PRAMANA — journal of physics
© Indian Academy of Sciences
Vol. 78, No. 5
May 2012
pp. 827–833

Effect of conduction band nonparabolicity on the optical properties in a single quantum well under hydrostatic pressure and electric field

S PANDA[1,*] and B K PANDA[2]
[1]Department of Mathematics; [2]Department of Physics, Ravenshaw University, Cuttack 753 003, India
*Corresponding author. E-mail: sudhira@iopb.res.in

MS received 9 June 2011; revised 11 October 2011; accepted 23 December 2011

Abstract. The effect of conduction band nonparabolicity on the linear and nonlinear optical properties such as absorption coefficients, and changes in the refractive index are calculated in the $Al_{0.3}Ga_{0.7}As/GaAs$ heterostructure-based symmetric rectangular quantum well under applied hydrostatic pressure and electric field. The electron envelope functions and energies are calculated in the effective mass equation including the conduction band nonparabolicity. The linear and nonlinear optical properties have been calculated in the density matrix formalism with two-level approximation. The conduction band nonparabolicity shifts the positions of the optical properties and decreases their strength compared to those without this correction. Both the optical properties are enhanced with the applied hydrostatic pressure. While the absorption coefficients are bleached under the combined effect of high pressure and electric field, the bleaching effect is reduced when nonparabolicity is included.

Keywords. Quantum well; nonparabolicity correction; nonlinear optics; hydrostatic pressure; electric field.

PACS Nos 73.21.Fg; 42.65.K; 47.85.Dk

When polarized light is incident on the growth direction of the quantum well (QW), the degenerate energy levels in the well will cause a narrow absorption spectrum where the photon energy at the peak corresponds to the intersub-band transition energy. The absorption coefficients are calculated using the density matrix method outlined in the theory of nonlinear optics [1]. In this theory, the contribution of the nonlinear term which depends on the strength of optical intensity is quite significant and it is just opposite to the linear term [2,3]. The optical properties such as the absorption coefficients and the changes in the real part of the refraction index have been calculated in the single rectangular [2,3], the double rectangular [4], the triple rectangular [5], the single asymmetric [6] and the single diffusion modified [7] QWs as a function of the incident optical field. The absorption

DOI: 10.1007/s12043-012-0270-0; ***e*Publication: 18 April 2012**

coefficients have been calculated in the QWs under a DC electric field which is perpendicular to the growth direction of the QW. The electric field not only influences the intersub-band transition energies but also shifts the wave functions in the direction of the field. As a result of this, the strength of the absorption coefficients is enhanced in the QW compared to those without the field [2,7,8]. The total absorption coefficient can be bleached at sufficiently high incident optical intensity [2,8].

The energy level at the bottom of a sub-band in a QW can often be determined to a reasonable accuracy by the parabolic band. However, for sub-bands fairly far from the bulk conduction band edge, the correction due to nonparabolicity can be important [9,10]. In a narrow QW under a strong magnetic field, the optical absorption coefficients calculated with the nonparabolicity correction shows remarkable deviation from results obtained using parabolic energy approximation [11]. The influence of nonparabolicity on the electronic states is important for calculating dark current in a QW [12]. It is therefore expected that the nonparabolicity correction of the electronic states will be important for calculating absorption coefficients in a QW under applied hydrostatic pressure and electric field.

The diamond-anvil cell (DAC) technique [13,14] makes it possible to perform experimental measurements of the electronic and optical properties of heterostructure systems at high pressure under cryogenic temperature. The electronic states are highly influenced by the hydrostatic pressure since it decreases the well width and barrier height. Recently, the study of electronic and optical properties of a QW under applied hydrostatic pressure has attracted a renewed interest. Several properties of the QW such as the second harmonic generation [15], the optical phonon-assisted electron mobility [16], the donor binding energies [17–23] and the Lande $g_{\parallel}$ and g-factor anisotropy [24] have been studied in AlGaAs/GaAs single QW under hydrostatic pressure. It is therefore expected that the absorption coefficients calculated under hydrostatic pressure will be remarkably different from those without the pressure.

