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전자 포텐셜 변형과 포논 상호작용에 의한 준 이차원 Si 구조의 전도 현상 해석

Quantum Transition Properties of Quasi-Two Dimensional Si System in Electron Deformation Potential Phonon Interacting

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Abstract - We investigated theoretically the quantum optical transition properties of Si, in quasi 2-Dimensinal Landau splitting system, based on quantum transport theory. We apply the quantum transport theory (QTR) to the system in the confinement of electrons by square well confinement potential under linearly polarized oscillating field. We use the projected Liouville equation method with Equilibrium Average Projection Scheme (EAPS). In order to analyze the quantum transition, we compare the temperature and the magnetic field dependencies of the QTLW and the QTLS on four transition processes, namely, the intra-leval transition process , the inter-leval transition process , the phonon emission transition process and the phonon absorption transition process.

Key Words : Si, Quantum transport theory, Equilibrium average projection scheme (EAPS), Response formula and the scattering factor formula, Electron phonon coupling system, The quantum transition line shapes (QTLS) and the quantum transition line widths (QTLW)

1. Introduction

The study of magneto-optical transitions is known to be a good tool for investigating the transport behavior of electrons in low-dimensional electron systems. There are many theories regarding the quantum transport problems in various methodologies, among them we use the projected Liouville equation method with the Equilibrium Average Projection Scheme (EAPS).

There are many theories regarding the quantum transport problems in various methodologies, such as the Boltzmann transport theory[1], the Green's function approach[2, 3], the force-balance approach[4], Feynman's path-integral approach[5] and the projection operator approach[6, 7]. Alternatively, in similar methodologies by Zwanzig[8], by directly using a projection operator on the Liouville equation, Kenkre's group suggested a response function which contains Kubo's theory as the lowest-order approximation[8, 9]. The study of the quantum transport theories based on the projected Liouville equation method provides a useful tool for investigating the scattering mechanism of solids. Using the projected Liouville equation method with the Equilibrium Average Projection Scheme (EAPS), we have suggested a new quantum transport theory of linear-nonlinear form[11].

The merit of using EAPS is that the quantum response function and the scattering factor formular can be obtained in a one step process by expanding the quantum transport theory (QTR). The merit of using EAPS is that the quantum response function and the scattering factor formula can be obtained in a one-step process by expanding the quantum transport theory. In the previous work, we applied the EAPS theory in Ge and Si, since there are abundant experimental date in non-confining potential systems. We compared our results of numerical calculations of the EAPS theory with existing experimental data and showed a good agreement between them. This indicated that the EAPS theory is useful in analyzing many-body systems. But, the previous work restricted for non-confining potential systems with the extremely weak coupling (EWC) approximation. The optical power absorption spectrum of the transitions measured in experiments is directly related to the electric conductivity tensor, and the spectrum's linewidth to its line-shape function. Hence, it is important to obtain an explicit expression of the line-shape function for a given confining potential system on the basis of a theoretical formulation. Recently, we suggested a more precise

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procedure of expanding and application of EAPS in Low-dimensional electron systems with the moderately weak coupling(MWC) approximation in Ref. [14-16]. In the MWC scheme, the distribution components can provide an adequate explanation of the quantum transition processes. In a previous work of EWC scheme, the intermediate states of quantum transition processes do not appear.

In this work, we investigate the optical Quantum Transition Line Shapes(QTLSs) which show the absorption power and the Quantum Transition Line Widths(QTLWs), which show the scattering effect in the electron-deformation potential phonon interacting system. The analysis of the temperature and the magnetic field dependence of the QTLWs are very difficult in alternative theories or experiment, because the absorption power in the various external field wavelengths is required to be calculated or observed. The QTR theory of EAPS is advantageous in this respect as it allows the QTLWs to be directly obtained, through EAPS, in the various external field wavelengths. In short the calculation of the absorption power is not required to obtain the QTLW. With the numerical calculation, we analyzed the temperature and the magnetic – field dependences of the QTLWs and QTLSs in various cases. In order to analyze the quantum transition, we compare the temperature and the magnetic field dependencies of the QTLWs and the QTLSs on two transition processes, namely, the phonon emission transition process and the phonon absorption transition process.

