Influence of phonon confinement on the optically detected electron-phonon resonance linewidth in quantum wells

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Abstract. We investigate the influence of phonon confinement on the optically detected electron-phonon resonance (ODEPR) effect and ODEPR line-width in quantum wells. The obtained numerical result for the GaAs/AlAs quantum well shows that the ODEPR line-widths depend on the well’s width and temperature. Besides, in the two cases of confined and bulk phonons, the linewidth (LW) decreases with the increase of well’s width and increases with the increase of temperature. Furthermore, in the small range of the well’s width, the influence of phonon confinement plays an important role and cannot be neglected in considering the ODEPR line-width.

1. Introduction

Electrophonon resonance (EPR) effects in low-dimensional electron gas systems have generated considerable interest in recent year [1]. EPR effects can only be observed for the resonant scattering of electrons confined in electric subband levels by longitudinal optical (LO) phonon whenever the LO phonon energy is equal to the energy separation between two electric subband levels. Scattering process with LO phonons is dominant in limiting the mobility of electrons in the polar semiconductors for temperature $T > 50$ K [2]. EPR was introduced by Bryskin and Firsov [2] who predicted EPR for non-degenerate semiconductors in a very strong electric fields.

The absorption line-width (LW) is well-known as a good tool for investigating the scattering mechanisms of carriers. Hence, it can be used to probe electron-phonon scattering processes. The absorption LW was investigated based on the interaction of electrons and bulk phonons, but the absorption LW in quantum wells (QWs) due to confined electrons and confined LO-phonons interaction is still open for study.

Phonon confinement is an essential part of the description of electrophonon interactions [3]. It causes the increase of electrophonon scattering rates [4] and significant nonlinearities in the dispersion relations of acoustic phonon modes, and modifies the phonon density of states [5]. There have been many models dealing theoretically with phonon modes, such as the Huang-Zhu (HZ) model, the slab mode model and guided mode model [6]. Phonon confinement is shown to be important whenever the transverse dimensions of a quantum well are smaller than...
the phonon coherence length \( [3] \) and should be taken into account in order to obtain realistic estimates for electron-phonon scattering in low-dimensional structures \([7]\). Phonon confinement affects ODEPR mainly through changes in the selection rules for transitions involving subband of electrons, phonon modes. Phonon confinement also affects the ODEPR linewidth (ODEPRLW) through changes in the probability of the electron-phonon scattering. The linewidth is defined as the profile of curves describing the dependence of the absorption power on the photon energy or frequency \([8]\). The linewidth has been measured in various kinds of semiconductors, such as quantum wells \([9]\), quantum wires \([10]\), and quantum dots \([11]\). These results show that the absorption linewidth has a weak dependence on temperature and has a strong dependence on the sample size. However, in these studies, the absorption linewidth was investigated based on the interaction of electrons and bulk phonons, so that the absorption linewidth in quantum wells (QWs) due to confined optical phonon-electron interaction is still open for study. Recently, our group has proposed a method, called the profile method. This method can be used to computationally obtain the linewidth from graphs of the absorption power \([12]\), and we used this method to determine the cyclotron resonance linewidth in cylindrical quantum wires \([13]\) and the influence of phonon confinement on the optically detected electrophonon resonance linewidth in GaAs/AlAs quantum wires \([14, 15]\).

In the present work, we investigate the ODEPRLW in QWs, the dependence of the ODEPRLW on the well’s width and the temperature of system is obtained. The results of the present work are fairly different from the previous theoretical results because the phonon confinement is considered. The paper is organized as follows. In Section 2, we introduce several models of the phonon confinement in QWs. Calculations of analytical expression of the absorption power in QWs are presented in Section 3. The graphical dependence of the absorption power on the photon energy in the GaAs/AlAs QW is shown in Section 4. From this dependence, we obtain the linewidth and examine not only the location of resonance peaks, but also the dependence of the linewidth on temperature and well’s width. Finally, remarks and conclusions are shown in Section 5.

2. Confined phonon models

For a square well of infinite height, the one-electron eigenfunctions, \( \psi_{k_x,k_y,n}(\mathbf{r}) \), and the eigenvalues, \( E_n(k_x, k_y) \), in the conduction band are, respectively, given by \([2]\)

\[
\psi_{k_x,k_y,n}(\mathbf{r}) \equiv \langle \mathbf{r} | k_x, k_y, n \rangle = \frac{1}{\sqrt{L_x L_y}} e^{ik_x x} e^{ik_y y} \varphi_n(z) = \sqrt{\frac{2}{L_x L_y L_z}} e^{ik_x x} e^{ik_y y} \sin \left( \frac{n \pi z}{L_z} + \frac{n \pi y}{2} \right),
\]

\[
E_n(k_x, k_y) = \frac{k_y^2}{2m^*} + n^2 \varepsilon_0,
\]