The donor binding energies in quantum wells under the combined effect of hydrostatic pressure and electric field have been studied [25,26]. The absorption coefficient and change in refractive index under the combined effect of hydrostatic pressure and electric field have also been studied [27]. However, the effect of nonparabolicity correction on the physical and optical properties in a QW structure under the combined effect of hydrostatic pressure and electric field has not been carried out. In order to fill up this gap, the present paper aims to study the effect of conduction band nonparabolicity on the linear and nonlinear optical absorption coefficients and changes in the real part of the refractive index in a single symmetric rectangular quantum well (RQW) based on $Al_{0.3}Ga_{0.7}As/GaAs$ heterostructures under the combined influence of hydrostatic pressure and electric field.

The energy levels and the corresponding envelope functions in the RQW can be determined from the effective mass equation with nonparabolicity correction [10–12]

$$\left[-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m_{\perp}^{*}(z, E_n, P)}\frac{\partial}{\partial z} + V(z, P) + eFz\right]\Psi_n(z) = E_n\Psi_n(z), \tag{1}$$

where $V(z, P)$ is the confining potential under hydrostatic pressure P, $m_{\perp}^{*}(z, E_n, P)$ is the position-dependent effective mass along the growth direction under P and F is the applied electric field perpendicular to the growth direction. The pressure-dependent well width is reduced as [15] $W = L[1 - (S_{11} + 2S_{12})P]$, where L is the original well width and $S_{11} = 1.16 \times 10^{-3}$ kbar^{-1} and $S_{12} = -3.7 \times 10^{-4}$ kbar^{-1} are the compliance constants of GaAs. Under the applied hydrostatic pressure, the barrier height is reduced as $V_0(x, P) = Q_c \Delta E_g(x, P)$ where $Q_c = 0.6$ is the conduction band offset and $\Delta E_g(x, P) = (1.155x + 0.37x^2 - 1.3 \times 10^{-3} x P)$eV is the pressure-dependent band gap difference between $Al_xGa_{1-x}As$ and GaAs with P measured in kbar [15]. The nonparabolic effective mass in the growth direction is defined as [10]

$$m_{\perp}^{*}(x, E_n, P) = \frac{m^*(x, P)}{\alpha(x, E_n, P)}[1 - \sqrt{1 - 2\alpha(x, E_n, P)}], \tag{2}$$

where $\alpha(x, E_n, P) = 4\gamma(x) m^*(x, P)[E_n - V_0(x, P)]/\hbar^2$ and the nonparabolicity correction $\gamma(x) = 95.3475 + 265.4429x$. The pressure-dependent effective mass is defined as [15]

$$m^*(x, P) = \left[\frac{1}{1 + 2E_p/E_g(P) + E_p/[E_g(P) + \Delta_0]} + 0.0856x + 0.0231x^2\right] m_0, \tag{3}$$

where m_0 is the electron rest mass, $E_p = 7.51$ eV, $\Delta_0 = 0.341$ eV and the pressure-dependent energy gap in GaAs $E_g(P) = (1.424 + 1.26 \times 10^{-2} P - 3.77 \times 10^{-5} P^2]$ eV. The energy for the nth state including the transverse kinetic energy is obtained as $\mathcal{E}_n(k_{\parallel}, P) = E_n + \hbar^2 k_{\parallel}^2 / 2m_{\parallel}^*(0, E_n, P)$, where the effective mass perpendicular to the growth direction is defined as [10]

$$m_{\parallel}^{*}(x, E_n, P) = \frac{m^*(x, P)}{\sqrt{1 - 2\alpha(x, E_n, P)}}. \tag{4}$$

Both parallel and perpendicular effective masses are enhanced in the well region while these are reduced in the barrier region.