2. The Absorption Power Formula and Scattering Factor Function

We suppose that an oscillatory electric field $E(t)=E_0\, e^{j\omega t}$ is applied along the z-axis, which gives the absorption power delivered to the system as $P(\omega)=(E_0^2/2)Re[\sigma(\omega)]$, where "Re" denotes the real component and $\sigma(\omega)$ is the optical conductivity tensor which is the coeffitient of the formula. Here the absorption power represents the optical QTLS, and the scattering factor function represents the optical QTLW. In order to apply the linear response formula, the first term of the Eq. (3.9) of reference[11], to the optical quantum transition system, we replace the dynamic variable with $r_k \equiv J^-$, $L_i^{'}X$ with $L_j^{'}X \equiv (-i/\omega)[J^+, X]$, and $J_i \equiv J^+$ for the current system under an oscillating external field of frequency ω. If we selet a linearly polarized electric field, we have the time dependent Hamiltonian as $H^{'}(t) \equiv H^{'}E_i(t)$ and $H^{'} \equiv (-i/\omega)J_x^{(L)}$. The corresponding Liouvill operators is $L_i^{'}X \equiv (-i/\omega)[J_x^{(L)}, X]$. We also consider the time independent operator corresponding to expectation of dynamic variable, r_k as $J_x^{(R)}$. Then we consider two current operators as $J_x^{(R)} \equiv \tilde{g}_{(sys)} \sum_\beta \sqrt{N_\beta}\ \alpha_\beta^+\ \alpha_{\beta+1}$ and $J_x^{(L)} \equiv \tilde{g}_{(sys)} \sum_\beta \sqrt{(N_\beta+1)}\ \alpha_{\beta+1}^+\ \alpha_\beta$. where $\tilde{g}_{(sys)} \equiv (-ie\bar{h}/m_e^*)\sqrt{1/l_0^2}$. $\tilde{g}_{(sys)}$ can be changed for other systems and external fields. We can easily obtain the ohmic linear current under linearly polarized external field (LF) from the response formula with the EAPS, while recent research on the response formula was restricted to the ohmic circlar current under the circlar polarized external field

When a static magnetic field $\vec{B}=B_z\hat{Z}$ is applied to an electron system, the single electron energy state is quantized to the Landau levels. We select a system of electrons confined in an infinite square well potential (SQWP) between $z=0$ and $z=L_z$ in the z-direction. We use the eigenvalue and eigenstate of Ref. [10] of the square well potential system. We suppose that an oscillatory electric field $E(t)=E_0e^{j\omega t}$ is applied along the z-axis, which gives the absorption power delivered to the system as $P(\omega)=(E_0^2/2)Re[\sigma(\omega)]$, where "Re" denotes the real component and $\sigma(\omega)$ is the optical conductivity tensor which is the coefficient of the current formula. Here the absorption power represents the optical QTLS, and the scattering factor function represents the optical QTLW. We consider the electron-phonon interacting system and then we have the Hamiltonian of the system as

$$H_s = H_e + H_P + V = \sum_\beta \langle\beta|h_0|\beta\rangle a_\beta^+ a_\beta + \sum_q \hbar\omega_q b_q^+ b_q + \sum_q \sum_{\alpha,\mu} C_{\alpha,\mu}(q) a_q^+ a_\mu \left(b_q + b_{-q}^+\right) \tag{1}$$

Here H_e is the electron Hamiltonian, h_0 is a single-electron Hamiltonian, H_p is the phonon Hamiltonian and V is the electron-phonon(or impurity) interaction Hamiltonian. The $b_1(b_2^+)$are the annihilation operator(creation operator) of boson particle, and $\vec{q}$ is phonon(or impurity) wave vector. The interaction Hamiltonian of electron- phonon (or impurity)- interacting system is $V \equiv \sum_q \sum_{\alpha,\mu} C_{\alpha,\mu}(q) a_\alpha^+ a_\mu (b_q + b_{-q}^+)$ where the coupling matrix element of electron-phonon interaction $C_{\alpha,\mu}(q)$ is $C_{\alpha,\mu}(q) \equiv V_q < \alpha|\exp(i\vec{q}\cdot\vec{r})|\mu >$, $\vec{r}$ is the position vector of electron and V_q is coupling coefficient of the materials.

