} < N_{\beta}$, the $K$-matrix is expressed as follows:
\[ K_{\alpha \beta}^{\nu \delta} = \left( \frac{N_0 \gamma_0}{N_0 + 1} \right)^2 \left( \sqrt{N_0 + 1} \right)^2 \left( \sqrt{N_0 + 1} \right)^2 \exp(-\epsilon_i) \left[ L_{\nu \delta}^{\nu \delta}(t) L_{\nu \delta}^{\nu \delta}(t) \right]. \]

and where the Legendre function is expressed as follows:

\[ L_{\nu \delta}(t) = \frac{1}{n} \exp\left( \frac{1}{\tau} \int_{-\alpha}^{\alpha} \left[ t^{\nu \delta} \exp(-\epsilon_i) \right] \frac{r}{2} \left( q_i^2 + q_j^2 \right). \]

The matrix element of the confinement potential is

\[ |F_{\nu \delta}(q)| = \int \delta_{\nu \delta}(z) \exp(iqz) \delta_r^m(z) dq \]

Subsequently, through continuous approximation, we derived the integrand of the scattering factor as follows:

\[ Y_{\nu \delta} = Y_{\nu \delta}^{\nu \delta} + Y_{\nu \delta}^{\nu \delta} + Y_{\nu \delta}^{\nu \delta}. \]

Furthermore, we have the following:

\[ Y_{\nu \delta}^{\nu \delta} = S_{\nu \delta} \left( \delta_r \right) \left[ (N_0 + 1)(f_{\nu \delta} - f_{\nu \delta}) \right], \]

\[ Y_{\nu \delta}^{\nu \delta} = -S_{\nu \delta} \left( \delta_r \right) \left[ (N_0 + 1)(f_{\nu \delta} + f_{\nu \delta}) \right], \]

\[ Y_{\nu \delta}^{\nu \delta} = U_{\nu \delta} \left( \delta_r \right) \left[ (N_0 + 1)(f_{\nu \delta} + f_{\nu \delta}) \right]. \]

Using the interacting matrix, we have the following:

\[ S_{\nu \delta} \left( \delta_r \right) \left[ \left( q_i^2 + q_j^2 \right) \right], \]

\[ + \left[ \left( q_i^2 + q_j^2 \right) \right], \]

\[ + \left[ \left( q_i^2 + q_j^2 \right) \right]. \]

3.2. A realistic recipe

Following Meijer and Polder [18], we adopted the isotropic interaction formalism to choose the interaction factor \( V_q \) expressed as follows:

\[ |V_q| = \frac{1}{2 \hbar \epsilon_q} \frac{1}{2 \hbar \epsilon_q}. \]

Here, \( \epsilon_q \) refers to the electrochemical constant, \( \nu \) to the sound velocity in solid, \( \Omega \) to the volume of the system, \( \epsilon_q \) to the permittivity of free space, and \( \Sigma \) to the dielectric constant. The Fermi-Dirac distribution functions are \( f_1 = 1/[e^{\epsilon_q/2} + 1] \) and \( f_2 = 1/[e^{\epsilon_q/2} + 1] \), in which the eigenvalues are expressed as follows:

\[ \epsilon_q = \left[ \frac{N_0 + 1}{2} \hbar \omega_q + \frac{\hbar k_i^2}{2m} (\epsilon_q - \epsilon_i) \right], \]

\[ \epsilon_q^* = \left[ \frac{N_0 + 1}{2} \hbar \omega_q + \frac{\hbar k_i^2}{2m} (\epsilon_q - \epsilon_i) \right], \]

where \( k_i \) is the \( z \) component of the electron wave vector and the chemical potential energy:

\[ \epsilon_q = \left[ \frac{N_0 + 1}{2} \hbar \omega_q + \frac{\hbar k_i^2}{2m} (\epsilon_q - \epsilon_i) \right]. \]

The aforementioned result can be directly used for numerical analysis through a wave vector integration.

4. Results and discussion

We calculated the line-widths for both GaAs, which is a typical sphalerite material, and CdS, which is a typical wurtzite material. Notably, since the theory was proven valid in the case of an infinite square well potential, it is expected that it will provide a good interpretation for the two aforementioned piezoelectric materials. We analyzed the line-widths in GaAs and CdS using Eqs. (4) and (5). Notably, electron-piezoelectric phonon scattering is known to be dominant in pure GaAs and CdS. We used \( m^* = 0.066 m_e \) and \( m = 0.4 m_e \) as the effective masses, and the constants of GaAs were as follows:

\[ \rho = 5.36 \times 10^3 \text{ kg/m}^3, \]

\[ k = 2.52 \times 10^4 \text{ eV/K}, \]

\[ \varepsilon = 204 \text{ K}, \]

\[ \lambda = 2.98 \times 10^{-12} \text{ cm}^3/\text{N}. \]

For CdS, we had the following values:

\[ m^* = 0.7 m_e \]

\[ m = 0.19 \text{ m_e} \]

\[ \rho = 2.52 \times 10^4 \text{ eV/K}, \]

\[ \varepsilon = 2.98 \times 10^{-12} \text{ cm}^3/\text{N}. \]

Furthermore, \( \delta_q \) was replaced by \( 2.52 \text{ eV} \) as an approximation; it was concluded that the variation with the temperature was extremely insignificant. A more accurate value of \( \delta_q(T) \) can be obtained by using Eq. (15) if the characteristic constants \( k \) and \( \xi \) are available. Furthermore, we chose \( \delta_q = 8.854 \times 10^{-12} \text{ cm}^3/\text{N}. \)

