Effects of hydrostatic pressure, temperature, electric field and aluminum concentration on the electronic states in GaAs/Ga$_{1-x}$Al$_x$As concentric double quantum rings

H M Baghramyan$^1$, M G Barseghyan$^{1,2,4}$, C A Duque$^3$ and A A Kirakosyan$^1$

$^1$Department of Solid State Physics, Yerevan State University, 1 Alex Manoogian, Yerevan 0025, Armenia
$^2$Base College of Yerevan State University of Architecture and Construction, 105 Vahan Teryan, Yerevan 0009, Armenia
$^3$Instituto de Física, Universidad de Antioquia, AA 1226, Medellín, Colombia

Email: mbarsegh@ysu.am

Abstract. Using the effective mass approximation and transfer matrix formalism the ground state energy of an electron in GaAs/Ga$_{1-x}$Al$_x$As concentric double quantum rings is calculated taking into account the combined effects of electric field, hydrostatic pressure, temperature and aluminum concentration. The ground state energy dependences on the mentioned factors are presented for different values of the sizes of rings and electric field strength. It is found that the considered effects mainly depend on the dimensions of quantum rings.

1. Introduction
Nowadays it is possible to make high-quality semiconductor quantum rings using the self-assembly technique [1,2]. Semiconductor quantum rings have attracted intensive interest due to their unique topological geometry and energy spectrum. Very recently lattice-matched GaAs/GaAlAs concentric double quantum rings (CDQRs) were fabricated by means of the droplet epitaxy technique with high uniformity and excellent rotational symmetry. The making of these concentric structures is clearly demonstrated by images of atomic force microscopy [3].

Recently there has been considerable interest in the properties of single [4-6] and few electron states [7-9], exciton states [3,10], the spin-orbit interaction [11,12] as well as the impurity effects [13] in vertically and laterally coupled double quantum rings. The theoretical investigation of CDQRs under the magnetic field applied perpendicularly to the ring plane is reported in [4,5]. Electron-hole transition energies are calculated as a function of the system geometry confinement, within a single-particle picture, neglecting interaction effects. The effect of hydrostatic pressure on electronic states in GaAs/Ga$_{0.7}$Al$_{0.3}$As CDQRs under axial magnetic field is investigated in [6]. For both symmetric and asymmetric CDQRs it is found that the electron-heavy hole transition energies augment with the applied pressure is mainly due to the pressure-induced increase in the GaAs gap.

In this work the effects of growth-direction applied electric field, hydrostatic pressure, temperature and aluminum concentration on the ground state energy in GaAs/Ga$_{1-x}$Al$_x$As CDQRs are studied. The...
paper is organized as follows: in Section 2 we describe the theoretical framework, Section 3 is dedicated to the results and discussion and, finally, our conclusions are given in Section 4.

2. Theoretical framework

In figure 1 the schematic view of the CDQRs is presented. The dimensions of heterostructure (radii, widths and the thickness of rings) and the direction of the applied electric field are depicted.

Figure 1. The CDQR heterostructure: $L_1$ is the width of the inner ring, $L_2$ is the width of the coupling barrier, $L_3$ is the width of the outer ring, $\rho_i^{\text{in}}$ and $\rho_i^{\text{out}}$ are the inner and outer radii of the inner ring, $\rho_o^{\text{in}}$ and $\rho_o^{\text{out}}$ are the inner and outer radii of the outer ring, $H$ is the thickness of rings, and $\vec{F}$ is the applied electric field strength.

The sizes of the structure depend on the pressure ($P$) according to the expressions [6, 14]

$$H(P) = H(0) \left[1 - (S_{11} + 2 S_{12}) P\right], \quad \rho(P) = \rho(0) \left[1 - 2 (S_{11} + 2 S_{12}) P\right]^{1/2},$$

where $S_{11}$ and $S_{12}$ are the components of the compliance tensor in GaAs ($S_{11} = 1.16 \times 10^{-3}$ kbar$^{-1}$ and $S_{12} = -3.7 \times 10^{-4}$ kbar$^{-1}$).

