C-V Data and Geometry Parameters of Self-Assembled InAs/GaAs Quantum Rings

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ABSTRACT

The problem of the interpretation of the recent C-V data given in W. Lei, et al. (Appl. Phys. Lett. 96, 033111 (2010)) for InAs/GaAs quantum rings (QR) is considered. We show that the single-electron spectrum calculations, based on a variant of the oscillator model of this paper, do not correspond to the experimentally proposed geometry of QR. We use the QR geometry that is follows from the oscillator model, due to relation between confinement potential parameters of the oscillator model and real sizes of quantum objects, to calculate the electron energy in a magnetic field. The original effective model, based on three-dimensional single band ***kp***-approximation with energy dependence of effective mass, is applied. These calculations give good fit for experimental data.

Keywords: quantum rings, single electron levels, optical properties

1 INTRODUCTION

Well-established process of QDs formation by epitaxial growth and consecutive transformation of QDs into InAs/GaAs quantum rings (QR) [1, 2] allows production of 3D structures with lateral size of about 40-60 nm and height of 2-8 nm. In produced QRs it is possible to directly observe discreet energy spectra by applying capacitance-voltage (CV) and far infrared spectroscopy (FIR). However, known theoretical studies have some limitations in interpreting the experiments:

(i) The derived value of the energy-gate-voltage conversion coefficient ($f \approx 2$) is in a disagreement with that obtained from CV experiments [2,3] ($f \approx 8$).

(ii) 3D geometry corresponding to the QR fabrication process has sufficiently different descriptions in theoretical works [1,2,3].

In the present work we focus on these problems and on the interpretation of the recent CV data given in [1]. We show that a variant of oscillator model [2-6] used in [1] does not resolve (i) and (ii). The calculations [1] with QR geometry parameters reported in [2] (Geometry 1) give a good fit for experimental data for additional single electron energy in a magnetic field with $f \approx 7-8$. At the same time, [1] ignores the relation between confinement potential parameters of the oscillator model and real sizes of quantum objects. According to [5] the adopted oscillator energy corresponds to a length l as following:

$$l = \sqrt{2\hbar / m\omega}\,. \qquad (1)$$

This relation defines the width $d = 2l$ for the considered rings.

We use the QR geometry which is following from the oscillator model [1] to calculate the electron energy in a magnetic field. The effective model [7], based on single band ***kp***-approximation with energy dependence of effective mass in three-dimensional, is applied. The numerical results are presented. These results are compared with experimental C-V data. Our calculations with this Geometry 2 give the value $f \approx 7$. However, the calculations with the experimental reported geometry [1,2] lead to the "old" value for f ($f \approx 2$) ([2,3,7]). We compare also results of the calculations for electron excitation energies, obtained for the QR geometry of [1], with one for the "recalculated" QR geometry. Relation between ideal ring approximation and our three dimensional model is studied.

2 EFFECTIVE MODEL

We assume that the quantum rings composed of InGaAs in an GaAs substrate. This heterostructure is modeled utilizing a ***kp***-perturbation single subband approach with an energy dependent quasi-particle effective mass. The problem is mathematically expressed by the following Schrodinger equation

$$\left(\hat{H}_{kp} + V_c(\mathbf{r}) + V_s(r)\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r})\,. \qquad (2)$$

Here $\hat{H}_{kp}$ is the single band kp-Hamiltonian operator $\hat{H}_{kp} = -\nabla \frac{\hbar^2}{2m^*}\nabla$, $m^* = m^*(\mathbf{r}, E)$ is the electron effective mass, which depends on energy and electron position, and $V_c(\mathbf{r})$ is the band gap potential, $V_c(\mathbf{r}) = 0$ inside the QR and is equal to E_c outside the QR, where E_c is defined by the conduction (or valence) band offset for the bulk. $V_s(\mathbf{r})$ is effective potential simulating the strain effect [8]. The effective potential $V_s(\mathbf{r})$ has an attractive character and acts inside the volume of the QD. The magnitude of the potential can be chosen to reproduce experimental data. In Fig. 1 we show the band gap model for InGaAs/GaAs heterostructure used in the present work. For example, the magnitude of V_s for conduction (valence) band chosen in [8] is 0.21 eV (0.28 eV).

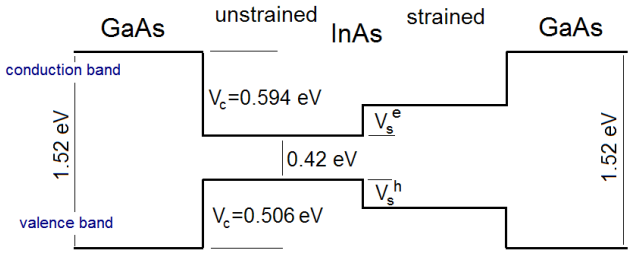

Figure 1. Band structure model for InGaAs/GaAs heterostructure.