where \( \mathbf{r} \) is the position vector of electron; \( k_x \) and \( k_y \) are, respectively, the wave-vector component of the electron in the \( x \) and \( y \) direction; \( m^* \) being the effective mass of an electron and \( \varepsilon_0 = \frac{\pi^2 \hbar^2}{2m^* L_z^2} \) is the energy of the lowest electric subband, \( n \) is the electric subband quantum number \( (n = 1, 2, 3, \cdots) \); \( L_x, L_y, \) and \( L_z \) are, respectively, the \( x \)-, \( y \)-, and \( z \)-directional normalization lengths. The electron wave function \( \varphi_n(z) \) in \( z \)-direction (well centered at \( z = 0 \)) as determined by the barrier potential \( V(z) \) \( (V(z) = 0 \) for \( |z| < L_z/2 \) and \( V(z) = \infty \) for \( |z| > L_z/2 \)) \([16]\).

The matrix element for electron-confined phonon interaction in quantum well in the extreme quantum limits can be written as \([17]\)

\[
|\langle i | H_{e-ph} | f \rangle|^2 = |C_{i,f}(\mathbf{q})|^2 = |C_m(q_\perp)|^2 |G_{n_i,n_f}(q_z)|^2 \delta_{k_{\perp,i},k_{\perp,f}+q_\perp},
\]
where
\[ |C_m(q_\perp)|^2 = \frac{2\pi e^2 \hbar \omega_m q_\perp}{\epsilon_0 \Omega} \left( \frac{1}{\chi_\infty} - \frac{1}{\chi_0} \right) \frac{1}{q_\perp^2 + q_m^2}, \] (4)

where \( \chi_0, \chi_\infty, \epsilon_0 \) and \( \Omega \) are the static, high-frequency, vacuum dielectric constants and the normalization volume of specimen, respectively; \( q_\perp \) is a two dimensional vector in the \((x, y)\) plane of phonon; \( q_m = m\pi/L_z \). The term \( G_{m,n_f}^{m_\alpha}(q_z) \) is given by
\[ G_{m,n_f}^{m_\alpha}(q_z) = \int_{L_z/2}^{L_z/2} \varphi_{n_f}^*(z) u_{m\alpha}(z) \varphi_{n_i}(z) dz, \] (5)

where \( \alpha \) distinguishes the even (-) and odd (+) confined phonon mode, \( u_{m\alpha}(z) \) being the parallel component of displacement vector of \( m \)-th phonon mode in the direction of spatial confinement. It is different for different models and has been calculated for some confined models such as the HZ model, slab mode model, and guided mode model [17]. In the next section, we will use the HZ model to calculate the optical absorption power in quantum wells because among these models, the HZ model has received wide acceptance and best describes the electron-phonon interaction in quasi-two-dimensional systems [18]. For example, calculations of electron intra- and inter-subband scattering rates in GaAs quantum wells due to confined LO phonons using the HZ model [19] have been found to be in good agreement with experimental results [20]. For this model [17]
\[ u_{m+}(z) = \sin \left( \frac{\mu_m \pi z}{L_z} \right) + \frac{C_m}{2} \frac{\mu_m \pi z}{L_z}, \quad m = 3, 5, 7, \ldots, \] (6)

where, \( \mu_m \) and \( C_m \) are constants: \( \mu_3 = 2.8606, \mu_5 = 4.918, \mu_7 = 6.95, \ldots, \) and \( C_3 = 1.9523, C_5 = -1.983, C_7 = 1.992, \ldots \)
\[ u_{m-}(z) = \cos \left( \frac{m \pi z}{L_z} \right) - (-1)^{m/2}, \quad m = 2, 4, 6, \ldots. \] (7)

The overlap integral (5) can be evaluated for intra-subband transition \((1 \rightarrow 1)\), and is obtained for the HZ model as
\[ G_{11}^{m+} = 0, \quad m = 3, 5, 7, \ldots, \] (8)
\[ G_{11}^{m-} = \frac{3}{2} \delta_{m,2} - (-1)^{m/2}(1 - \delta_{m,2}), \quad m = 2, 4, 6, \ldots. \] (9)