The Hamiltonian of the electron in CDQRs in the effective mass and parabolic band approximations under the combined effects of pressure, temperature and applied electric field is given by the expression

$$\hat{H} = \hat{H}_{\rho \varphi} + \hat{H}_z,$$

where

$$\hat{H}_{\rho \varphi} = -\frac{\hbar^2}{2} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \frac{\rho}{m(x,P,T)} \frac{\partial}{\partial \rho} \right) + \frac{1}{m(x,P,T)} \frac{\partial^2}{\partial \varphi^2} \right) + V_{\rho}(\rho,x,P,T),$$

$$\hat{H}_z = -\frac{\hbar^2}{2 m(0,P,T)} \frac{\partial^2}{\partial z^2} + V_z(z,P).$$

In the expression (3) $m(x,P,T)$ is the aluminum concentration ($x$), temperature ($T$) and pressure dependent electron effective mass and it is given by [15]

$$m(x,P,T) = m_0 \left[1 + \frac{\Pi^2(x)}{3} \left( \frac{2}{E_g(x,P,T)} + \frac{1}{E_g(x,P,T) + \Delta_0(x)} \right) + \delta(x) \right]^{-1},$$

where $m_0$ is the free electron mass, $\Pi(x)$ is the interband matrix element [$\Pi^2(x) = 28900 - 6290 \cdot x$], and $\Delta_0(x)$ is the valence-band spin-orbit splitting [$\Delta_0(x) = 341 - 66 \cdot x$]. The remote-band effects are taken into account via the $\delta(x)$ parameter, which is given by $\delta(x) = -3.935 + 0.488 \cdot x + 4.938 \cdot x^2$. The energy gap at the $i$-point ($i = \Gamma, X$) of the conduction band is given by the expression
\[ E_i(x, P, T) = a_i + b_i x + c_i x^2 + \alpha_i P - \beta_i T^2 \left( \gamma_i + T \right)^{-1}, \]  

where the values of parameters \( a_i, b_i, c_i, \alpha_i, \beta_i \), and \( \gamma_i \) are given in the table 1.

The confining potentials are defined taking into account the crossover between the \( \Gamma \) and \( X \) minima of the conduction band [15-17]. There are two critical values of pressure at which the crossover can be observed: 1) at \( P_i(x, T) \) there is a crossover between the \( \Gamma \) and \( X \) points at the Ga\textsubscript{i-x}Al\textsubscript{x}As barrier with energies \( E_{g_i}(x, P, T) \) and \( E_{g_i}^X(x, P, T) \) respectively and 2) at \( P_\ell(x, T) \) the crossover is between the \( \Gamma \) point at the GaAs well and the \( X \) point at the Ga\textsubscript{i-x}Al\textsubscript{x}As barrier. In the direct gap regime \( (P < P_i) \) the confining potential height is independent on pressure and obtained as a fraction \( r \) of the difference between the Ga\textsubscript{i-x}Al\textsubscript{x}As and GaAs energy gaps at the \( \Gamma \) point. If \( P_i < P < P_\ell \) the position of the \( X \) minimum is lower than the \( \Gamma \) one and the height of the confining potential decreases with pressure and can be defined as a fraction \( r \) of the energy \( E_{g_i}^X(x, P, T) - E_{g_i}^X(0, P, T) + S_{1\chi}(x, P, T) \), where \( S_{1\chi}(x, P, T) = S_0(P - P_\chi(x, T)) \) is the \( \Gamma-X \) mixing strength coefficient and \( S_0 = 250 \text{ meV} \) is the adjustable parameter which fits the experimental measurements [16]. If \( P > P_\ell(x, T) \) a type I-type II semiconductor heterostructure transition occurs. It is necessary to note that \( \Gamma-X \) crossover can be observed with variation of aluminum concentration. If \( x_\chi \approx 0.38 \) \( (P = 0 \text{ and } T = 4 \text{ K}) \) crossover takes place at the barriers and there is no observed crossover with variation of temperature. Below the pressure values considered are between 0 and \( P_\ell(x, T) \), and \( x \) will be taken to lie between 0 and \( x_\chi \).

With the inclusion of the crossover effect the confining potential in radial direction is defined by

\[
V_\rho(x, P, T) = \begin{cases} 
0, & \text{if } \rho_{1\text{in}}^i \leq \rho \leq \rho_{1\text{out}}^i \text{ and } \rho_{2\text{in}}^i \leq \rho \leq \rho_{2\text{out}}^i, \\
V_\rho(x, P, T), & \text{if } \rho < \rho_{1\text{in}}^i, \rho_{2\text{in}}^i < \rho < \rho_{1\text{out}}^i \text{ and } \rho > \rho_{2\text{out}}^i,
\end{cases}
\]

where

\[
V_\rho(x, P, T) = r \begin{cases} 
E_{g_i}^\Gamma(x, P, T) - E_{g_i}^\Gamma(0, P, T), & \text{if } P \leq P_i(x, T), \\
E_{g_i}^X(x, P, T) - E_{g_i}^X(0, P, T) + S_{1\chi}(x, P, T), & \text{if } P_i(x, T) < P \leq P_\ell(x, T),
\end{cases}
\]

