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The hydrostatic pressure effects on intersubband optical absorption of n -type δ -doped quantum well in GaAs

O. Oubram^{a,*}, O. Navarro^a, L.M. Gaggero-Sager^b, J.C. Martínez-Orozco^c, I. Rodríguez-Vargas^c

^a Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de Mèxico, Apartado Postal 70-360, 04510, México. D.F, Mexico ^b Facultad de Ciencias, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, Col. Chamilpa Cuernavaca, Morelos 62210, Mexico ^c Unidad Académica de Física, Universidad Autónoma de Zacatecas, Calzada Solidaridad Esquina con Paseo la Bufa S/N, Zacatecas, Zac., 98060, Mexico

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ABSTRACT

We have theoretically calculated the effects of hydrostatic pressure on subband structure and optical transitions in n -delta-doped quantum well (DDQW) in GaAs for different values of energy. The electronic structure of DDQW under the hydrostatic pressure is determined by solving the Schrödinger equation and a simple algebraic method. From our calculations, it is found that the subband energies and intersubband optical absorption is quite sensitive to the applied hydrostatic pressure. This gives a new degree of freedom in various device applications based on the intersubband transitions of electrons.

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1. Introduction

Devices with delta (δ , planar)-doped semiconductor structures have recently attracted much attention because of their potential technological applications in electronic and photonic devices [1–8]. The δ -doping technique has been used widely to introduce carrierconfinement effects [1,3,9–14]. Due to this property of localizing impurities in space, δ -doping is used in devices to give rise to quantum confinement of carriers [6,8,12–16].

Such δ -doped semiconductor structures are important for various devices such as high-power FETs, and infrared devices based on the intersubband transition of electrons.

Recently, more attention has been paid to study experimentally and theoretically the optical properties of nanostructures such as quantum dots (QD), quantum wires, and quantum wells [17–29].

It is to be noted that external factors such as shallow impurity, temperature, electric and magnetic fields, and pressure can change the optical and transport properties of nanostructures [9,21–24,27,29–31]. This why in the past few years, many researchers have studied effect of the external factors on the electronic and optical properties of low dimensional semiconductor structures.

The effects of the hydrostatic pressure applied on two-dimensional structures have been studied by several authors [23,25,30,32,33]. The hydrostatic pressure dependence of the intersubband optical absorption is also interesting for potential

E-mail address: oubram@uaem.mx (O. Oubram).

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device applications. Intersubband absorption in quantum wells have been proposed or demonstrated experimentally to be very useful for far-infrared detectors [34,35], electro-optical modulators [36,37], and infrared lasers [38]. One of the most remarkable features of two-Dimensional Electronic Gas (2DEG) is the intersubband optical transitions between the size quantized subbands in the same band.

The intersubband optical absorption in simple and double quantum wells, grooves, dots and wires under pressure [24-28,39-42] has been studied. For instance, Raigoza et al. [19] have calculated optical absorption spectra in symmetrical doped quantum well structures in the presence of applied pressure, they observed a blue shift in the optical transitions with increasing of the pressure. Barseghyan et al. [20] investigated the influence of externally applied hydrostatic pressure on the binding energy and photoionization in GaAs– $Ga_{1-x}Al_xAs$ cylindrical QD. The pressure effect on intersubband optical absorption in a V-groove quantum wire was studied by Khordad et al. [26]. They deduced that this coefficient increases towards high energies as the pressure increases. Karabulut et al. [27] investigated the dependence of optical absorption in asymmetric double quantum wells with the hydrostatic pressure. The effects of hydrostatic pressure on the optical absorption coefficient in the QD have been computed by Galindez et al. [40] and Shijun Liang et al. [28].

Even though considerable attention has been given to the study of the optical properties in semiconductor structures, the effect of pressure on these properties have not been well understood in DDQW. In this work, we studied the intersubband absorption



^{*} Corresponding author. Tel.: +52 555 623 28 97.

coefficients changes in *n*-type DDQW in GaAs under the influence of hydrostatic pressure. It is used an algebraic formulation to obtain the linear absorption coefficient and electronic structure. Particularly, we solve the Schrödinger equation for P = 0 kbar and then applied the algebraic formalism to solve it in the full range of hydrostatic pressures of interest. It is showed that the intersubband transitions are quite sensitive to the hydrostatic pressure.