3. Analytical results

In this section, we utilize the HZ model for confined phonon to calculate the absorption power in above mentioned quantum wells, subjected to an electric field with amplitude \( E_0 \) and frequency \( \omega \). The absorption power is obtained by using the operator projection technique to calculate the conductivity tensor \((\sigma_{zz}(\omega))\). Finally, absorption power with confined phonons can be written as
\[ P(\omega) = \frac{E_0^2}{2} \text{Re}[\sigma_{zz}(\omega)] = \frac{E_0^2}{2\omega} \sum_{\alpha,\beta} (j_z)_{\alpha,\beta} (j_z)_{\beta,\alpha} \left( \frac{f_\alpha - f_\beta}{(\hbar \omega - E_{\alpha,\beta})^2 + \hbar^2 B_{\alpha,\beta}^2(\omega)} \right), \] (10)
\[ (j_z)_{\alpha,\beta} = \frac{2e\pi\hbar}{\Omega m^*} n_\beta \delta(k_{\perp,\beta} - k_{\perp,\alpha}) \left[ \frac{1 - (-1)^{n_\alpha + n_\beta}}{n_\alpha + n_\beta} + \frac{1 - (-1)^{n_\alpha - n_\beta}}{n_\alpha - n_\beta} \right], \] (11)
\[ (j_z)_{\beta,\alpha} = \frac{2e\pi\hbar}{\Omega m^*} n_\alpha \delta(k_{\perp,\alpha} - k_{\perp,\beta}) \left[ \frac{1 - (-1)^{n_\alpha + n_\beta}}{n_\alpha + n_\beta} + \frac{1 - (-1)^{n_\beta - n_\alpha}}{n_\beta - n_\alpha} \right]. \] (12)
\( f_\alpha \) and \( f_\beta \) are the Fermi-Dirac distribution function of electron at state \(|\alpha\rangle\) and \(|\beta\rangle\),

\[
B_{\alpha,\beta}(\omega) = C_0^m \sum_n |G_{n,\alpha,\beta}(q_z)|^2 \sum_{n_q} \frac{m^* k_{1}^+ (k_{1,\beta} - k_{1}^+)}{\hbar^2 |k_{1}^+|^2} \times \left\{ \left[ f_\alpha (1 + N_q) - (f_\alpha + N_q) f_\eta (k_{1}^+) \right] - \left[ N_q f_\alpha - (1 + N_q - f_\alpha) f_\eta (k_{1}^-) \right] \right\} \times \left\{ (1 + N_q - f_\beta) f_\eta (k_{2}^+) - N_q f_\beta - \left[ (f_\beta + N_q) f_\eta (k_{2}^-) - (1 + N_q) f_\beta \right] \right\},
\]

(13)

where \( N_q \) is the Planck distribution function for confined phonon at the state \(|q\rangle = |m, q_\perp\rangle\),

\[
C_0^m = \frac{2\pi e^2 \hbar \omega_{m,q_\perp}}{\varepsilon_0 \Omega} \left( \frac{1}{\chi_{\infty}} - \frac{1}{\chi_0} \right),
\]

(14)

\[
k_{1,\pm} = \left\{ k_{1,\beta}^2 + \frac{2m^*}{\hbar^2} [(n_\eta^2 - n_\beta^2) \varepsilon_0 + \hbar (\omega \pm \omega_{LO,m,q_\perp})] \right\}^{1/2},
\]

(15)

\[
k_{2,\pm} = \left\{ k_{2,\alpha}^2 + \frac{2m^*}{\hbar^2} [(n_\alpha^2 - n_\beta^2) \varepsilon_0 + \hbar (\omega \pm \omega_{LO,m,q_\perp})] \right\}^{1/2}.
\]

(16)

We can see that these analytical results appear very involved. However, physical conclusion can be drawn from graphical representations and numerical results, obtained from adequate computational methods.

4. Numerical results and Discussion

To clarify the obtained results we numerically evaluate the absorption power, \( P(\omega) \), for a specific GaAs/AlAs QW. The absorption power is considered to be a function of the photon energy. The parameters used in our computational evaluation are as follows [21]: \( \chi_{\infty} = 10.9, \chi_0 = 12.9, m^* = 0.067 \times m_0 \) (\( m_0 \) being the mass of free electron), \( \hbar \omega_0 = 36.25 \text{ meV}, E_0 = 5.0 \times 10^6 \text{ Vm}^{-1}, \) and \( \beta = 4.73 \times 10^3 \text{ ms}^{-1}. \) The following conclusions are obtained in the extreme quantum limit, where the low subbands of confined phonon for Huang-Zhu model \( m = 2 \) and \( m = 4; n_\alpha = 1, n_\beta = 2 \) for confined electron.

Dependence of the absorption power in QW on the photon energy for two different models of phonons is shown in figure 1. The solid curve corresponds to confined phonon, i.e., the energy of confined phonon for \( m = 2 \), \( \hbar \omega_{m,q_\perp} = \hbar \sqrt{\omega_0^2 - \beta^2 (m^* L_z)^2} = 36.22 \text{ meV}, \varepsilon_0 = 28.67 \text{ meV} \) (for \( L_z = 14 \text{ nm} \)). From the graph we can see that each peak describes a specific resonance. By using the computational method, we easily determine from the left to the right (of solid curve).
The dependence of the absorption power on the photon energy in the case of confined phonon is presented in figure 1a. The graph exhibits four peaks which can be explained as follows:

- The first peak corresponds to the photon energy $\hbar \omega = 36.22$ meV, which satisfies the condition $\hbar \omega = \hbar \omega_{m,\vec{q}}$. This is the condition for intrasubband transitions.

