Size Related Contribution to Electron Energy of the Quantum Ring

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ABSTRACT

The semiconductor quantum ring (QR) is studied under energy dependent effective mass approximation. The 3D ground state energy problem is solved numerically by the finite element method. General relation for the size dependence of the QR confinement energy was derived. Several cases related to experimentally achievable QR/substrate configurations of InAs/GaAs, Ge/Si, and CdTe/CdS were studied. The QR confined energy problem in an external magnetic field was also solved in order to compare relative contributions of the external magnetic field and size factors.

Keywords: quantum ring, effective mass approximation, QR size parameters, external magnetic field effect.

1 INTRODUCTION

In last years theoretical interest in the self-assembled heterostructures such as quantum rings (QR) has increased significantly [1-8]. One of the prospective approaches to study the energy properties of QR and QD is the quasi-particle energy dependent effective mass approximation [6-9]. For nanoscopic quantum objects this approach (non-parabolic approximation) is proven to be more constructive than parabolic (E ~p2) approximation, traditionally applied in the macroscopic scale. In the present paper the ***kp***-perturbation theory in a single subband approach [10] is applied to a model of QR, in which the energy dispersion is defined by the Kane formula [9]. The 3D confined energy problem is solved numerically by the finite element method. Effect of QR geometry on the energy properties of QR is studied, and the magnitude of the non-parabolic contribution estimated. As a result, general relation for the size dependence of the QR confinement energy is obtained. Calculations were then extended to include several experimentally achievable QR/substrate configurations of InAs/GaAs, Ge/Si, and CdTe/CdS. Confined energy an external magnetic field is also solved in order to compare relative contributions of the external magnetic field and size factors.

2 MODEL

The semiconductor quantum ring located on the top of the substrate is considered (Fig. 1). Geometrical parameters of QR are the height H, radial width ΔR, and inner radius R_1, where $H/\Delta R < 1$ (wide ring). Discontinuity of conduction-band edge of the QR and substrate material forms a band gap potential, which induces confinement electron states in QR. The ***kp***-perturbation theory in a single subband approach [10] is used for description of electron states of QR; the non-parabolicity effect in energy is taken into account by applying the Kane formula [9].

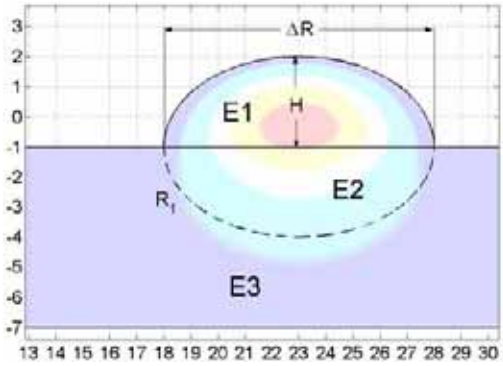


Figure 1 Cross section of quantum ring E1 and substrate E2+E3.

3 EQUATIONS

The electron confinement energy E and the wave function $\Psi(\mathbf{r})$ are the solutions of the Schrödinger equation:

$$\left(H_{kp} + V_c(\mathbf{r})\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \qquad (1)$$

Here H_{kp} is the one band ***kp*** Hamiltonian operator $H_{kp} = -\nabla \frac{\hbar^2}{2m^*(E,\mathbf{r})}\nabla$, $m^*(E,\mathbf{r})$ is the electron effective mass, and $V_c(r)$ is the band gap potential. $V_c(r)$=0 inside the QR, and it is equal to the confinement potential E_c outside of the QR: The spatial dependence of the electron effective mass is given as m^*(E,r)= m_i^*(E), i=1,2,3, where m_1^* is the effective mass in the material of QR (r ∈ E1), and $m_2^*(E)$ and m_3^* are the effective mass of the substrate material (***r***∈ E2 and E3).