This value was obtained to reproduce results of the 8-th band ***kp***-calculations of Ref [9] for InAs/GaAs QD. To reproduce the experimental data from [2], the V_s value of 0.31 eV was used in [7] for conduction band.

The Ben-Daniel-Duke boundary conditions are used on interface of the material of QR and substrate. Introducing a constant magnetic field in the z direction ($\mathbf{B} = B\hat{z}$) the Schrödinger equation in cylindrical coordinates can be written in following form:

$$-\frac{\hbar^2}{2}\left(\frac{\partial}{\partial\rho}\left(\frac{1}{m^*}\frac{\partial\Phi_{n,l}}{\partial\rho}\right)+\frac{1}{m^*\rho}\frac{\partial\Phi_{n,l}}{\partial\rho}-\frac{l^2}{m^*\rho^2}\Phi_{n,l}\right)+$$

$$+\frac{\hbar l\omega_c}{2}\Phi_{n,l}+\frac{m^*\omega_c^2\rho^2}{8}\Phi_{n,l}+\left[V_c(\rho,z)+V_s(\rho,z)-E\right]\Phi_{n,l}$$

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\Phi_{n,l}}{\partial z^2}=0. \qquad (3)$$

Here we separated an angle coordinate

$$\Psi_{n,l}(\rho,z,\varphi)=\Phi_{n,l}(\rho,z)e^{il\varphi}, \qquad (4)$$

where $n=1,2,3...$ and $l=\pm0,\pm1,\pm2,...$ are orbital quantum numbers. $\omega_c=|e|B/m^*$ is the cyclotron frequency. The first magnetic field term in (3) is the orbital Zeeman term, the second - so called diamagnetic term. The electron spin Zeeman effect has been ignored here since it is considered to be small. The energy dependence of the electron effective mass $m^*=m^*(\rho,z,E)$ is defined [7] by the Kane formula [10] (in present work - for the QR material). Eq. (3) with this functional dependence can be solved by iterative procedure. The effective mass of electrons in QR is changed from initial balk values to the value corresponding to electron energy by Kane formula. Results of such calculations (see [7]) for the InAs/GaAs QR are shown in Fig. 2. The effective mass of the InAs QR is close to one of the balk value for the GaAs substrate due to weak confinement of an electron in considered QR. Note that, as it is clear from Fig. 2 for QD (with the shape proposed in [2]), the confinement of the electron is stronger. Thus effective mass is relatively smaller. In this work we used the GaAs balk value for the electron effective mass in QR. The same assumption was also used in [1].

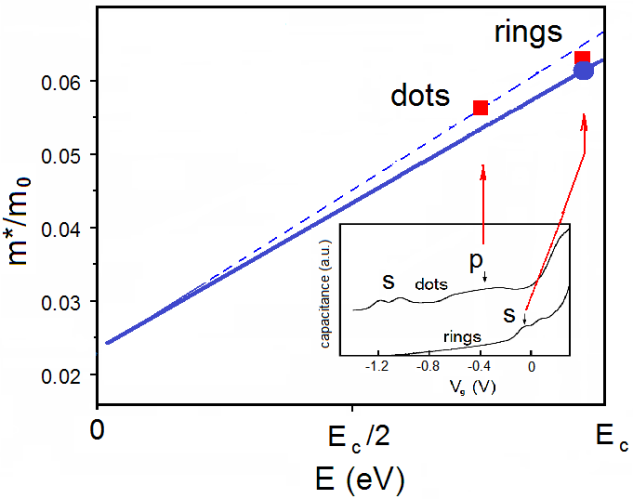

Figure 2. Calculated (circle) and experimentally obtained [2-3] (squares) values for the electron effective mass and s and p -level energy of QD and QR. Solid line is derived by the Kane formula. Dashed line connects bulk values of the effective mass. The insert: the capacitance-gate voltage traces [2].

To indicate the electron localization in QR ,we used the electron effective radius $R_{n,l}$ which is defined as root mean square (rms) radius by the relation:

$$R^2{}_{n,l}=\int|\Phi^N{}_{n,l}(\rho,z)|^2\,\rho^3 d\rho dz,$$

where $\Phi^N{}_{n,l}(\rho,z)$ is the normalized wave function of an electron.

3 RESULTS OF CALCULATIONS

The geometry of the self-assembled QRs, reported in [1,2], is shown in Fig. 3 (Geometry 1). The InGaAs QRs are a height of about 2 nm, an outer diameter of about 49 nm, and an inner diameter of about 20 nm.

