Effect of interdiffusion and external magnetic field on electronic states and light absorption in Gaussian-shaped double quantum ring

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\section{Introduction}
One of the promising courses of development of present day optoelectronics and computational electronics is the transition to zero dimensional (0D) nanostructures, such as quantum dots (QD) [1] and quantum rings (QR) [2]. Optoelectronic devices based on QD systems possess a number of advantages: temperature stability, wide spectral range, small dark current, high signal-to-noise ratio, and the possibility of the absorption of incident light beam as well as the multiexcitonic absorption [3,4]. Electrons confined in a nanometer-sized QR manifest their quantum nature by an oscillatory behavior of their energy levels as a function of an applied magnetic field (the Aharonov-Bohm effect). This effect originates from the periodic dependence of the phase of the electron wave function on the magnetic flux through the ring [5] and is usually associated with the occurrence of persistent currents [6–11]. Using the droplet epitaxial technique, authors of [12] performed self-assembly of concentric double quantum rings (DQR) with high uniformity and excellent rotational symmetry. The intraband optical absorption in QRs has attracted an enormous interest in recent years [13–15] because of a large optical nonlinearity in these structures. Note that both linear and nonlinear intraband optical transitions can be used for practical applications in photodetectors and high-speed electro-optical-devices [16–19]. It is shown that the post growth rapid thermal annealing (RTA) plays a major role in modifying the electronic structure and in the improvement of material quality due to the interdiffusion of the compound materials of heterojunction [20–23]. Recently several works have been done to theoretically predict the necessary conditions of realization of layered nanostructures (QR, spherical layer et al.) with desirable optical characteristics [24–26]. Theoretical calculations indicate to the blue shift of the interband absorption spectrum of QDs [27,28] and QD superlattices [29,30] due to interdiffusion, which is in accordance with experiment [23]. However a redshift is theoretically predicted for intersubband absorption threshold in QR superlattices [31]. In Ref. [32] RTA was used to improve the optical quality of strain-free DQR solar cells fabricated by droplet epitaxy. The shape of DQRs obtained in [32] can be successfully modeled by two shifted Gaussians as it was shown in [31]. Our previous works are devoted to the theoretical investigation of the effect of interdiffusion on electronic band structure of the SL composed of Gaussian-shaped (GS) DQRs and on the intraband nonlinear absorption spectrum of a GSDQR [31,33]. In the present work the effect of interdiffusion and the external magnetic field on electron and heavy hole (HH) energy spectrum and interband absorption coefficient of a Ga\textsubscript{1−\textit{x}}Al\textsubscript{x}As/GaAs GSDQR is considered. The article is organized as follows. In Section 2 the theoretical model to calculate electron energy spectrum and interband absorption coefficient is described. Section 3 is...
devoted to the discussion of the obtained results and the conclusions are presented in Section 4.

2. Theory

In the framework of effective mass approach the Hamiltonian of electron (HH) in GSDQR in the presence of transversal magnetic field can be written in the following form:

$$\hat{H}(\vec{r}) = \hat{H}_0(\vec{r}) + V_{\text{fr}}(r, z; L)$$

where \(\hat{H}_0\) is the Hamiltonian in cylindrical quantum dot (CQD) with infinitely high potential barriers and with enough large radius \(R_0\) and height \(h_0\), \(m_{\text{eff}}^{\text{HH}}\) is the electron (HH) effective mass, \(\omega_0 = eB/m_e\) is the cyclotron frequency, \(B\) is the magnetic field induction which is directed along the QR's z axis. The Zeeman term for electron (HH) in the considered material is of order 1 meV (0.1 meV) for \(B \lesssim 10\) T and hence is omitted in the Hamiltonian [34]. In Eq. (1)

$$V_{\text{fr}}(r, z; L) = V_0 \left(1 - \frac{1}{2} \text{erf}\left(\frac{z}{L}\right) - \exp\left(-\frac{r^2}{L^2}\right) \right)$$

is the potential of GSDQR which is obtained as a solution of diffusion equation [33], \(L = 2\sqrt{D\tau}\) is the diffusion parameter, \(D\) is the diffusion coefficient, \(r\) is time, \(V_0 = 1247 Q_0\) (meV) is the potential barriers’ height before the interdiffusion (\(\tau\) is the Al initial concentration and \(Q = 0.6(0.4)\) is the conduction (valence) band offset for GaAs material) [33], \(\text{erf}(\xi)\) is the error function, \(h_0\) is the modified Bessel function of the zero order. The surface which covers the GSDQR can be expressed by the following dependence of \(z\) coordinate on the radial coordinate \(r\) (\(r = \sqrt{x^2 + y^2}\)):

