Orissa Journal of Physics
ISSN 0974-8202

Vol. 24, No.2
August 2017
pp. 177-182

Polaronic Correction on Absorption Coefficient in GaAs / $Al_xGa_{1-x}As$ Single Quantum Well

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Received: 15.6.2017 ; *Revised : 2.7.2017* ; *Accepted : 25.7. 2017*

Abstract : Polaronic effect on the optical absorption coefficient is studied theoretically. In a rectangular quantum well based on AlGaAs/GaAs heterostructures. The electron-phonon interaction term modifies the electron wave function which affects the dipole matrix elements. The modified dipole matrix elements lower the total optical absorption coefficient due to increase in the nonlinear term.

PACS numbers: 68.65-k, 71.45 Gm, 71.10 Ca, 73.21-b

The heterojunctions $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}$ as form a single symmetric rectangular quantum well (QW) with a confining potential whose height is decided by the aluminum concentration x. The nonlinear effects can be enhanced dramatically in the QW systems compared to bulk materials due to quantum confinement of electrons in the well. The nonlinear optical properties in semiconductor quantum well (QW) system have attracted much attention for device applications [1]. Among the optical processes, more attention has been paid to the nonlinear optical absorption coefficient since it is the primary mechanism for governing the photo detection process [2].

When an electron moves in a QW system, its coulomb field displaces both positive and negative ions with respect to each other so that a virtual phonon field is set in the system. A polaron is constituted when the electron is surrounded by the cloud of virtual phonons [3]. In the Frohlich's polaron theory, a conduction electron interacts with the long-wavelength longitudinal optic (LO) phonon mode and the radius of the polaron is far larger then the elementary cell of the material. Such a condition is valid for GaAs and AlGaAs which form the QW.

The strength of the absorption process depends on the dipole matrix elements which are calculated using the electron wave functions in the QW.

However, the weak electron-phonon interaction in the Frohlich form can modify the electron wave function. As a result of this the dipole matrix elements are modified. The optical properties are modified since the dipole matrix elements govern these quantities. The effect of polaron on the optical rectification[4], the second harmonic generation[5] and the third harmonic generation[6] have been found significant. In the present work, the effect of polaron on the optical absorption coefficient has been studied.

The energy levels En and the corresponding envelope functions $\phi_n(z)$ in a QW can be determined from the effective mass equation,

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m*(z)}\frac{\partial}{\partial z}+V(z)\right]\phi_n(z)=E_n\phi_n(z) \quad (1)$$

Where $V(z)$ is the confining potential and $m^*(z)$ is the position-dependent effective mass.

For a rectangular QW with well width l, the energy levels for n=1,3,5,….. states are obtained from the roots of the transcendental equation,

$$\tan\left(k_n\frac{l}{2}\right)=\frac{m*(0)k_n'}{m*(x)k_n} \quad (2)$$

Where $k_n=\sqrt{2m^*(0)E_n}/\hbar$ and $k_n'=\sqrt{2m^*(x)[V_0(x)-E_n]}/\hbar$ with $V_0(x)$ as the barrier height. For an electron in the conduction band, V_0=0.6(1.155 x +0.37 x^2) eV and $m^*(x)$=(0.0632+0.0856 x +0.0231 x^2)m_0, m_0 being the electron rest mass. The envelope functions corresponding to n=1,3,5,….states are obtained as

$$\varphi_n(z) = \begin{cases} C_n\cos(k_n z) & |z|<\frac{l}{2} \\ C_n\cos(k_n z\, l/2)e^{-k_n^1(|z|-\frac{l}{2})} & |z|\geq\frac{l}{2} \end{cases} \quad (3)$$

Where C_n is the normalization constant. It is obtained as

$$C_n=\left[\frac{2k_n}{k_n l+\sin(k_n l)+2k_n cos^2(k_n l/2)/k_n^1}\right]^{1/2} \quad (4)$$

The energy levels for n=2,4,6,….states are obtained from the roots of the transcendental equation,

$$cot\left(k_n\frac{l}{2}\right)=-\frac{m*(0)k_n'}{m*(x)k_n} \quad (5)$$

The corresponding anti-symmetric wave function is obtained as

$$\varphi_n(z) = \begin{cases} D_n \sin(k_n z) & |z| < \frac{l}{2} \\ \sin(z) D_n \sin(k_n l/2) e^{-k_n'(|z|-\frac{l}{2})} & |z| \geq \frac{l}{2} \end{cases} \quad (6)$$

The normalization constant D_n is obtained as

$$D_n = \left[\frac{2k_n}{k_n l + \sin(k_n l) + 2k_n \sin^2(k_n l/2)/k_n'}\right]^{1/2} \quad (7)$$