2. Theoretical background

In the effective mass approximation the Schrödinger equation for a n -type DDQW under hydrostatic pressure is given by:

$$-\frac{\hbar^2}{2m^*(P)}\frac{d^2\psi(z,P)}{dz^2} + V(z,P)\psi(z,P) = E(P)\psi(z,P),$$
(1)

where *P* is the hydrostatic pressure in units of kbar, V(z,P) is the pressure dependent confinement potential and $m^*(P)$ is the pressure dependent effective mass. Usually, the electronic structure calculations in GaAs *n* -type DDQW can be carried out by solving a single band effective mass Schrödinger equation with a V-shaped Thomas-Fermi potential or by means of a self-consistent approach for each value of *P*.

A convenient way to perform such analysis is introducing effective atomic units. We suppose that at low hydrostatic pressure all physical proprieties can be expressed in effective mass and dielectric constant. This means that distances are given in terms of the effective Bohr radius, $a_0^*(P) = \epsilon(P)\hbar/m^*e^2$, and the energies in units of the effective Rydberg, $R_y^*(P) = e^2/2\epsilon(P)a_0^*(P)$. Here, $\epsilon(P)$ is the pressure dependent dielectric constant. Furthermore, the wave function, energy, confinement potential and position will be write as: $\psi(P) = \psi^* \times a_0^{*-(1/2)}(P)$, $E(P) = E^* \times R_y^*(P)$, $V(z, P) = V^* \times R_y^*(P)$ and $z = z^* \times a_0^*(P)$, respectively.

Within this context, the Schrödinger equation can be written as:

$$-\frac{d^2\psi^*}{dz^{*2}} + V^*\psi^* = E^*\psi^*.$$
 (2)

The inclusion of pressure effects is made via the variation of the main input parameters upon *P* [23,43]. At the GaAs Γ -point conduction band minimum, the following relation for the related energy band gap holds;

$$E_{gap}(P) = E_1 + \beta P, \tag{3}$$

where $E_1 = 1519$ meV, and $\beta = 10.7$ meV/kbar. The variation of the static dielectric constant is given by [42]:

$$\varepsilon(P) = 12.65e^{-1.67P \times 10^{-3}},\tag{4}$$

and the corresponding electron effective mass is given by [18,39]:

$$m^{*}(P) = \left[1 + \frac{2 \times 7510}{E_{gap}(P)} + \frac{7510}{E_{gap}(P) + 341}\right]^{-1} m_{0}.$$
 (5)

The variation of P in this work lies within the range between 0 kbar and 10 kbar. We restrict ourselves to consider values of P below the point of transition from the direct to the indirect energy gap regimes, induced by pressure in GaAs. The confinement potential can be related to the well known Thomas-Fermi potential by means of the following relations,

$$V^* = \frac{V(z, P = 0)}{R_v^*(P = 0)},$$
(6)

Where V(z, P = 0) is the δ -doped well potential at P = 0, and is described within the self-consistent Thomas-Fermi approach [44] by:

$$V(z, P = 0) = -\frac{\alpha_n^2}{(\alpha_n |z| + z_{0n})^4},$$
(7)

with $\alpha_n = 2/(15\pi)$ and $z_{0n} = (\alpha_n^3/\pi N_{2d})^{1/5}$, N_{2d} is the twodimensional impurity density of the *n*-type DDQW.