The effective mass equation in eq. (1) under zero bias can be solved using the analytic method of Nag and Mukhopadhyay [10]. The energy levels and envelope functions in the well are obtained by matching $\Psi(z)$ and $1/m_{\parallel}(z, E_n, P)\partial_z \Psi(z)$ at the boundaries of the well $\pm W/2$. The eigenstates in the well under the applied electric field can be solved by first transforming the coordinate z to dimensionless coordinate Z and then matching the Airy function and its derivative with parallel mass at the boundary of the well [12].

With the calculated ground and first excited state electron energy levels and envelope functions in a quantum well, the optical properties can be calculated in the density matrix formalism [2,3]. Assuming that a monochromatic incident field $E(t) = \bar{E} e^{i\omega t} + \bar{E}^* e^{i\omega t}$ is applied to a two-level system, the polarization response is written as

$$P(t) = \epsilon_0 \chi^{(1)}(\omega) e^{i\omega t} + \epsilon_0 \chi^{(3)}(\omega) e^{i\omega t}, \tag{5}$$

where ϵ_0 is the permittivity in free space, and $\chi^{(1)}(\omega)$ and $\chi^{(3)}(\omega)$ are the linear and nonlinear susceptibilities, respectively. The DC optical rectification and higher-order harmonics in ω are not considered here since these are negligibly small in a symmetric well. In a two-level system, using the density compact matrix formalism with iterative procedure [2,3], the linear and nonlinear susceptibilities are obtained as

$$\epsilon_0 \chi^{(1)}(\omega) = \frac{e^2[\rho(E_1) - \rho(E_2)]|M_{21}|^2}{E_{21} - \hbar\omega - i\Gamma_{21}}, \tag{6}$$

$$\begin{aligned}\epsilon_0 \chi^{(3)}(\omega) = & -\frac{e^4[\rho(E_1) - \rho(E_2)]|M_{21}|^2 I}{E_{21} - \hbar\omega - i\Gamma_{21}} \\ & \times \left[\frac{4|M_{21}|^2}{(E_{21} - \hbar\omega)^2 + \Gamma_{21}^2} - \frac{|M_{22} - M_{11}|^2}{(E_{21} - i\Gamma_{21})(E_{21} - \hbar\omega - i\Gamma_{21}}\right],\end{aligned} \tag{7}$$

where the energy separation $E_{21} = E_2 - E_1$, the optical intensity $I = |\bar{E}|^2$, $\rho(E_i)$ is the density of states for the ith state, eM_{ij} is the dipole moment and Γ_{21} is the lineshape. The density of states for the ith state is given as

$$\rho(E_i) = \left(\frac{m_{\parallel}^*(0, E_i, P) k_B T}{W \pi \hbar^2}\right) \log\left(1 + \exp\left[\frac{(E_F - E_i)}{k_B T}\right]\right). \tag{8}$$

M_{ij} is defined as

$$M_{ij} = \int_{-\infty}^{\infty} dz \Psi_i^*(z) z \Psi_j(z), \qquad i, j = 1, 2. \tag{9}$$

Under zero-bias, M_{11} and M_{22} vanishes in a symmetric single RQW.

The lineshape is calculated taking rates from the tunnelling and scattering processes as

$$\Gamma_{21} = \frac{\hbar}{2}\left(\frac{1}{\tau_1^{\rm tun}} + \frac{1}{\tau_2^{\rm tun}} + \frac{1}{\tau_1^{\rm scat}} + \frac{1}{\tau_2^{\rm scat}}\right), \tag{10}$$

where $\tau_i^{\rm tun}$ and $\tau_i^{\rm scat}$ are the mean tunnelling and scattering rates for the ith level at temperature T. The method for calculating $\tau_i^{\rm tun}$ is given in detail in our earlier work [12]. The mean scattering rates with the longitudinal optic (LO) phonon are calculated in the Fermi golden rule by taking absorption of phonons [9]. The scattering rates under hydrostatic pressure and applied electric field are calculated taking the pressure-dependent static dielectric constant $\epsilon_0(P) = 13.1 - 0.0088P$ [28], high-frequency dielectric constant $\epsilon_\infty(P) = 10.89 + 0.0219P$ [28], phonon energy $\hbar\omega_{\rm LO}(P) = (36.25 - 0.0485P)$ [29] and temperature $T = 77$ K.