The QR geometry constructed with the parameters m, ω of [1] is shown in Fig. 3 (Geometry 2). We used the values m =0.067 m_0 and ω=15 meV in Eq. (1). The radius of QR center is defined to be 20 nm.

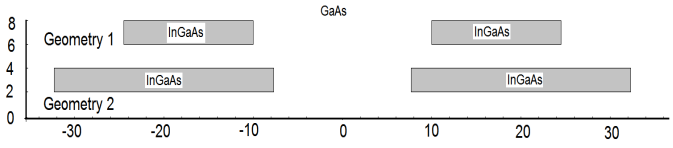

Figure 3. QR cross sections corresponding to Geometry 1 and Geometry 2; sizes are in nm.

To calculate energies of a single electron in QR, we solved numerically the eigenvalue problem (3)-(4) using the finite elements method.

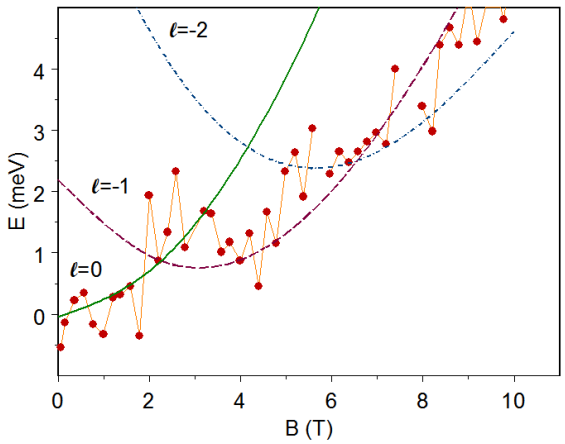

Figure 4. Additional energy of electron ground state for QR in a magnetic field. The experimental energies (circles) are obtained in [1] by using a linear approximation $\Delta E = e\Delta V_g / f$, with the lever arm $f = 7.84$. The lines $l = 0,-1,-2$ are result of our calculations multiplied by factor 1.18 [1].

The result of the calculations for additional energy of electron ground state for QR in a magnetic field are shown in Fig. 4. The picture of changing orbital quantum number of the ground state is the same to one obtained in [1] within oscillator model. The changing occurred at 2.2 T (and 6.7 T). Obtained curve well fits the experimental data. However, this result of [1] we cannot reproduce using the proposed in [1] geometry of QR (Geometry 1). The correspondence between confinement potential parameters of the oscillator model and real sizes of quantum objects can be formalized by the Eq. (1). By this method we reproduce result of [1] as it shown in Fig. 4. The strength parameter of the effective potential, in case the Geometry 2 used, was chosen to be 0.382 eV, which is close to that for QD from [8], where $V_s(\mathbf{r})$=0.31 eV. The difference is explained by quantum object topology dependence of the effective potentials (see [7], also).

Note that the considered QRs are the plane quantum rings with the condition $H << D$ that enhances the role of lateral size confinement effect. To represent qualitatively the situation shown in the Fig. 2, we used approximation in which the 3D QR is replaced by the ideal quantum ring of radius R in a perpendicular magnetic field B. Additional electron energy, due to the magnetic field, can be calculated by the formula: $E = \hbar^2/(2m^* R^2)(l + \Phi/\Phi_0)^2$ [10], where $\Phi = \pi R^2 B$, $\Phi_0 = h/e$ ($\Phi_0 = 4135.7$ Tnm^2). The Aharonov-Bohm (AB) period ΔB is estimated by the following relation $\Delta B = \Phi_0/\pi/R^2$. Using rms radius as R (R=20.5 nm) one can obtain $\Delta B/2$=1.56 T and $\Delta B/2 + \Delta B$=4.68 T for the ideal ring. This result is far from the result of 3D calculations shown in Fig. 2.

We obtained better agreement using the radius of most probably localization of electron $R_{loc.}$, defined at the maximum of square of the wave function. The electron mostly localized near 17.1 nm for B=0. With these values, the single ideal ring estimate leads for $\Delta B/2$ and $\Delta B/2 + \Delta B$ to the values of 2.25 T and 6.75 T, respectively, that agrees with the result of 3D calculations (see Fig. 4). Obviously, the reason for this agreement is the condition $H << D$ for the considered QR geometry as it was mentioned above. The profile of square wave function is presented in Fig. 5 to show the mostly localized position of the electron in QR for B=0. Note that this value is weakly depended on the magnetic field. It is shown in Fig. 6 where the $R_{loc.}$ of electron ground state is presented as a function of the magnetic field. The $R_{loc.}(B)$ is changed in interval of ± 1 nm around the mean value $R_{loc.}(0)$ of 17 nm. We can conclude, that the radius of most localized position of electron is more proper, in this contest, for comparison of the ideal and realistic rings, than the rms radius which is defined as an integral characteristic of the wave function.