It is worth mentioning that the solution of the Eq. (2) is energy levels E_i^* , and their corresponding wave functions ψ_i^* . Their correspondence for a value of *P* is:

$$E_i(P) = E_i^* \times R_v^*(P), \tag{8}$$

and

$$\psi_i(P) = \psi_i^* \times a_0^{*-\frac{1}{2}}(P).$$
(9)

After obtain the subband energies and their corresponding wave functions, the linear absorption coefficient $\alpha(\omega)$ for the intersubband transitions can be readily calculated as:

$$\alpha(\omega) = \frac{\omega\mu ce^2}{n_F} \left| M_{fi} \right|^2 \frac{m^* k_B T}{L_{\text{eff}} \pi \hbar^2} \times \ln \left\{ \frac{1 + \exp[(E_F - E_i)/k_B T]}{1 + \exp\left[\left(E_F - E_f\right)/k_B T\right]} \right\}$$
$$\times \frac{\hbar/\tau_{\text{in}}}{\left(E_f - E_i - \hbar\omega\right)^2 + \left(\hbar/\tau_{\text{in}}\right)^2},$$
(10)

with the matrix element given by

$$M_{fi} = \int_{-L_0/2}^{L_0/2} \psi_f^*(z) z \psi_i(z) dz, \qquad (11)$$

 E_i and E_f denote the quantized energy levels for the initial and final states, respectively, μ is the permeability, c is the speed of light in free space, L_{eff} is the effective spatial extent of electrons in subbands, n_r is the refractive index, τ_{in} is the intersubband relaxation time (τ_{in} is a constant and takes the numerical value of 0.14 ps following [29,45]).

We introduce the relative absorption coefficient $\alpha_{rel}(\omega, P)$:

$$\alpha_{\rm rel}(\omega, P) = \frac{\alpha(\omega, P)}{\alpha_{10}(\Omega, P = 0)},\tag{12}$$

where $\alpha_{10}(\Omega, P = 0)$ is the linear absorption coefficient for the intersubband transitions between the ground state and the first excited state at P = 0 kbar, and $\Omega = \arg[\max(\alpha_{1-0}(\omega, P = 0))]$ presents the value of resonance for intersubband transition 1–0.

Now, we write expression (12) in relative effective atomic units at T = 0 K,

$$\begin{aligned} \alpha_{\rm rel}(\omega,P) &= \frac{\omega}{\Omega} \times \left| \frac{M_{fi}(0)}{M_{10}(0)} \right|^2 \times \frac{m^*(P)}{m^*(0)} \times \frac{\varepsilon(0)}{\varepsilon(P)} \times \frac{\Delta E_{fi}(0)}{\Delta E_{10}(0)} \\ &\times \frac{(\Delta E_{10}(0) - \hbar\Omega)^2 + (\hbar/\tau_{in})^2}{\left(\Delta E_{fi}(0) \frac{m^*(P)}{m^*(0)} \frac{\varepsilon(0)^2}{\varepsilon(P)^2} - \hbar\omega \right)^2 + (\hbar/\tau_{in})^2}, \end{aligned}$$
(13)

where $\Delta E_{fi}(0) = E_f(0) - E_i(0)$ denote quantized energy between the final state and initial state at P = 0 kbar.

And we define the relative element matrix as:

$$M_{\rm fi_{\rm rel}} = \frac{M_{\rm fi}(P)}{M_{10}(0)}.$$
 (14)

Writing this expression in effective atomic units, will arrive at this reduce expression,



Fig. 1. The confining δ -potential profile, the subband energies with their wave functions for P = 0 kbar (Solid curves) and P = 5 kbar (dashed curves).



3. Results and discussion

Variation of the confinement potential profile, subband energy levels and wave functions associated to these energy levels in the DDQW, far a doping concentration $N_{2d} = 7.5 \times 10^{12}$ cm⁻², are presented in Fig. 1. The Fermi energy level is set at 0 meV. Solid (dashed) curves correspond to P = 0 (P = 5 kbar). As can be seen in Fig. 1, with the increase of the hydrostatic pressure the potential and the eigenfunctions are more confined.

It is well known that application of hydrostatic pressure results in a modification of the physical properties [18,25,46], this mainly due to deformation of the interatomic bonds [47].

While pressure increases, the dielectric constant decreases and the effective mass increases [18] leading to a decreasing in effective Bohr radius and an increasing in effective Rydberg (see Fig. 2). So, the eigenfunction is more confined and eigenvalues more localized (see Eq. (8) and Eq. (9)).