The absorption coefficient is obtained as $\alpha(\omega) = \omega\sqrt{\mu/\epsilon_R}\ {\rm Im}[\chi(\omega)]$, where μ is the permeability of the material and ϵ_R is the real part of the permittivity, respectively. The change in refractive index is related to $\chi(\omega)$ as $\Delta n(\omega)/n_r = {\rm Re}[\chi(\omega)/2n_r^2]$ where n_r is the refractive index. The total absorption coefficient and change in the real part of the refractive index are calculated by summing their linear and nonlinear parts.

The single symmetric quantum well with 80 Å well width and an aluminium concentration $x = 0.3$ is a two-level system since it contains two energy levels. Several quantities such as the energy separation, the Fermi energy, the dipole moment and the linewidth which are required for calculating optical properties of this well are tabulated in table 1. While the nonparabolicity decreases the energy separation and the dipole moment due to narrowing of the well width and speading of envelope function, it increases the

Table 1. Energy separation (E_{21}), Fermi energy (E_F), dipole moment (M_{21}) and linewidth (Γ_{21}) in $Al_{0.3}Ga_{0.7}As/GaAs$ symmetric RQW under hydrostatic pressures $P = 0$, 20 and 50 kbar and electric field strength $F = 0$ and 100 kV/cm.

		$F = 0$ kV/cm		$F = 100$ kV/cm	
Quantity	Pressure (kbar)	Parabolic	Nonparabolic	Parabolic	Nonparabolic
	0	120	116	119	114
E_{21} (meV)	20	111	108	110	107
	50	102	100	102	99
	0	22.82	27.99	21.95	27.19
E_F (meV)	20	18.82	23.71	17.93	22.91
	50	14.76	19.35	13.86	18.56
	0	0	0	−4.10	−503.76
M_{11} (Å)	20	0	0	−4.18	−503.76
	50	0	0	−4.26	−503.77
	0	22.10	21.36	21.53	17.22
M_{21} (Å)	20	21.49	20.68	21.21	16.53
	50	20.85	19.98	20.67	15.77
	0	0	0	−20.82	−514.10
M_{22} (Å)	20	0	0	−9.45	−508.28
	50	0	0	−4.98	−505.48
	0	1.20	1.24	1.08	1.09
Γ_{21} (meV)	20	0.91	0.93	0.85	0.85
	50	0.42	0.39	0.38	0.38

Fermi energy and the linewidth due to increase in nonparabolic effective mass in the well region. However, the effect of nonparabolicity is weak when the hydrostatic pressure is high.

The absorption coefficients and changes in refractive index with and without the nonparabolicity effects under 0, 20 and 50 kbar hydrostatic pressures are calculated taking $n_r = 3.3$, $\epsilon_R = n_r^2\epsilon_0$, $\mu = 12.8$, $I = 0.1$ MW/cm^2, $T = 77$ K and $F = 0$ kV/cm and shown in figure 1. The resonant energies of absorption corresponding to the peak positions of the linear and nonlinear absorption coefficients decrease with increasing pressure. The strength of absorption coefficients decreases with increasing pressure. Similar effects are found in the changes of refractive index. Both the effects can be easily understood in terms of the decreasing energy level separation and scattering rate with the applied pressure. The nonparabolicity decreases the strength of both linear and nonlinear optical properties. The total absorption coefficient is bleached at $P = 50$ kbar due to large nonlinear absorption coefficient.

The total absorption coefficients and changes in refractive index with and without the nonparabolicity correction for different hydrostatic pressures under the electric field strength $F = 100$ kV/cm are shown in figure 2. The effect of hydrostatic pressure on the optical properties under electric field is the same as those in figure 1 calculated under zero bias. The deviation between optical properties calculated with and without the nonparabolicity correction increases with applied electric field. At high pressure, the bleaching effect is reduced with the inclusion of nonparabolicity effect.