The wave function in the QW structure is defined as $\phi_{n,k_t}(r_t, z) = e^{ik_t.r_t}\phi_n(z)$ with the energy $E_{n,k_t} = E_n + \hbar^2 k_t^2/2m^*(0)$

Using the compact density matrix method and usual interactive procedure[7], the electronic polarization in a QW under the optical field with frequency ω normal to the growth direction can be expanded in Taylor series as,

$$p(t) = \epsilon_0 \chi^{(1)}(\omega) \mathrm{E} e^{i\omega t} + \epsilon_0 \chi^{(3)}(\omega) \mathrm{E} e^{i\omega t}, \quad (8)$$

Where ϵ_0 is the vacuum permittivity, $\chi^{(1)}(\omega)$ and $\chi^{(3)}(\omega)$ are the linear and nonlinear susceptibility, respectively . The higher terms are neglected. The analytic forms of $\chi^{(1)}(\omega)$ and $\chi^{(3)}(\omega)$ have been derived by modeling the QW as a two-level system[2]. The absorption coefficient is related to susceptibility as $\alpha(\omega) = \omega\sqrt{\mu/\epsilon_R} Im[\epsilon_0 \chi(\omega)]$. The analytic expressions for the linear absorption coefficient is obtained as

$$\alpha^{(1)}(\omega) = \omega \sqrt{\frac{\mu}{\epsilon_R}} \frac{|M_{21}|^2 \sigma_s \hbar \Gamma_{21}}{(E_{21} - \hbar\omega)^2 + (\hbar\Gamma_{21})^2} \quad (9)$$

Where μ is the permeability of system, ϵ_R is the real part of the permittivity, σ_s is the sheet carrier density in the QW, $E_{21} = E_2 - E_1$ and $\Gamma_{21} = \Gamma_1 + \Gamma_2$ is the lineshape.

The third order nonlinear absorption coefficient,

$$\alpha^{(3)}(\omega, I) = -\omega \sqrt{\frac{\mu}{\epsilon_R}} \frac{I}{2\epsilon_0 n_r c} \frac{|M_{21}|^2 \sigma_s \hbar \Gamma_{21}}{[(E_{21} - \hbar\omega)^2 + (\hbar\Gamma_{21})^2]^2}$$

$$\left[4|M_{21}|^2 - \frac{|M_{22} - M_{11}|^2 [3E_{21}^2 - 4E_{21}\hbar\omega + \hbar^2\omega^2 - \hbar^2\Gamma_{21}^2]}{E_{21}^2 + (\hbar\Gamma_{21})^2}\right], \quad (10)$$

Where I is the optical intensity and M_{ij} is the dipole moment matrix element. In the symmetric rectangular QW , M_{11} and M_{22} vanish.

Taking the weak electron-LO phonon coupling interaction, the wave function can be calculated using the perturbation method as,

$$\psi_{n,k_t}(r_t,z) = \varphi_{n,k_t}(r_t,z) + \sum_{m\neq n}\sum_{k_t'} \frac{\left\langle \varphi_{m,k_t'}(r_t,z)\middle|H_{e-ph}\middle|\varphi_{n,k_t}(r_t,z)\right\rangle}{E_{n,k_t'}-E_{n,k_t}+\hbar\omega_{LO}} \varphi_{m,k_t'}(r_t,z) \tag{11}$$

Where the phonon emission process is taken into consideration. The electron-LO phonon interaction Hamiltonian in the Frohlich form is given as,

$$H_{e-ph} = \sum_{q_t}\sum_{q_z}\left[i\frac{4\pi\alpha}{\Omega q^2}\hbar\omega_{LO} r_s b_{qt} e^{-iq_{t.r_t}} e^{-iq_z z} + c.c\right] \tag{12}$$

Where $r_p = (\hbar/2m^*(0)\omega_{LO})^{1/4}$is the polaron radius. Since the second term corresponds to phonon emission process, it contributes to Eq.(11).

The dipole momentum including the polaron correction is defined as

$$M_{ij} = \int \Psi_{i,k_t}(r_t,z) z \Psi_{j,k_t}(r_t,z) d^3r \tag{13}$$

The lineshape due to the electron-LO phonon interaction is calculated using the Fermi golden rule as,

$$\Gamma_n(k_t) = 2\pi \sum_m \sum_{k_t'} \left| < \Phi_{m,k_t'}(r_t,z)\middle|H_{e-ph}\middle|\Phi_{n.k_t}(r_t,z) > \right|^2 f(E_{n,k_t})\left[1 - f(E_{m,k_t'})\right] \times \delta(E_{m,k_t'} - E_{n,k_t} + \hbar\omega_{LO}) \tag{14}$$