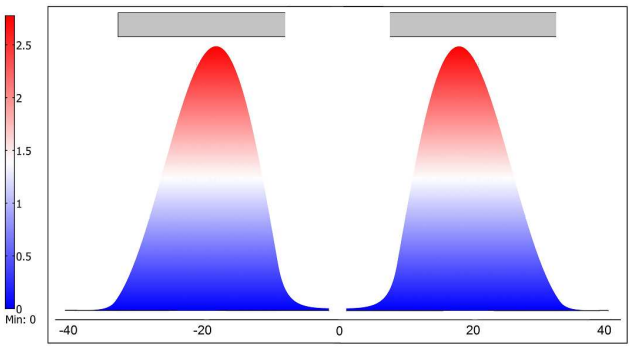

Figure 5. Square wave function of electron ground state for B=0 and l=0. The QR cross section (Geometry 2 in Fig. 1) is shown in inset. The size is given in nm.

It is interesting to compare the result of calculations with the QR geometry parameters corresponding to Geometry 1 and Geometry 2 in Fig. 1 with the FIR data, reported in [3]. The results are presented in Fig. 7. One can see that the QR geometry proposed in [1] leads to significant deference between the FIR data and our calculations (see Fig. 7b), whereas the results obtained with Geometry 2 are in satisfactory agreement with the data (Fig. 7). We can conclude again that the QR geometry of [1] does not provide adequate description of electron properties of the InAs/GaAs QRs measured in [1,2].

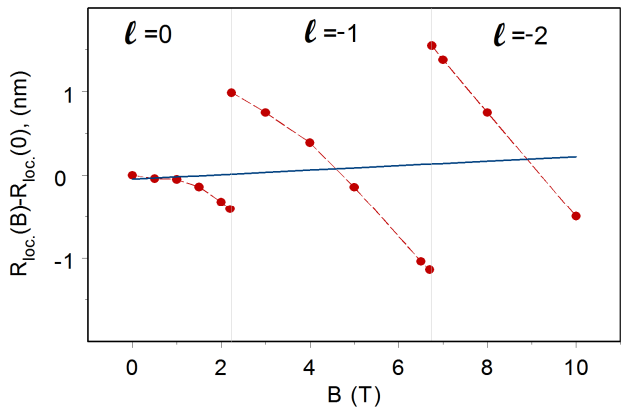

Figure 6. The radius ($R_{loc.}$) of the most localized position of electron as a function of the magnetic field B. The electron ground state is considered. The circles mean the calculated values and solid line is result of the least squares method fitting for the calculated values. The orbital quantum number of ground state is shown.

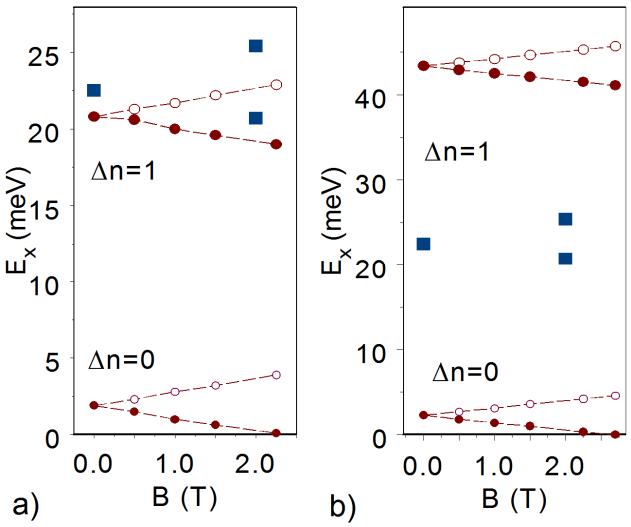

Figure 7. Solid squares present the observed resonance positions [3] of the FIR transmissions at various magnetic field strength B. Calculated energies of the excited states with $|\Delta l|=1$ are marked by the circles. a) QR with shape given by Geometry 2 in Fig. 1, b) QR with shape given by Geometry 1. The orbital quantum numbers of ground state is $l=0$. The quantum numbers n is changed as it shown.

4 CONCLUSION

To summarize, we stress that the problem of reliable theoretical interpretation of the C-V (and FIR) data for InAs/GaAs quantum rings is far from resolved. The oscillator model that is quite wildly utilized in literature can be used carefully not to lose the relation between the model assumptions and real QR geometry. Obtained in present work simple geometry can be considered as one of possible variants of geometry for experimentally fabricated QR.

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