Modeling of InAs/GaAs quantum ring capacitance spectroscopy in the nonparabolic approximation

I. Filikhin, V. M. Suslov,* and B. Vlahovic†
Department of Physics, North Carolina Central University, Durham, North Carolina 27707, USA
(Received 15 February 2006; revised manuscript received 30 March 2006; published 17 May 2006)

A three-dimensional model of InAs/GaAs quantum rings based on a single sub-band approach with an energy dependence of the electron effective mass is used to describe the capacitance-voltage spectroscopy by Lorke et al. [Phys. Rev. Lett. 84, 2223 (2000)]. The confinement states energy problem is solved numerically using the finite elements method. Observed deviation of an electron effective mass from the bulk value is explained by the nonparabolic effect. Additional energy of the electron ground state due to an external magnetic field is estimated and compared with the capacitance-voltage data. The model is also applied to describe the far-infrared measurements.

DOI: 10.1103/PhysRevB.73.205332

PHYSICAL REVIEW B 73, 205332 (2006)

I. INTRODUCTION

InAs/GaAs self-assembled nanosize quantum dots (QD) and quantum rings (QR) have displayed properties similar to those of atomlike objects.1,2 Important information about the electron structure of QD (QR) populated with a few electrons can be provided by the capacitance-voltage (CV) spectroscopy.3,4 In the experiments of Miller et al.5 CV spectroscopy was successfully employed to define the low-lying electron states of InAs/GaAs QDs. For quantum rings similar experiments were performed by Lorke et al.6 Theoretical studies5–7 using simple models have encountered some difficulties in interpreting the experimental data. These works have been restricted to parabolic infinite confinement potentials and planar models of the quantum objects. Since an observed deviation of electron effective mass in QD (QR) from the bulk value cannot be explained in the framework of these models, the effective mass was considered as a phenomenological input parameter. More sophisticated three-dimensional (3D) models were introduced in the works by Refs. 8–14. These models took into account the nonparabolic effect connected with changing the electron effective mass relative to its bulk value. However, in Refs. 10 and 11 the geometry employed to describe the quantum rings was far from realistic and in Refs. 12–14 the potential model was restricted by the band-gap potential only.

In this paper a 3D model of QD (QR) with an energy dependent electron effective mass is presented.12,13,16 In the model the energy dispersion is defined by the Kane’s formula17 and the kp-perturbation theory18 in a single subband approach is applied. The geometrical parameters chosen for the QD (QR) are those occurring in the actual InAs/GaAs QD and/or QR fabrication process, for which experimental CV and far-infrared (FIR) data are available.5–7 The resulting nonlinear confined energy problem12,13,16 is solved numerically by an iterative method. We use the CV spectroscopy measurements for the electron s-shell energy to define an effective potential which simulates the total effect of the band-gap deformation potential, the strain induced, and the piezoelectricity.10,11 In this way the model enables us to reproduce the experimental observed change of the electron effective mass in quantum dots (rings). We calculate the energy of single electron levels for quantum rings in a magnetic field and compare the results with the CV and the FIR spectroscopy data.

II. MODEL INPUT

The InAs quantum dot (ring) with a height $H$ and radius $R$ (outer radius $R_2$ and inner radius $R_1$) is embedded in a GaAs substrate. The average measurements of InAs/GaAs quantum dots reported in Ref. 5 are $H=7$ nm and $R=10$ nm. The InAs/GaAs self-assembled quantum rings derived from quantum dots have the following average sizes:5 the inner radius is about 10 nm, the height $H$ is about 1.5 nm, and the outer radius is about 40 nm. Maximal thickness for a QR has been reaching with a radius of 15 nm. The suggested geometry is shown in Fig. 1. This QR geometry is in agreement with data from the atomic microscope scanning of uncapped QR given in Ref. 10. In the picture the depth of the central hole of the QR is two times larger than the height of the visible part of the quantum rings. To choose the profile of the quantum ring, we take into account the distribution of the InAs material suggested in Ref. 19. Note that for this geometry the volume of InAs quantum rings is bigger than the volume of the initial InAs quantum dots. We explain this fact as due to the diffusion of GaAs substrate material into the quantum ring. The influence of this diffusion on the parameters of the QR and/or substrate materials is not taken into account in our model.

III. FORMALISM

The discontinuity in the conduction-band edge of the QD and the substrate causes a band-gap potential, which induces
confinement of electron states. The energies and wave functions of a single electron in the InAs/GaAs structure are the solutions of the nonlinear Schrödinger equation:
\[
[H_{kp}(n^*) + V_\epsilon(r)]\Psi(r) = E\Psi(r),
\]
where \(H_{kp}(n^*) = \mathbf{p} / 2m^* \mathbf{p} \) is a single band \( kp \)-Hamiltonian operator, \( m^* \) is the electron effective mass dependent on the energy \( E \), and position vector \( r \); \( n^* = m^*(E, r) \). \( V_\epsilon(r) \) is the band-gap potential which is zero inside the QD, and \( E \) outside the QD: \( V_\epsilon(r) = E_c \) for \( r \) in substrate. The value \( E_c \) is defined by the energy misalignment between the conduction-band edges of the QD and the substrate (\( E_g^\text{QR} \)): \( E_c = 0.7(E_g^\text{QR} - E_g^\text{QR}). \) Within each subdomain (QD and substrate) the effective mass \( m_i^*(E, r), i = 1, 2 \) is independent on the coordinates: \( m_1^* \) is the effective electron mass of the QD (\( r \) \( \in \) QD) and \( m_2^* \) is one of the substrate (\( r \) \( \in \) substrate), respectively. A detailed description of the model is given in Refs. 13–15.