\( r \) being the fraction of band gap discontinuity. The confining potential in \( z \)-direction

\[
V_z(z, P) = \begin{cases} 
-eFz, & \text{if } |z| \leq H(P)/2, \\
\infty, & \text{if } |z| > H(P)/2.
\end{cases}
\]

Table 1. Parameters for energy gap [15]

| Type         | \( a_i \) (meV) | \( b_i \) (meV) | \( c_i \) (meV) | \( \alpha_i \) (meV/kbar) | \( \beta_i \) (meV/K) | \( \gamma_i \) (K) |
|--------------|-----------------|-----------------|-----------------|---------------------------|----------------------|------------------|
| \( \Gamma \)-minimum | 1519.4          | 1360            | 220             | 10.7                      | 0.5405               | 204              |
| \( X \)-minimum | 1981            | 207             | 55              | -1.35                     | 0.46                 | 204              |

The eigenfunctions of the Hamiltonian (2) can be presented in the form

\( \Phi(\rho, \varphi, z) = (2\pi)^{-1/2} e^{i\mu \varphi} f(\rho) g(z) \), where \( \mu = 0, \pm 1, \pm 2, \ldots \) is the magnetic quantum number. In the next only the ground state of electron is taken into account and, consequently, only the value \( \mu = 0 \) is needed. Then \( f(\rho) \) and \( g(z) \) will be the eigenfunctions of the Hamiltonians (3) and (4) respectively with the corresponding eigenvalues \( \varepsilon_{\rho} \) and \( \varepsilon_{z} \). \( f(\rho) \) is a linear combination of Bessel functions. In
order to find \( \varepsilon_p \), the transfer matrix formalism is used [19], whereas in \( z \)-direction the Schrödinger equation can be modified to the Airy equation [20].

3. Results and discussion

In the calculations we have taken \( r = 0.6 \). At \( T = 4K \) the first crossover pressure occurs at \( P_c = 8.37 \) kbar. In figure 2 the ground state energy as a function of pressure (a), (b) and the probability density in radial direction for several values of pressure (c) are presented (in all figures of this section the fixed values of CDQRs’ sizes are given for \( P = 0 \)).

As it is shown in figure 2 (a) the energy is a decreasing function of the electric field strength and pressure. For \( P \leq P_c \) the radial-confining potential height is constant and the energy decrease is due only to the increasing of the electron effective mass. If \( P > P_c \) the decrease in the electron energy with pressure is faster, because besides the decrease associated with the augment of the electron effective mass, now there is a reduction associated with the fall in the radial-potential barrier height. For electric field strength of 400 kV/cm it is also shown the energy dependence without including the \( \Gamma - X \) crossover. It should be noted that the energy variations due to the changes of the structure sizes with pressure (see equation (1)) are very small compared with the variations associated with pressure-related changes in the effective mass and height of the confining potential. In figure 2 (b) the energy is a decreasing function of the ring thickness. It is clear that the stronger size-quantization effect and pressure influences are larger for smaller values of ring thickness. This last effect is related to the fact that in \( z \)-direction the electron energy changes with pressure are only due to the variation of the effective mass with pressure. The effects associated with the effective mass are stronger for smaller values of ring thickness. From figure 2 (c) it is seen that the probability density is greater in the inner ring (although the widths of the rings are equal) because of the unique topological geometry of the rings. Also we observe that if \( P \leq P_c \) the maximum value of probability density increases within the inner ring and decreases in outer ring. If \( P > P_c \), the opposite situation is observed. This is because in the region \( P \leq P_c \) there will be only an increase of the electron effective mass with the pressure, with the augment of the probability density in the inner ring and a decrease of it in the outer ring. When \( P > P_c \) the radial potential height is also reduced, causing the increase of the tunneling probability from inner to outer ring.

The ground state energy as a function of temperature and the probability density in radial direction for several values of temperature are presented in figure 3 (a), (b) and (c), respectively. In figures 3 (a)
and (b) the energy increase with temperature can be explained by the effective mass reduction. Also the energy is a decreasing function of the electric field strength and the quantum rings thickness and the influence of temperature is larger for smaller values of ring thickness. From figure 3 (c) it is observed the expected decrease of the probability density within the inner ring (because of the effective mass decrease with temperature).

In figure 4 are presented the ground state energy as a function of aluminum concentration (a) and probability density in radial direction for several values of $x$ (b). The energy is an increasing function of $x$ given the strengthening of the radial-confining potential for bigger barrier heights (although the effective mass in the barrier region is larger as well, leading to the decrease of energy).