$$z(r) = h_0 \exp[-\alpha^2(r - r_1)^2] + h_2 \exp[-\beta^2(r - r_2)^2],$$

where \(\alpha, \beta, h_0\) and \(h_2\) are Gaussian parameters, \(r_1\) and \(r_2\) are the values of \(r\) at which the inner and the outer Gaussians have maximum, respectively. In Fig. 1 the shape of GSDQR (a) and the profile of its diffused potential (b) are illustrated for the values of parameters: \(h_1 = 3\) nm, \(h_2 = 5\) nm, \(R_0 = 1.5\), \(r_1 = R/3\), \(r_2 = 2R/3\), \(\alpha = \beta = 0.25\) nm⁻¹, \(L = 1\) nm and \(R = 30\) nm. The CQD, \(\hat{H}_0\), the eigenfunctions in which are considered material is of order 1 meV (0.1 meV) for \(B \lesssim 10\) T and hence is omitted in the Hamiltonian [34]. In Eq. (1)

$$\sum_n c_n \phi_n(z, r, \varphi),$$

where

$$\phi_n(z, r, \varphi) = \left(\frac{2}{h_0}\right)^{1/2} \sin\left(\frac{\pi n}{h_0} z\right)$$

are the eigenfunctions \(\hat{H}_0(\vec{r})\), \(J_{k_n}\) is the first kind Bessel function of the \(l\)-th order, \(k_{n,l}\) is its \(n\)-th root, \(n\) are the quantum numbers \(n, n\) and \(l\).

Let us now consider the absorption of a plane monochromatic electromagnetic wave caused by the optical interband transitions. Calculations show that the third order interband absorption coefficient is more than \(10^2\) times smaller than the linear one when the intensity of the incident radiation does not exceed 5 kW/cm², so we will consider here only the first order perturbation theory which leads to the following expression for the absorption coefficient [35]:

$$\alpha(\omega) = \delta_{n,m} \delta_{l,i} \frac{4 \pi e^2 \eta_0 \langle M_{1l}^2 \rangle (\langle \psi, \psi \rangle)^2}{\hbar c \sqrt{\epsilon} (E_n - E_l - \hbar\omega)^2 + \Gamma_n^2},$$

where

$$\langle M_{1l}^2 \rangle = \frac{\hbar^2 \langle p_{1l}^2 \rangle}{m_0 (E_n - E_l)^3},$$

is the mean square of the coordinate interband matrix element,

$$\langle p_{1l}^2 \rangle \approx 5.4 e_c m_0,$$

is the mean square of the momentum interband matrix element for unpolarized light in GaAs material [35], \(\omega\) is the incident photon frequency, \(E_n\) and \(E_l\) are the energies in conduction and valence band, respectively, \(\Gamma_n\) is the Lorentzian broadening parameter, \(\eta_0\) is the concentration of QRs, \(\epsilon\) is the dielectric constant, \(e\) and \(m_0\) are the charge and the mass of free electron, respectively, \(\hbar\) is the reduced Planck constant, \(c\) is the light velocity, \(\delta_{n,l}\) is the Kronecker delta symbol.

3. Discussion

The numerical calculations are made for a Ga_{1-x}Al_{x}As/GaAs GSDQR with following values of parameters: \(m_e^* = 0.067 m_0\), \(m_{\text{eff}}^{\text{HH}} = 0.62 m_0\), \(x = 0.33\) and \(\Gamma_n = 2\) meV. Fig. 2 demonstrates the dependencies of the electron (Fig. 2a–c) and HH (Fig. 2d–f) energies corresponding to the value of the radial quantum number \(n = 1\) and for different values of the azimuthal quantum number \(l\) on magnetic field induction in GSDQR. Three different values of the diffusion parameter \(L = 0\) (Fig. 2a and d), \(L = 0.5\) nm (Fig. 2b and e) and \(L = 1\) nm (Fig. 2c and f) have been considered. The interdiffusion process leads to the narrowing of the potential well at it’s lower part, and to the decreasing
of the confining potential depth in one hand and to the widening of upper part of the potential well and erosion of the potential barriers (see Fig. 1b) in other hand. The behaviors of the particle energies are caused by the competition of these changes in the potential profile as well as by the particle effective mass and the position of the corresponding energy level. As is seen from the Fig. 2 for a given value of magnetic field induction, the increase of diffusion length leads to the shift far from the confining potential bottom of almost all the energy levels of electron and the levels of HH corresponding to the values of $l = \pm 3, \pm 4, \pm 6$ and $\pm 7$. However one can observe a nonmonotonic change in the energies of some levels (for example the levels corresponding to the values of $l = \pm 5$ for electron and $l = \pm 2$ and $\pm 5$ for HH) with the increase of the diffusion parameter. Namely, these energies are firstly shifted to the potential well bottom at $L = 0.5$ nm but with further increase of $L$ an opposite shift is observed. The change in the energy due to the increasing of magnetic field induction has an oscillatory behavior due to the crossings of the levels corresponding to different values of $l$. However, the Aharonov-Bohm oscillations are not observed clearly because of the considerable tunneling of electron through the barrier between the central region of the QR. One can also observe that the oscillating behavior of the electron ground state energy gradually disappears with the increase of diffusion parameter. However for HH the ground state energy oscillations in the region of the values of magnetic field induction $B = 0 – 10$ T are not observable. From the behaviors of the curves in Fig. 2 one can conclude that both interdiffusion and magnetic field leads to the change of the arrangement of the quantum states by their energy.