For CdS, we had the following values:

\[ m^* = 0.19 m_e, \]

\[ m = 0.7 m_e \]

\[ \rho = 4.82 \times 10^4 \text{ kg/m}^3, \]

\[ k = 2.52 \times 10^4 \text{ eV/K}, \]

\[ \varepsilon = 2.56 \text{ eV}, \]

\[ \delta_q = 8.58 \times 10^{-14} \text{ eV/K}, \]

\[ \delta_q = 235 \text{ K}. \]

Figure 3 compares the temperature dependence of \( \gamma_{\text{ode}}(T) \) of GaAs (upper side) with that of \( \gamma_{\text{ode}}(T) \) of CdS (lower side) for \( \lambda = 220, 394, 513, 550, \) and 720 μm. As illustrated in Fig. 3, \( \gamma_{\text{ode}}(T) \) of GaAs and CdS increases with increasing temperature. Furthermore, in Fig. 4, the magnetic field dependence of the line-widths, \( \gamma_{\text{ode}}(B) \) of GaAs (upper side) and \( \gamma_{\text{ode}}(B) \) of CdS (lower side) are observed at \( T = 50 \) and 70 K.
As depicted in Fig. 4, \( \gamma_{\text{total}}^{\text{GaAs}} \) of GaAs increases with increasing temperature; however, the \( \gamma_{\text{total}}^{\text{GaAs}} \) decreases when the magnetic field is larger than \( B = 4.2 \) T at \( T = 50 \) and 70 K. There are two different regions in the magnetic field dependence of the line-widths: a high-magnetic field region, where the line-widths increase with a decreasing magnetic field, and a low-magnetic field region, where an increase in the line-widths is observed. Theoretically, the line-widths show a maximum at \( B = 4.2 \) T, which is possibly because of the coupling between the Landau levels and the electric structure of GaAs. We assume that the scattering is affected in high-magnetic field regions as there is no correlation between the resonance field and the Fermi-Dirac distribution function. In addition, the advantages of the EAPT theory are evident in the calculation of line-widths for various cases. The results thus obtained indicate that the EAPT is advantageous in explaining the resonant phenomena based on the quantum transition and the scattering effects on a microscopic level.

5. Concluding remarks

The EAPT theory provides an easy approach for analyzing the temperature dependence of line-widths. We found that the line-widths of GaAs and CdS increased with increasing temperature. We also found that the \( \gamma_{\text{total}}^{\text{GaAs}} \) of GaAs < \( \gamma_{\text{total}}^{\text{CdS}} \) CdS in the magnetic field region \( B > 4.2 \) T, which is believed to be as a result of the geometrical structure of the zinc-blended semiconductors. We also presented reasonable resonating pictures of the line-shapes. Furthermore, if we go beyond the quantum limit specified by \( \hbar \omega_c \gg k_B T \), the result is expected to be different; this is because higher order terms in addition to other coherent parts would have to be included in the calculation of the line-widths, and we intend to investigate this topic in the future.

Appendix

We performed further calculations using the moderate MWCA estimate the Hamiltonian commutator as follows.

\[
\begin{align*}
\{ a_j^\dagger a_i^\dagger a_i a_j, a_k^\dagger a_l \} &= \delta_{ij}, \quad a_j^\dagger a_i^\dagger a_i a_j = a_j^\dagger a_i^\dagger a_j^\dagger a_i^\dagger \delta_{ij} = 0, \\
\{ b_k^\dagger b_l^\dagger b_l b_k, a_i a_j \} &= -a_i^\dagger a_i^\dagger a_j a_j^\dagger + a_j^\dagger, \quad a_i^\dagger a_j a_i^\dagger a_j^\dagger = a_j^\dagger a_i^\dagger a_i a_j^\dagger = a_j^\dagger, \\
\{ a_j^\dagger a_i^\dagger a_i^\dagger a_i a_j, a_k^\dagger a_l^\dagger b_{k'} b_{l'} \} &= a_j^\dagger a_i^\dagger a_i^\dagger a_i a_j^\dagger (\delta_{k'l'} + \delta_{kl}), \\
L_{\text{p}, a_j} &= \sum_i \hbar \omega_i \left[ b_i^\dagger b_i^\dagger b_i + b_i b_i^\dagger \right] = -\hbar a_j, \\
L_{\text{p}, b_{k'} b_{l'}} &= \sum_i \hbar \omega_i \left[ b_i^\dagger b_i^\dagger b_i + b_i b_i^\dagger \right], \\
\end{align*}
\]

Figure 3. Temperature dependence of the line-widths, \( \gamma_{\text{total}}(T) \) of GaAs (upper side) and CdS (lower side) for \( \lambda = 220, 394, 513, 550, \) and 720 \( \mu \)m.

Figure 4. Magnetic field dependence of line-widths, \( \gamma_{\text{total}}(T) \) of GaAs (upper side) and CdS (lower side) at \( T = 50 \) and 70 K.
Therefore, we obtained the following relations:

\[ L_{b_q^i} = \sum_{\mu} \hbar \alpha \left[ b_{\mu}^* b_{\sigma}^* b_{\mu} b_{\sigma} \right] = -\hbar \alpha \cdot b_{\sigma}^i, \]

Then, using the equilibrium average relations, we have the following:

\[ \text{Tr} \{ \rho (H) a_\sigma a_\sigma^* \} = f_\sigma, \]
\[ \text{Tr} \{ \rho (H) a_\sigma^* a_\sigma \} = 1 - f_\sigma, \]
\[ N_{\sigma} = \langle b_{\sigma}^i b_{\sigma}^i \rangle = n_{\sigma} \delta_{\sigma, 0}, \]
\[ N_{\sigma}^* = \langle b_{\sigma}^i \rangle = (\alpha_i + 1) \delta_{\sigma, 0}, \]

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