Within each of the regions E1, E2, E3 m_i^* does not depend on the coordinates. The effective mass m_3^* is equal to a constant bulk value. The energy dependence of the electron effective mass from the E1 and E2 subdomains is defined by the following formula [9]

$$\frac{m_0}{m^*} = \frac{2m_0P^2}{3\hbar^2}\left(\frac{2}{E_g+E} + \frac{1}{E_g+\Delta+E}\right). \qquad (2)$$

Here m_0 is free electron mass, P is Kane's momentum matrix element, E_g is the band gap, and Δ is the spin-orbit splitting of the valence band. The equation (1) satisfies the asymptotical boundary conditions: $\Psi(\mathbf{r})|_{|\mathbf{r}|\to\infty} \to 0$, r∈ substrate and $\Psi(\mathbf{r})|_{|\mathbf{r}|\in S} = 0$, where S is free surface of QR. On the surface of boundaries of regions the wave function is continuous with the first order derivative $(\vec{n},\vec{\nabla}\Psi)/m_i^*$, where $\vec{n}$ is the surface normal.

4 RESULTS

The non-linear Schrodinger equation (1) was solved by an iterative procedure. During each iteration step the problem (1) is reduced to linear equation which is written in cylindrical coordinates taking into account rotation symmetry of the problem [7, 8]. The finite elements method (FEM) within the MATLAB PDE toolbox has been used. The following typical QR/substrate structures with experimental parameters taken from [11] were chosen: InAs/GaAs, Ge/Si, CdTe/CdS (Tabl. 1)

QR/ Substrate	m_1^*/m_2^*	E_c (eV)	$\frac{2m_0P_1^2}{\hbar^2}/\frac{2m_0P_2^2}{\hbar^2}$	Δ_1/Δ_2
Ge/Si	0.041/0.200	0.46	16.3/4.0	0.028/0.04
InAs/GaAs	0.024/0.067	0.77	22.4/24.6	0.34/0.49
CdTe/CdS	0.11/0.20	0.66	15.8/12.0	0.80/0.07

Table 1: Parameters of the QR and substrate materials

Analysis of the results of numerical calculations shows that the ground state energy of QR can be best approximated as a power function of the inverse values of the height and the radial width:

$$E \approx a\left(\frac{1}{\Delta R}\right)^{\gamma} + b\left(\frac{1}{H}\right)^{\beta}, \qquad (3)$$

where the coefficients γ=3/2 and β=1 were obtained numerically by the least square method. An example of this relation is illustrated in Fig. 2 for InAs/GaAs QR. Parameters *a* and *b* are tend to remain constant except for extremely low values of *H* and *ΔR*. Our analysis also reveals a significant numerical difference between the energy of QR electron ground states, calculated in non-parabolic and parabolic approximations. The results of the calculation with parabolic approximation are represented in the Fig. 2 and Fig. 3 by the dashed lines. Computations of the electron confinement energy of QRs for different materials (Fig.2) show that the non-parabolic contribution is quite significant when chosen QR geometrical parameters are close to those of the QRs produced experimentally: H < 7 nm, R < 30 nm for InAs/GaAs H < 5 nm, R < 20 nm for Ge/Si; and H < 4 nm, R < 15 nm for CdTe/CdS. Magnitude of this effect for InAs/GaAs can be greater than 30%, as shown in Fig. 4, where ΔE is defined as the difference between the values of the electron confinement energy calculated in parabolic and nonparabolic approximations.

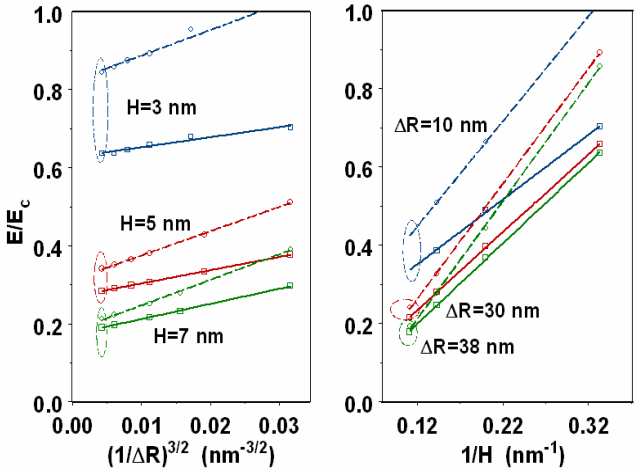


Figure 2. Normalized electron ground state energy of semi-ellipsoidal shape InAs/GaAs QR with parabolic (dashed line) and nonparabolic (solid lines) approximation as function of the QR size.