The influence of variation of the confining potential height is stronger). It can be also seen an augment of the distance between lines with temperature, which is because of the non-linear behavior of energy as a function of temperature (see figure 3). The probability density behavior is strongly dependent on the range of variation of the concentration: (1) the increase of $x$ in the range from 0.2 to 0.37 is reflected in the augment of the probability density in the inner ring while there will be a decrease of the probability density in the outer ring due to the increase of the confining potential height; (2) in the range from 0.1 to 0.01 the probability density both in the inner and outer rings decrease, because now the confining potential in radial direction become very small and the curve of probability density goes down as whole. Besides that, the energies don’t start from 0 values because in vertical direction the
potential is infinite, although if $x = 0$ there is no potential in radial direction.

4. Conclusions

In this work the combined effects of pressure, temperature, electric field and aluminum concentration on electronic states in GaAs/Ga$_{1-x}$Al$_x$As CDQRs are investigated using the effective mass and parabolic band approximations and the transfer matrix formalism. It is shown that the ground state energy is a decreasing function of electric field strength and pressure and an increasing function of temperature and aluminum concentration. We have shown that the effect of pressure and temperature is larger for smaller values of thickness of the rings. It is also found that the behavior of probability density is strongly dependent on the range of variation of the pressure and aluminum concentration. As a final conclusion it can be mentioned that our findings confirm that the pressure, the temperature, the electric field and the aluminum concentration could be suitable tools for tuning the electronic and optical properties of quantum rings.

Acknowledgments: This research was partially supported by Colombian Agencies: COLCIENCIAS, CODI-Universidad de Antioquia (Estrategia de Sostenibilidad Grupo de Materia Condensada-UdeA, 2011-2012), Facultad de Ciencias Exactas y Naturales-Universidad de Antioquia (CAD-exclusive dedication project 2011-2012) and “El Patrimonio Autónomo Fondo Nacional de Financiamiento para la Ciencia, la Tecnología y la Innovación Francisco José de Caldas” Contract RC – No. 275-2011. The work was developed with the help of CENAPAD-SP, Brazil. This work was partially supported by Armenian State Committee of Science (Project No.11B-1c039).

References
[1] Lorke A, Luyken R J, Govorov A O, Kotthaus J P, Garcia J M and Petroff P M 2000 Phys. Rev. Lett. 84 2223–6
[2] Lee J H, Wang Zh M, Abuwaar Z Y, Strom N W and Salamo G J 2006 Nanotechnology 17 3973–6
[3] Mano T, Kuroda T, Sanguinetti S, Ochiai T, Tateno T, Kim J, Noda T, Kawabe M, Sakoda K, Kido G and Koguchi N 2005 Nano Lett. 5 425–8
[4] Culchac F J, Porras-Montenegro N, Granada J C and Latgé A 2008 Microelectron. J. 39 402–6
[5] Culchac F J, Porras-Montenegro N and Latgé A 2008 J. Phys.: Condens. Matter 20 285215–20
[6] Culchac F J, Porras-Montenegro N, Granada J C and Latgé A 2009 J. Appl. Phys. 105, 094324–8
[7] Castelano L K, Hai G-Q, Partoens B and Peeters F M 2006 Phys. Rev. B 74 045313–7
[8] Liu Y M, Huang G M and Shi T Y 2008 Phys. Rev. B 77 115311–4
[9] Szafran B and Peeters F M 2005 Phys. Rev. B 72 155316–24
[10] Dias da Silva L G G V, Villas-Bôas J M and Ulloa S E 2007 Phys. Rev. B 76 155306–10
[11] Kuan Wen-Hsuan, Tang Chi-Shung and Chang Cheng-Hung 2007 Phys. Rev. B 75 155326–34
[12] Alves F M, Trallero-Giner C, Lopez-Richard V and Marques G E 2008 Phys. Rev. B 77 035434–40
[13] Farias G A, Degani M H, Freire J A K, Costa e Silva J and Ferreira R 2008 Phys. Rev. B 77 085316–24
[14] Elabsy A M 1993 Physica Scripta 48 376–8
[15] Reyes-Gómez E, Raigoza N and Oliveira L E 2008 Phys. Rev. B 77 115308–13
[16] Elabsy A M 1994 J. Phys.: Condens. Matter 6 10025–30
[17] Raigoza N, Morales A L, Montes A, Porras-Montenegro N and Duque C A 2004 Phys. Rev. B 69, 045323–30
[18] Aspnes D E 1976 Phys. Rev. B 14 5331–43
[19] Wojs A, Hawrylak P, Farad S and Jacak L 1996 Phys. Rev. B 54 5604–8
[20] Abramowitz M and Stegun I A 1964 Handbook of mathematical functions with formulas, graphs and mathematical tables (Courier Dover Publications: Mineola, New York) pp 446–52