In our calculation x=0.3 which yields the barrier height V_0=228meV. The barrier width l =70Å and for this well there are two energy levels with values 54.566 and 200meV. We have taken $\mu = 4\pi \times Hm^{-1}, \epsilon_R = n_r^2\epsilon_0, \eta_r = 3.3, \sigma_s = 5\times10^{16} cm^{-3}, \hbar\omega_{LO} = 36.25\, meV$ and $\alpha = 0.068$. The sheet carrier density $\sigma_s = 5\times10^{16} cm^{-3}$ yields the Fermi energy as 35.592meV from the charge neutrality condition. The calculated lineshape Γ_{21} due to electron-LO-phonon interaction is 3.092meV. When the electron-LO-phonon interaction is not included , the diagonal dipole moments M_{11} and M_{22} vanish whereas with the inclusion of interaction term M_{11} and M_{22} are 3.48 Å and -6.55 Å .The off-diagonal elements M_{12} and M_{22} are identical and it reduces from 19.34 Å to 18.57 Å when the interaction is included.

The total absorption coefficients $\alpha(\omega, I) = \alpha^{(1)}(\omega) + \alpha^{(3)}(\omega, I)$ as a function of the photon energy $\hbar\omega$ for two laser intensities are calculated with and without the electron-LO-phonon interaction and are shown in Fig.1. It is clear

that the electron-phonon interaction term reduces the absorption coefficient irrespective of the strength of laser field. Since M_{21} reduces when the electron-LO-phonon interaction term is included. $\alpha^{(1)}(\omega)$ is reduced. The magnitude of the nonlinear term $\alpha^{(3)}(\omega, I)$ is decided by $|M_{22} - M_{11}|$ which is 10.03Å when the electron-phonon interaction term is taken into account whereas it vanishes without the interaction. Since $\alpha^{(3)}$ is negative in nature $\alpha(\omega)$ is reduced when the electron-phonon interaction is taken into consideration. At higher I, $\alpha(\omega)$ is bleached.

In conclusion, the effect of electron-LO-phonon interaction on the optical absorption coefficient in a single QW is studied. The nonlinear absorption coefficient is increased due to dipole matrix elements modified by the electron-phonon interaction. Since the nonlinear absorption coefficient is negative in nature, the total absorption coefficient is reduced when the polaron effects are included.

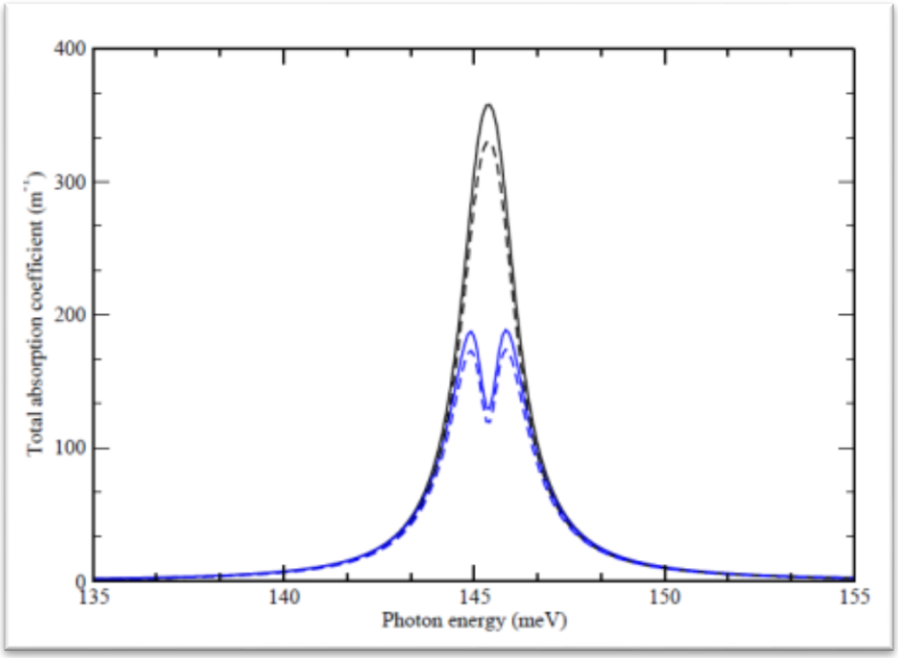

Figure. 1: total absorption coefficient as a function of photon energy. For two cases: (1) considering the electron-LO-phonon interaction (dashed line), (2) without considering the electron-LO-phonon interaction (solid line). The black and blue lines correspond to the calculations with laser intensities $1 \times 10^{10}$and 2×10^{10}mW/m^2,respectively.

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