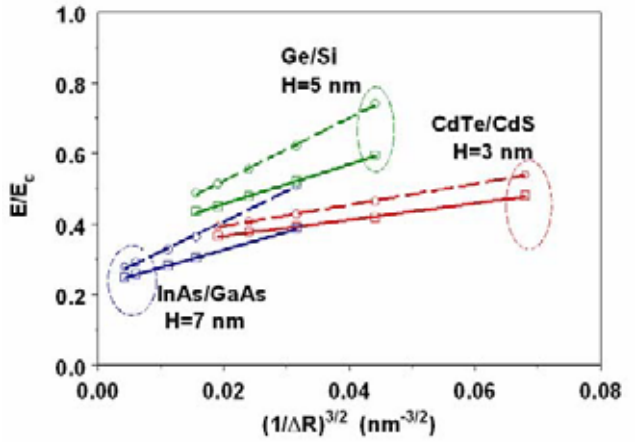


Figure 3. Normalized electron confinement energy of QRs of various materials in the parabolic (dashed line) and non-parabolic (solid lines) approximation.

As it can be seen from the Fig. 3, power coefficients γ and β in the relation (3) do not depend on QR/substrate materials. Their values are defined exclusively by the boundary conditions of the applied model. The model described above (Fig. 1) corresponds to the 2D problem with quantum well which has the infinity wall at one side (top side of the QR). For the model without the infinity wall (QR embedded into the substrate) γ=1, and β=1/3; in the infinity wall limit (isolated QR of the rectangular shape) both γ and β are equal to 2. These relations are illustrated in Fig. 5.

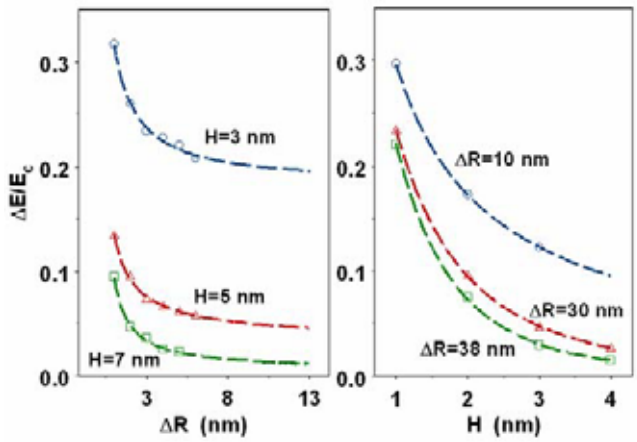
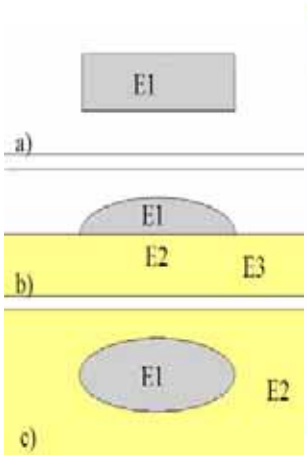


Figure 4 Non-parabolic contributions into the electron confinement energy of InAs/GaAs QR at different geometrical parameters.



Boundary conditions	γ	β
a) 'infinity wall'	2	2
b) 'infinity wall at one side'	3/2	1
c) 'no infinity wall'	1	1/3

Figure 5. Boundary conditions and respective power coefficients of the size-dependent electron confinement energy of QR. In the cross section of the QR/substrate structure the QR is marked as E1; E3 is the substrate; E2 is the area where QR acts to the substrate.

Another interesting geometrical effect is illustrated in Figure 6. It shows how the electron energy of QR is changing upon the "immersion" depth of the QR into the substrate (D is the immersion depth). This figure also demonstrates the shift of the QR ground state energy occurring during transition from the model c) to the model b) from Fig. 5 due to the depth variation.

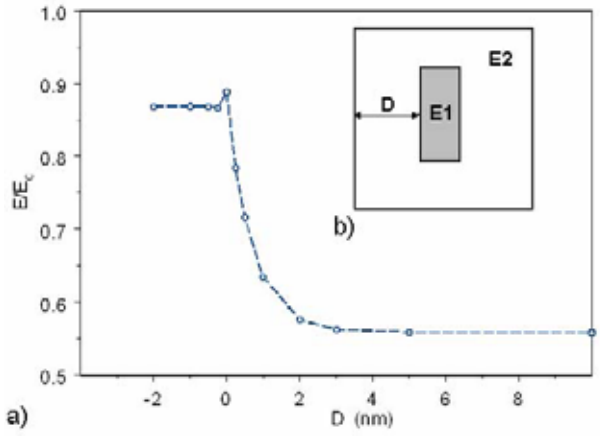


Figure 6. (a) Normalized electron ground state energy of cylindrical shape InAs/GaAs QR as a function of the QR immersion depth D; (b) cross section of QR/substrate configuration. H=2 nm, R_1=10 nm, R2=20 nm.