Fig. 3 shows the energy difference between two successive states as a function of pressure. Here, it can be observed that the energy difference increases when the pressure increases. The similar behavior of the energy difference was observed in V-groove quantum wire [26].



Fig. 2. Variation of effective Bohr radius and effective Rydberg versus hydrostatic pressure.



Fig. 3. The energy difference between two successive states as a function of hydrostatic pressure.

In Fig. 4 the relative lineal absorption coefficients are shown as a function of photon energy for three different pressures, P = 0 kbar, P = 5 kbar and P = 10 kbar for $N_{2d} = 7.5 \times 10^{12}$ cm⁻². It is seen from the figure that the relative lineal absorption coefficient will increase as the pressure increases. Also, the resonance peak positions shift to the higher photon energies (blue shift) as the hydrostatic pressure increases. The shift is due to the increment in the energy difference between the two different states as the hydrostatic pressure increases. Our results are compatible with others found in other quantum structures [20,26,28,39,48].

The forbidden transitions (2–0, 3–1, 4–1, 4–2, 5–2) in Fig. 4 without hydrostatic pressure keeps impossible when the hydrostatic pressure is nonzero, since the pressure doesn't break the symmetry in the system.

Fig. 5 shows the absorption peak of the dominant intersubband transitions (1-0) for different applied hydrostatic pressures. It seems clearly that when the pressure increases the absorption peak increases as well and additionally it shifts to higher energies.

Fig. 6 displays the relative absorption coefficient as a function of the photon energy for three different pressures, P = 0 kbar,



Fig. 4. The variation of the relative absorption coefficient for $N_{2d} = 7.5 \times 10^{12} \text{ cm}^{-2}$ as a function of the photon energy for different intersubband transitions for (a) P = 0 kbar, (b) P = 5 kbar and (c) P = 10 kbar.



Fig. 5. The relative absorption coefficient of the (1-0) intersubband transition as a function of the photon energy for P = 0 kbar-10 kbar with a step equal to 2 kbar. The energy resonance shows a clear blue shift.

P = 5 kbar and P = 10 kbar for $N_{2d} = 3 \times 10^{12}$ cm⁻². It is observed that only two intersubbands transition (1-0) and (3-2) are similar to those shown in Fig. 4. As the pressure increase, the relative linear coefficients increase and shift towards higher energies.

Furthermore, as a result of the increase in the pressure, the magnitude of the absorption coefficient increases and the intersubband absorption spectrum shows a blue shift. The obtained results give a new degree of freedom in device applications, such as photo-detectors, electro-optical modulators, and all optical switches.

Fig. 7 presents the dependence of the relative square dipole matrix element on the hydrostatic pressure. It is observed that the dipole matrix element decreases with pressure. When the pressure increases, the effective mass increases and the dielectric constant decreases on the contrary. This involves the square dipole matrix element to decrease (see Eq. (15)) as the pressure grows. On the other side, as the pressure goes up, the wave functions are very confined and become more compressed in the vicinity of z = 0. This decreasing of $|M_{firel}|^2$ was also seen in simple quantum wells under pressure [49].



Fig. 6. The variation of the relative absorption coefficient for $N_{2d} = 3 \times 10^{12} \text{ cm}^{-2}$ as a function of the photon energy for different intersubband transitions for (a) P = 0 kbar, (b) P = 5 kbar and (c) P = 10 kbar.



Fig. 7. Square dipole matrix element for the intersubband transitions between two successive states versus hydrostatic pressure.

4. Conclusions

In this work we have investigated the effect of the hydrostatic pressure on the subband structure and optical transitions in n-type δ -doped guantum well in GaAs. This effect could be explain only by the pressure effect on the electron effective mass and dielectric constant.

The combined algebraic formalism with the Schrödinger equation were used to determine the electronic structure. From our calculations, we have seen that the hydrostatic pressure can induce an energy separation between intersubband energies and confinement in wave functions.

We have seen that the absorption peaks change in magnitude and the absorption spectrum shifts to the blue as the hydrostatic pressure increases. These changes in the intersubband absorption peaks can be used in various optical device applications. Finally, our results are similar to those found in other structures.

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