Recently, we suggested the absorption power formula in Ref. [16] in confining potential systems. With the continuous approximation[15], in a right circularly polarized external field, the absorption power formula (or the QTLS formula) is obtained finally as

$$P(\omega) \propto \left(\frac{e^2\omega_c^2}{\pi^2\hbar\omega}\right)\left\{\frac{\gamma_{total}(\omega_c)\sum_{N_\alpha}\int_{-\infty}^{\infty} dk_{z\alpha}(N_\alpha+1)(f_\alpha - f_{\alpha+1})}{(\omega-\omega_c)^2 + (\gamma_{total}(\omega_c))^2}\right\} \tag{2}$$

where the scattering factor function(or QTLW) is given by

$$\gamma_{total}(\omega) \equiv \mathrm{Re}\,\Xi_{kl}(\omega) \equiv \sum_{\mp}\sum_{N_\alpha=0}\sum_{N_\beta=0}\gamma^{\mp}_{\alpha,\beta}$$

$$= \left(\frac{\Omega}{4\pi\hbar^2\upsilon_s}\right)\left(\frac{\pi}{L_z}(2+\delta(n_\alpha,n_\beta))\right)\left\{\frac{\sum_{\mp}\sum_{N_\alpha=0}\sum_{N_\beta=0}\int_{-\infty}^{\infty}dk_{z\alpha}\int_{-\infty}^{\infty}dq_z Y^{\mp}_{\alpha,\beta}}{\sum_{N_\alpha=0}^{\infty}\int_{-\infty}^{\infty}dk_{z\alpha}(N_\alpha+1)(f_{\alpha+1}-f_\alpha)}\right\}. \quad (3)$$

Recently, we suggested the final derivation of the integrand $Y^{\mp}_{\alpha,\beta}$ of the scattering factor in Ref. [16]. We use the result equations from Eq. (18) to Eq. (23) in Ref. [16].

Through the numerical calculation of the theoretical result, of QTLS and of the QTLW, we analyze absorption power and line widths of Si. In order to analyze the QTLW and the QTLS of Si, we use the material constant of table[1] and inserting these constants into result yields the line shapes from which the line width can be measured.

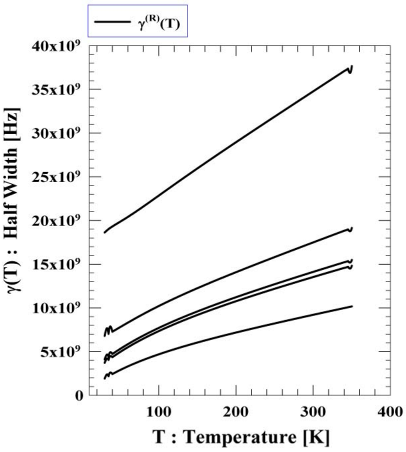
In order to analyze the quantum transition process, we denote the total QTLW as $r_{total} \equiv r_{em} + r_{ab}$, where, $r_{em} \equiv r^+_{0,0} + r^+_{0,1} + r^+_{1,0}$ and $r_{ab} \equiv r^-_{0,0} + r^-_{0,1} + r^-_{1,0}$ are the QTLW of the total phonon emission and absorption transition process, respectively.