The QR confined energy problem in external magnetic field was also solved in order to compare relative contributions of magnetic field, and size factors. The magnetic field addition to the potential is given by the formula

$$V_m(\rho) = \frac{1}{2m^*}(\beta\hbar l + \frac{\beta^2}{4}\rho^2), \qquad (4)$$

where $\beta = eB$, B is magnetic field strength and ρ is cylindrical coordinate of the electron. The external magnetic field here is normal to the plane of QR, and the spin of electron is not taken into the account. In a magnetic field there is specific effect for the electron ground state of QR [12]. Since the ground state energy of the QR always corresponds to the minimal electron energy, the resulting E is the envelope consisting of the consequent segments related to the angular momentum transitions of the states with l =0,-1,-2,…This effect is illustrated by Fig.7 where electron energy of InAs/GaAs QR is depicted as a function of magnetic field *B* for various orbital quantum numbers *l*. The results of calculation of the QR ground state energy in magnetic field at different H and ΔR are shown in Figure 8. It is clear that size-dependent energy variations can dominate the effect caused by the magnetic field. Apparently, in order to fully utilize the effect of the magnetic field on the electron ground state energy, the size precision of the manufactured QRs must be improved significantly.

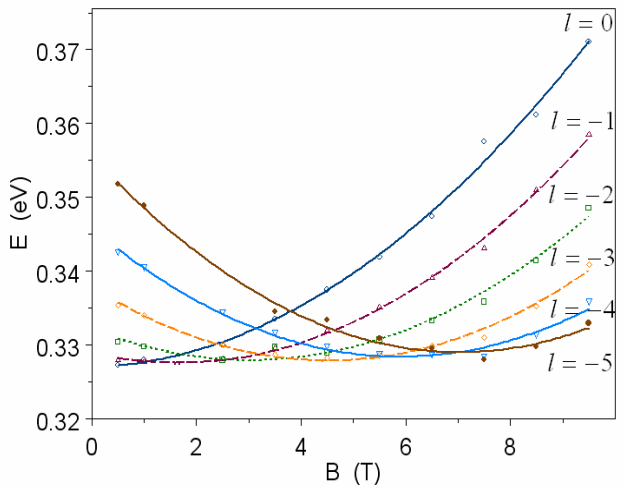


Figure 7. Electron energy of InAs/GaAs QR as a function of magnetic field B for various orbital quantum numbers l, H = 3 nm, ΔR = 19 nm.

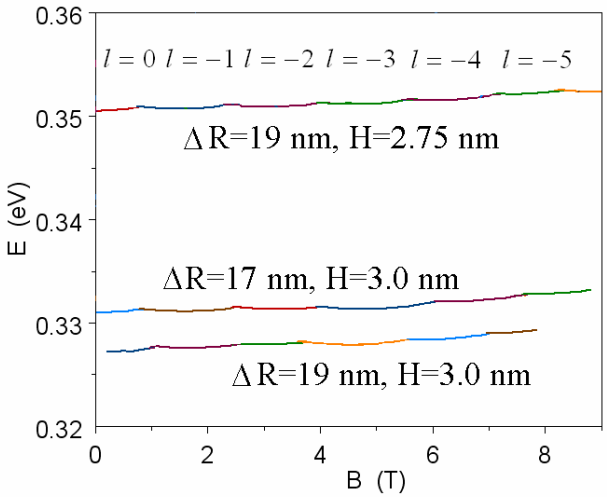


Figure 8 Electron ground state energy E in the magnetic field B at different geometrical parameters of QR. Inner radius R_1 = 20 nm.

5 CONCLUSION

The effect of geometry of the QR/substrate structures of several materials on the confinement energy is determined by relation (3), where the power coefficients γ and β are defined by the model boundary conditions only. It is shown that for wide QR the non-parabolicity effect does considerably alter the energy of the electron states, especially when the height or width of QR is relatively small. It is shown that the size-dependent energy variations can dominate the effect caused by the magnetic field.

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