The energy dependence\(^\text{17} \) of the electron effective mass is defined as
\[
\frac{m_0}{m^*} = \frac{2m_0P^2}{3h^2}\left(\frac{2}{E_g + E} + \frac{1}{E_g + \Delta + E}\right).
\]
Here \( m_0 \) is free electron mass, \( P \) is Kane's momentum matrix element, \( E_g \) is the band-gap energy, \( \Delta \) is the spin-orbit splitting of the valence band, and \( E \) is the ground state confinement energy. The parameters of the QD and substrate materials\(^\text{20} \) are as follows: \( m_{\text{bulk,1}}^*/m_{\text{bulk,2}}^* \approx 0.024/0.067, E_g^\text{QR}/E_g^\text{QR} \approx 0.42/1.52, E_c = 0.77 \text{ eV}, (2m_0P^2/h^2)/(2m_0P^2/h^2) = 20.5/24.6, \) and \( \Delta/\Delta_3 \approx 0.34/0.49. \)

The nonlinear Schrödinger equation (1) under a relationship (2) is to be solved by an iterative procedure: \(^\text{16} \)
\[
H_{kp}(m_i^{*,N-1})\Psi^N = E^N\Psi^N, m_i^{*,N} = f_i(E^N),
\]
where \( N \) is the iteration number, \( i = 1, 2 \) refers to system subdomains (\( i = 1 \) for the QD, and \( i = 2 \) for the substrate), and the function \( f_i \) is defined by Eq. (2). The initial values \( m_{i,0}^{*,0} \) are equal to bulk effective masses of the corresponding materials. For each iteration the problem (1) is reduced to a solution of the linear Schrödinger equation. Taking into account the axial symmetry of the quantum dot (ring), this equation may be written in the cylindrical coordinates \((\rho, z, \phi)\) as follows:
\[
-\frac{h^2}{2m}(\frac{1}{\rho} \frac{\partial^2 \Phi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Phi}{\partial \rho} + \frac{\partial^2 \Phi}{\partial z^2}) + V_\epsilon(\rho, z) - E \Phi(\rho, z) = 0.
\]

The wave function is at the form \( \Psi(r) = \Phi(\rho, z) \text{exp}(i l \delta) \), where \( l = 0, 1, \pm 2, \ldots \), is the electron orbital quantum number. The boundary conditions for this QR and/or substrate structure are \( \Phi(\rho, z) \to 0 \) when \( (\rho, z) \to \infty \), where \( (\rho, z) \) \( \in \) substrate. The wave function \( \Phi(\rho, z) \), and its first derivative in the form \( h^2/2m^* (n, \nabla) \Phi \), where \( n \) is the normal vector to the interface surface, have to be continuous throughout the subdomain interface. When quantum dots are in an external magnetic field, the magnetic potential term must be added to the potential of Eq. (1) (Ref. 15) in the form \( V_m(\rho) \)

\( = 1/2m^*(\beta h l + \beta^2/4p^2) \), where \( \beta = eB, B \) is the magnetic field strength, and \( e \) is the electron charge. We consider the case of a magnetic field normal to the plane of the QD and do not take into account the spin of electrons because the observed Zeeman spin splitting is small.\(^\text{21} \) The solutions of Eq. (4) were obtained by the finite elements method using FEMLAB software (http://www.comsol.com). The spatial domain of the solution was meshed with consecutively decreasing mesh size in order to determine an optimal mesh for the solution. Then the iterative procedure Eq. (3) was applied. This procedure usually required 3–6 iterations to achieve a convergence with a relative accuracy of \( 10^{-2} \) for the effective mass.

IV. NUMERICAL RESULTS

To reproduce the observed electron \( s \)-shell energy, we employed an effective potential which simulates the cumulative effect of the band-gap deformation potential, the strain-induced potential, and the piezoelectric potential.\(^\text{10,11} \) The effective potential \( V_s \) has an attractive character and acts within the volume of the quantum objects. Figure 2 shows the typical picture of the capacitance-gate-voltage traces obtained in CV measurements. Each peak of the traces corresponds to the tunneling of a single electron into the quantum dot or quantum ring. The corresponding energy spectrum is depicted in the inset of Fig. 2. The voltage-to-energy conversion coefficient \( f = (e\Delta V)/\Delta E \), used for the recalculation is equal to \( 7.5 \). It is important to note that the first level of the \( d \)-shell is located near the top of the potential well or the bottom of the conductor band of GaAs. In a weak magnetic field this state is confined due to the orbital Zeeman effect.\(^\text{5,22} \) Thus one can calculate the energy of the first \( s \)-shell level both for QD and for QR (relative to the top of the potential well). As one can see in Fig. 2 this energy is approximately equal to 180 meV for QD and to 30 meV for QR. The corresponding \( V_s \) potentials have the magnitude of 0.482 eV and 0.55 eV for QD and QR, respectively. CV and
MODELING OF InAs/GaAs QUANTUM RING