Table 1 Material constant of Si

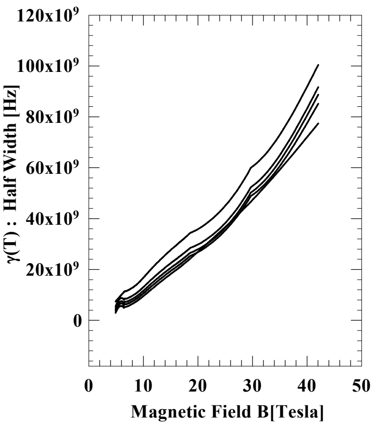
Symbol	Contents	Value
m^*	Effective mass of electron	$0.33m_0$
$\overline{m}$	Effective mass of hole	$0.58m_0$
ρ	Mass density	$2340kg/m^3$
κ	Characteristic constant	$4.37\times10^{-4}eV/K$
ξ	Characteristic constant	636
$\overline{K}$	Electromechanical constant	$2.98\times10^{-2}m/s$
$\overline{v_s}$	Speed of sound	$9030m/s$
$\tilde{\epsilon_s}$	Energy gap	$1.424eV$
E_1	Deformation potential constant	$7eV$
L_z	Length of well of z direction	$20\times10^{-9}m$

3. Results and Discussion

In Fig. 1(a) the temperature dependence of QTLW of Si, $r(T)$ is plotted. As shown in Fig. 1(a), $r(T)$ increase as temperatures increase for the external field wavelengths λ= 220, 394, 513, 550 and 720 μm. In Fig. 1(b), we plotted the magnetic field dependence of the QTLW, $r(B)$ of Si, at T= 50, 70, 90, 120 and 210 K. The results indicate that increase as the magnetic field. This result implies that the scattering effect of phonons enlarges with the increasing temperatures and the increasing magnetic field in Si.



(a)

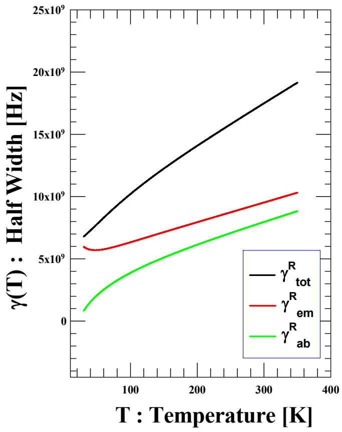


(b)

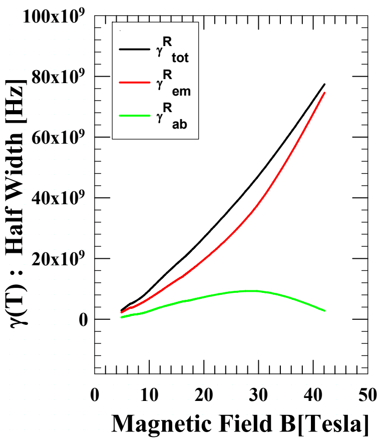
Fig. 1 (a) Temperature dependence of QTLW of Si, $r(T)$ with λ=220, 394, 513, 550 and 720 μm (from the top line to the bottom line), (b) Magnetic field dependence of QTLW of Si, $r(B)$ at T=50, 70, 90, 120 and 210 K (from the bottom line to the top line).

In Fig. 2(a), the temperature dependence of the QTLW, $r(T)_{total}$, $r(T)_{em}$ and $r(T)_{ab}$ of Si for external field wavelength λ=220 μm is shown. The QTLWs,$r(T)_{total}$, $r(T)_{em}$ and $r(T)_{ab}$ increase as the temperatures increase. The result implies that the phonon emission transition process prevails against the phonon absorption transition process because the $r(T)_{em}$is closer to $r(T)_{total}$. In Fig. 2(b), comparisons of the magnetic field dependence of QTLW, $r(B)_{total}$, $r(B)_{em}$and $r(B)_{ab}$ of Si, at T=50 K is shown. The QTLWs,$r(B)_{total}$, $r(B)_{em}$ and $r(B)_{ab}$ increase as the magnetic field while $r(B)_{ab}$ decreases as the magnetic field increase at the region 28 Tesla <B<50