Figs. 3 and 4 represent the spatial distribution of the electron probability density (PD) in the cases of $n l = 1, =0$ (a–c) and $n = 1, l = 1$ (d–f) (The PD for the $n = 1, l = -1$ state coincides with one for the state $n = 1, l = 1$). Fig. 3 corresponds to nondiffused structure, while Fig. 4 is for $L = 1$ nm. In each figure the first, second and third rows correspond to the values of magnetic field induction $B = 0$, $B = 10$ T and $B = 20$ T, respectively. As is seen from Fig. 3a and Fig. 4a in the case of $n = 1, l = 0$, and $B = 0$ electron is mostly localized in the outer ring. For an intermediate value of magnetic field induction ($B = 10$ T) we have almost the same picture as in the case of $B = 0$ with only a slight quantitative difference in the PD distribution. However for enough large values of $B (B = 20$ T) electron can also be found in the inner ring due to the increase of electron energy and tunneling effect through the barrier between the inner and the outer rings (Fig. 3c and Fig. 4c). Comparing Figs. 3a–c with Figs. 4a–c one can see almost the same impact of magnetic field on electron PD in nondiffused and diffused QRs. For the value of azimuthal quantum number $l = 1$ there is a considerable probability of being electron in the inner ring, which significantly increases with the increase of magnetic field induction and for $B = 20$ T becomes larger than in the outer ring (Figs. 3d–f).

Comparison of Figs. 3d–f with Figs. 4d–f shows that, in contrast with
the case of $n = 1, l = 0$, the impact of magnetic field on the state $n = 1, l = 1$ significantly depends on the value of diffusion parameter. Due to about 10 times larger effective mass of HH comparing with one of electron, the PD of HH in the $n = 1, l = 0$ state is almost not affected by interdiffusion and magnetic field. In this state HH is localized in the outer ring (Figs. 5 and 6a, b, c). In the case of $n = 1, l = 1$, we can see a very weak tunneling of HH into the inner ring for nondiffused structure (Figs. 5d–f) and significant tunneling to the central part of GSQR through the inner ring for diffused structure (Figs. 6d–f). The later is the consequence of the potential barriers’ erosion due to interdiffusion.

Finally, for $B = 20$ T we observe an ejection of HH from the inner ring to the outer one for diffused GSQR (Fig. 6f).

Fig. 7 shows the dependence of the interband absorption coefficient on incident photon energy for different values of magnetic field induction $B$ and diffusion length. According to the selection rule (see Eq. (6)), the values of the quantum numbers $n$ and $l$ in the initial and the final states must be the same. Figs. 7a–c correspond to the transitions between the states in the valence and the conduction bands with the quantum numbers of $n = 1, l = 0$, $n = 1, l = 1$ and $n = 1, l = −1$, respectively. The picks’ positions of the curves corre-
respond to the values of incident photon energy equal to the absorption threshold (energy differences between initial and final states). One can see from the Fig. 7 that both the magnetic field and the interdiffusion lead to a blue-shift of the absorption spectrum and to decreasing of the absorption intensity for all three transitions. The blue-shift is due to the increase of energy difference between the initial and the final states (Fig. 2) while the decrease of the absorption intensity is a result of the weaker envelope of the PD in the initial (see Figs. 5 and 6) and the final (see Figs. 3 and 4) states. The examination of the black lines \((B = 0)\) in Figs. 7a–c shows that the strongest absorption occurs for the transition between the \(n = 1, l = 0\) states, while for \(n = 1, l = 1\) and \(n = 1, l = -1\) states the absorption spectra are the same.

4. Conclusion

Summarizing, the effects of interdiffusion and magnetic field on the energy levels and PDs of electron and HH as well as on interband absorption coefficient in GSDQR are investigated by means of exact
field induction gradually disappears with the increase of diffusion parameter due to the enhanced tunneling of electron to the central region of the ring. For HH the ground state energy oscillations in the region of the values of magnetic field induction $B = 0 - 10$ T are not observable. The impact of the magnetic field on the PD in the $n = 1, l = 0$ state is almost the same for nondiffused and diffused structures while in the $n = 1, l = \pm 1$ states it significantly depends on diffusion parameter. Both the magnetic field and the interdiffusion lead to a blue-shift of the absorption spectrum and to decreasing of the absorption intensity for all three transitions. The obtained results indicate on the opportunity of flexible manipulation of energy states and absorption spectrum of GSDQRs by means of interdiffusion and the external magnetic field.

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