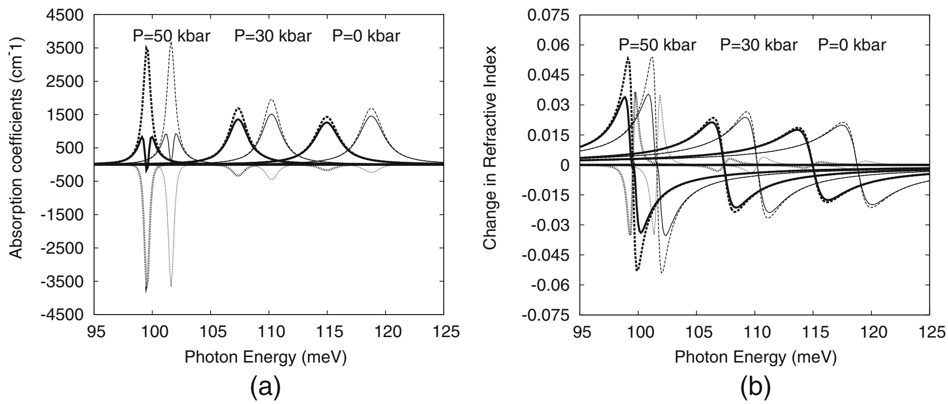

Figure 1. Optical properties of the single symmetric rectangular quantum well $Al_{0.3}Ga_{0.7}As/GaAs$ with well width $L = 80$ Å under 0, 20 and 50 kbar hydrostatic pressures and zero bias. Absorption coefficients (**a**) and changes in the real part of the refractive index (**b**) are plotted as a function of photon energy. The results with and without the nonparabolicity correction are shown by thick and thin lines, respectively. The dashed, dotted and solid lines correspond to linear, nonlinear and total optical properties.

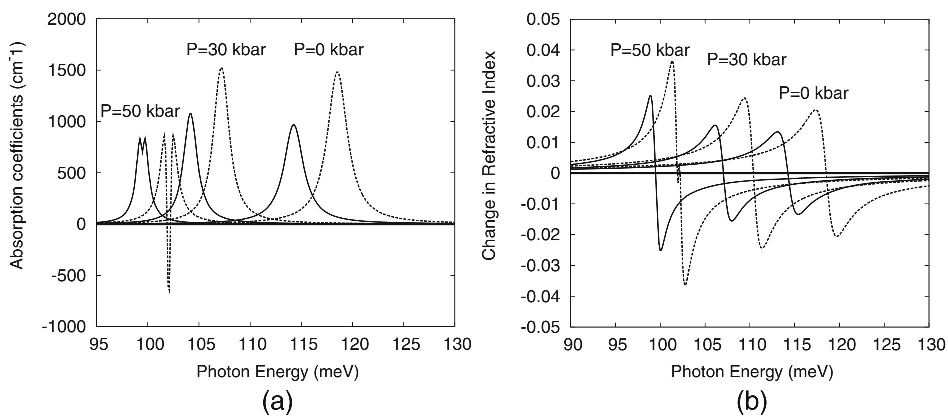

Figure 2. Absorption coefficients (**a**) and changes in the real part of the refractive index (**b**) with (solid line) and without (dashed line) the nonparabolicity corrections as a function of photon energy under 0, 20 and 50 kbar hydrostatic pressures and electric field $F = 100$ kV/cm.

In conclusion, the intersub-band transitions in quantum wells are important for designing devices based on these systems. In this work, we present a study of the linear and nonlinear absorption coefficients and changes in the refractive index as a function of the electric field and applied hydrostatic pressure in a symmetric RQW with and without the nonparabolicity corrections. The inclusion of nonparabolicity in the calculation of energies and wave functions in a QW shows that the ground state, as it is far away from the conduction band edge, is affected by the nonparabolicity effect. The applied hydrostatic pressure decreases the energy levels and the envelope functions are spread out to the barrier region. The energies and envelope functions are Stark shifted by the applied electric field. The hydrostatic pressure decreases the resonant peak position and increases the strength of the optical properties by decreasing energy separation and lineshape, respectively. At high pressure, the optical properties are bleached. The effect of electric field is to widen the separation of optical properties with and without the nonparabolicity and reduces the nonlinear contribution due to lower nonlinear effect.