Tesla. The contributions of two processes can be appeared differently in various cases in various systems. In this work, our results reveal that values of QTLW of Si are $r(T)_{ab} < r(T)_{em} < r(T)_{total}$ and $r(B)_{ab} < r(B)_{em} < r(B)_{total}$



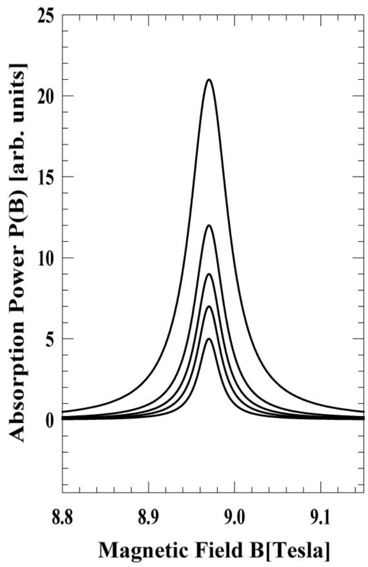
(a)



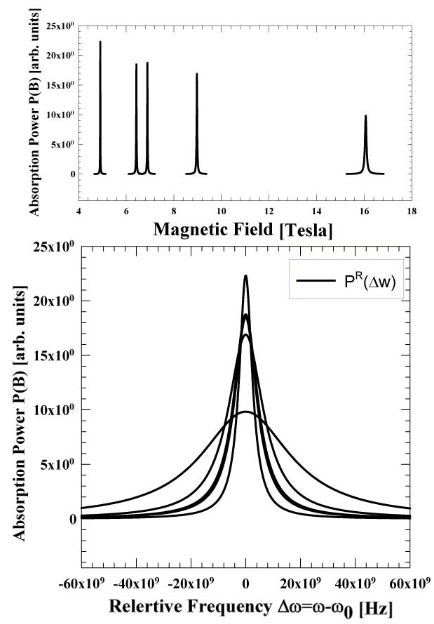
(b)

Fig. 2 (a) Comparisons of the temperature dependence of QTLW of Si, $r(B)_{total}$, $r(B)_{em}$ and $r(B)_{ab}$ with λ=394 μm, (b) Comparisons of the magnetic field dependence of QTLW of Si, $r(B)_{total}$, $r(B)_{em}$ and $r(B)_{ab}$ at 50 K.

Fig. 3(a) represents the magnetic field dependence of the absorption power $P(B)$ of the QTLS of Si for the external field wavelength λ=393 μm at several temperatures, T=50, 70, 90, 120 and 210 K. In order to compare the line of QTLS in the same graph, we plot the value of $P_{nr}(B) = \alpha P(B)$. As seen in Fig. 3(a), $P(B)$ increases as the temperature increases. Also, the linewidth increases with the increasing temperatures. In the Fig. 3(b), we can read the magnetic-field dependence of the maximum absorption power in upper figure. The bellow figure of Fig. 3(b) shows the relative frequency dependence of the absorption power(QTLS), $P(\Delta\omega)$ of Si, with λ=220, 394, 513, 550 and 720 μm at T=50K. The analysis of the relative frequency dependence of the absorption power(QTLS) represents the magnetic field dependency property of the absorption power given for an external field wavelength and the conditions of the system.



(a)



(b)

Fig. 3 (a) The Magnetic Field dependence of normalized $P(B)$ (QTLS) of Si with λ=393 μm the at T=50, 70, 90, 120 and 210K. (from the bottom line to top), (b) The relativity frequency dependence of $P(\Delta\omega)$ (QTLS) of Si and the magnetic field dependence of the absorption power, $P(B)$(QTLS) with λ= 220, 394, 513, 550 and 720 μm at T=50 K

4. Conclusion

In a summary, The approach to the analysis of quantum transition processes with ease is the merits of our EAPS theory. Through the analysis of this work, we found the increasing properties of QTLW and QTLS of Si with the temperature and the magnetic fields. We also found the dominant scattering processes are the phonon emission transition process. The results of this work will help to analyze experimental the scattering mechanisms in the electron-deformation potential interacting materials.

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