The Coulomb interaction between electrons depends on whether their spins are parallel or antiparallel as a result the s-shell splits into two levels. This splitting is reflected in the double peak of the s shell in the capacitance-voltage traces of Fig. 2. The observed magnitude of the splitting for quantum dots is about 20 meV. It is shown in Ref. 22 that traces of Fig. 2. The observed magnitude of the splitting for quantum dots and rings changes from 0.024 to 0.063 respectively. We found that the Kane's formula describes these variations well. In Fig. 3 the results of our calculations are shown together with the experimental data. The calculated values are shown by solid circles. They lie on the curve defined by Kane's formula. The observed data are shown by solid squares. The dashed line connecting the bulk value is shown to guide the eyes. The calculated values for the effective masses for quantum dots and rings are 0.543 and 0.061 respectively.

The Coulomb interaction depends on whether their spins are parallel or antiparallel as a result the s-shell splits into two levels. This splitting is reflected in the double peak of the s shell in the capacitance-voltage traces of Fig. 2. The observed magnitude of the splitting for quantum dots is about 20 meV. It is shown in Ref. 22 that the perturbation theory when taking into account the electron-electron interaction in the first order is appropriate to adequately describe the CV data. We have performed the perturbation theory calculation using obtained wave functions of a single electron in order to take into account the Coulomb interaction of s-shell electrons, similarly to the approach. Our calculation gives the value of 18.9 meV, which coincides with the calculation of Ref. 22 where the parabolic potential model was used with an electron effective mass equal to the experimental value of 0.057. For quantum rings we obtained a value of 7 meV, which is less than the value of 20 meV reported in Ref. 6. However, like ours, other calculations also do not match the experimental value.

There are two types of QR experimental data that are difficult to describe theoretically. One is the FIR spectroscopy of quantum rings in a magnetic field given in Refs. 6 and 7. The parabolic potential model was used in Ref. 7 to describe single electron data. The parameters of the model were adjusted to reproduce the Aharonov-Bohm-like (AB) oscillation about 8 T obtained in the CV data interpretation of Ref. 6. Our calculation, however, does not confirm the existence of the first AB-like oscillation at 8 T. Results of our calculation (open circles) and those from Ref. 7 (solid lines with small crosses) are shown in Fig. 4 together with experimental data (various symbols). Note that the first AB-like oscillation from our calculation is about 3 T. One can see that our results reproduce qualitatively the experimental pictures of the |Δl|=1 resonances. However, the resonances that are marked by large crosses in Fig. 4 cannot be described by our model. We agree with the conclusion reached in Ref. 7 that these resonances can be described as resonances of quantum rings with a different geometry. This is confirmed, in particular, by the fact that the excitation energy of Δn=1 levels is very sensitive to a small change in the QR averaged geometry that we adopted in our calculations. Other calculations in Ref. 11 have been performed in the framework of a model similar to the one presented here. Those results cannot be compared directly with the FIR experiments because the values of the parameters of the quantum rings chosen in Ref. 11 lead to an unrealistically large volume.

The second difficulty is related to the explanation of the CV measurements of additional ground state energy for a QR in a magnetic field. Calculations using a parabolic potential model for QR have described the experimental data qualitatively. However, to reach an agreement with the experiments, in these calculations it is necessary to choose for the voltage-to-energy conversion coefficient f a value of 1.8.
whereas the experimental value is 7. Our calculations with the geometry of Fig. 1 lead to similar results, except for the existence of a first AB-like oscillation at 8 T. They are shown in Fig. 5 along with the experimental data from Ref. 7. The existence of oscillations at 3 and 9 T is not noticeable when using the small energy-gate-voltage coefficient. It is possible to get good agreement with the data also with $f=7$ by using a special set of QR geometry parameters.$^{14}$ In Ref. 14 the geometry of quantum rings was chosen to satisfy the condition that the volumes of the quantum ring and of the initial quantum dot be equal. However, in the model presented in that work only the band-gap potential was taken into account. Thus the location of the $s$-shell levels relatively to the top of potential well does not agree with the picture of electron spectra shown in Fig. 2.

V. CONCLUSION

A single subband model of QD and/or substrate semiconductor structure, with the energy dependence of the electron effective mass defined by Kane’s formula and a realistic 3D geometry taken into account, describes quantitatively the CV spectroscopy measurements. The model we have presented does also allow us to estimate correctly the change in the effective mass due to the nonparabolic effect.

ACKNOWLEDGMENTS

The authors wish to thank A. Soldi for useful remarks and discussion. This project was supported by the Department of Defence through Grant No. DAAD 19-01-1-0795. I.F. is also partly supported by NASA Grant No. NAG3-804.