- The second peak corresponds to the photon energy of $\hbar \omega = 49.79$ meV, which satisfies the condition $\hbar \omega = (n_\beta^2 - n_\alpha^2)\varepsilon_0 - \hbar \omega_{m,\vec{q}_\perp}$, i.e., $49.79$ meV=$(2^2 - 1^2) \times 28.67$ meV - 36.22 meV. This condition implies that an electron in the $n_\alpha = 1$ can move to $n_\beta = 2$ by absorbing of a photon with energy $\hbar \omega$ along with the absorption of a phonon with energy $\hbar \omega_{m,\vec{q}_\perp}$. This is the condition for optically detected electrophonon resonance (ODEPR).

- The third peak corresponds to the photon energy $\hbar \omega = 86.01$ meV, which satisfies the condition $\hbar \omega = (n_\beta^2 - n_\alpha^2)\varepsilon_0$, i.e., $86.01$ meV= $(2^2 - 1^2) \times 28.67$ meV. This condition implies that an electron in the $n_\alpha = 1$ can move to $n_\beta = 2$ by absorbing a photon with energy $\hbar \omega$. This is the condition for direct transitions.

- The fourth peak corresponds to the energy $\hbar \omega = 122.23$ meV, which satisfies the condition $\hbar \omega = (n_\beta^2 - n_\alpha^2)\varepsilon_0 + \hbar \omega_{m,\vec{q}_\perp}$, i.e., $122.23$ meV=$(2^2 - 1^2) \times 28.67$ meV + 36.22 meV. This condition implies that an electron in the $n_\alpha = 1$ can move to $n_\beta = 2$ by absorbing a photon with energy $\hbar \omega$ along with the emission of a phonon with energy $\hbar \omega_{m,\vec{q}_\perp}$. This is the condition for optically detected electrophonon resonance (ODEPR).

The dependence of the absorption power in QW on the photon energy for two different models of phonon at the fourth peak on the figure 1a is showed in figure 1b. In the case of bulk phonon this peak is located at the photon energy of 122.27 meV, while it is at 122.23 meV in the case of confined phonon. The difference between these two values is insignificant and can be neglected.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{Dependence of the absorption power in QW on the photon energy for two different models of phonon. Here, $T=200$ K, $L_z=14$ nm. The solid and the dashed curves correspond to confined phonons and bulk phonons, respectively. (a) All peaks, (b) At the fourth peak in (a).}
\end{figure}

The dependence of the linewidth on temperature in both models of phonon is showed in figure 2a. From the figure we can see that the linewidth increases with the temperature. This is reasonable because the possibility of the electron-phonon scattering rises as the temperature increases. It is also seen that linewidths of the ODEPR peak in the cases of confined phonons are...
larger than the bulk one. This is because when phonons are confined the probability electron-phonon scattering is increased.

The dependence of the linewidth on the well’s width in both models of phonon is showed in figure 2b. It can be seen from the figure that the linewidths decrease with the well’s width. This can be explained physically by the fact that the possibility of electron-phonon scattering decreases when the well’s width increases. Furthermore, the LW in the confined phonon cases vary faster and have greater values than it does in the bulk phonon case. In addition, the LW for the confined phonon with \( m = 4 \) varies faster and has a greater value than it does for the confined phonon with \( m = 2 \) and the smaller the well’s width is, the more pronounced the difference is. Thus, as the well’s width decreases, the phonon confinement becomes more important and cannot be neglected. For well with width so large, the influence of phonon confinement on the LW is very small and can be ignored.

5. Conclusions

In the present paper, we have obtained analytical expressions for the absorption power in quantum wells due to electrons-confined optical phonons interaction. Carrying out numerical computations and graphically plotting the dependence of the absorption power on the photon energy, we can find the resonant peaks. Besides, using the profile method, we have determined the linewidth based on graphs of the absorption power versus the photon energy with the help of the computational program. From the numerical results, we can write out some important remarks as follows: The effect of the phonon confinement on the peak location is very weak, so for theoretical studies on determining the peak locations that do not require a high precision, we can ignore the phonon confinement effect. In both bulk and confined phonon models, the linewidth increases with the increase of temperature and decreases with the increase of well’s width. However, the linewidth in the case of confined phonon model varies faster and has a greater value than it does in the case of bulk phonon model. The linewidth in the case of strong confined phonon (with \( m = 4 \)) varies faster and has a greater value than it does in the case of weak confined phonon (with \( m = 2 \)). The effect of the phonon confinement on the linewidth is very weak and can ignore when the well’s width is larger 20 nm, but the phonon confinement cannot be neglected, especially at small well’s width.

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