Acknowledgement

One of the authors, Sudhira Panda, acknowledges the financial support of the Department of Science and Technology (DST) SR/WOS-A/PS-33/2007 to carry out this work.

References

[1] R W Boyd, *Nonlinear optics* (Academic Press, Boston, 1992)
[2] D Ahn and S L Chuang, *IEEE J. Quatum Electron.* **QE-23**, 2196 (1987)
[3] K J Kuhn, G U Iyengar and S Yee, *J. Appl. Phys.* **70**, 5010 (1991)
[4] E Ozturk, H Sari and I Sokman, *Eur. Phys. J. Appl. Phys.* **35**, 1 (2006)
[5] E Ozturk and I Sokman, *Eur. Phys. J. Appl. Phys.* **51**, 10303 (2010)
[6] M Bedoya and A S Camacho, *Phys. Rev.* **B72**, 155318 (2005)
[7] S Panda, B K Panda, C D Beling and S Fung, *J. Appl. Phys.* **80**, 1532 (1996)
[8] E Ozturk, *Eur. Phys. J.* **B75**, 197 (2010)
[9] P Harrison, *Quantum wells, wires and dots* (John Wiley and Sons, Ltd., England, 2001)
[10] B R Nag and S Mukhopadhyay, *Phys. Status Solidi* **B175**, 103 (1993)
[11] L Y Yu, J C Cao and C Zhang, *J. Appl. Phys.* **99**, 123706 (2006)
[12] S Panda, B K Panda and S Fung, *J. Appl. Phys.* **101**, 043705 (2007)
[13] *Physics of solids under pressure* edited by J S Schilling and R N Shelton (North-Halland, New York, 1981)
[14] A Jayaram, *Rev. Mod. Phys.* **55**, 65 (1983)
[15] I Karabulut, U Atav, H Safak and M Tomak, *Physica* **B393**, 133 (2007)
[16] X P Bai and S L Ban, *Eur. Phys. J.* **B58**, 31 (2007)
[17] A M Elabsy, *J. Phys.: Condens. Matter* **6**, 10025 (1994)
[18] A M Elabsy, *Phys. Scr.* **48**, 376 (1993)
[19] S L Ban and X X Liang, *J. Lumin.* **94–95**, 417 (2001)
[20] A Montes, A L Morales and C A Duque, *Surf. Rev. Lett.* **9**, 1753 (2002)
[21] G J Zhao, X K Liang and S L Ban, *Phys. Lett.* **A319**, 191 (2003)
[22] J W Gonzalez, N Porras-Montenegro and C A Duque, *Braz. J. Phys.* **36**, 944 (2006)
[23] E C Niculescu and N Eseanu, *Eur. Phys. J.* **B75**, 247 (2010)
[24] N Porras-Montenegro, C A Duque, E Reyes-Gomez and L E Oliveira, *J. Phys.: Condens. Matter* **20**, 465220 (2008)
[25] A L Morales, A Montes, S Y Lopez and C A Duque, *J. Phys.: Condens. Matter* **14**, 987 (2002)
[26] E C Niculescu and N Eseanu, *Eur. Phys. J.* **B75**, 247 (2010)
[27] I Karabulut, M E Mora-Ramos and C A Duque, *J. Lumin.* **131**, 1502 (2011)
[28] A El Moussaouy, D Bria and A Nougaoui, *Physica* **B370**, 178 (2005)
[29] U D Venkateswaran, L J Cui, B A Weinstein and F A Chambers, *Phys. Rev.* **B45**, 9237 (1992)