

InAs/GaAs quantum ring in energy dependent quasi-particle effective mass approximation

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ABSTRACT

Three-dimensional InAs/GaAs quantum ring is studied under the energy dependent quasi-particle effective mass approximation. The confined energy problem is solved numerically by the finite element kp -perturbation method in a single subband approach. The influence of the quantum ring geometry on energy states and the electron effective mass are investigated. The limits of applicability of the considered model are also discussed.

Keywords: InAs/GaAs semiconductor, quantum ring, electron properties, computer simulation

1. INTRODUCTION

The possibility of fabrication of the semiconductor nanostructures with wide range of geometries, including quantum dots (QD) and quantum rings (QR), provides new basis for experimental and theoretical study of the nanoscale systems. Current theoretical analysis of properties of the QR, however, is limited to only several studies. In this paper we are extending the energy dependent effective mass approach [1] with an emphasis on numerical calculations of the effect of QR geometry on energy properties of both QR and surrounding substrate. We have estimated the magnitude of the non-parabolic contribution to the electron effective mass and energy states of the QR-substrate carriers. Model limitations are discussed.

2. MODEL DESCRIPTION

The InAs (QR) of an ellipsoidal shape is considered. The ring is embedded into the GaAs substrate. Geometrical parameters of the QR are height H , radial width ΔR and inner radius R_1 . These parameters are assumed to satisfy the relation $H/\Delta R < 1$ (narrow ring). The quantum ring cross section is schematically shown in Fig.1.

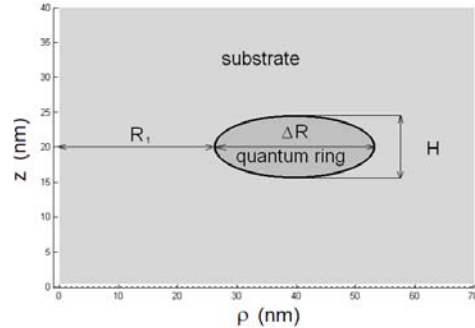


Figure 1. Quantum ring cross section. The geometrical parameters are shown: H – height, ΔR - radial width, R_1 - inner radius.

The discontinuity of conduction-band edge of the QR and the substrate forms a band gap potential which induces confinement electron states. This 3D heterogeneous structure is modeled utilizing the kp -perturbation single subband basis approach [2] with energy dependent quasi-particle effective mass. The energies and wave functions of a single electron in a semiconductor structure are solutions of the time-independent Schrödinger equation:

$$(H_{kp} + V(\mathbf{r}))\Psi(\mathbf{r}) = E\Psi(\mathbf{r}), \quad (1)$$

where $\Psi(\mathbf{r})$ is the wave function, E is the confinement energy, H_{kp} is the one band kp Hamiltonian operator

$$H_{kp} = -\nabla \frac{\hbar^2}{2m^*(E, \mathbf{r})} \nabla, \quad m^*(E, \mathbf{r}) \text{ is the electron}$$

effective mass dependent on the energy and position vector; and $V(\mathbf{r})$ is the band gap potential which is equal to zero in the QR, and is equal to V_0 outside of the QR:

$$V(\mathbf{r}) = \begin{cases} 0, & \in QR, \\ V_0, & r \notin QR. \end{cases}$$

The value V_0 is proportional to the energy misalignment of the valence band edges of the InAs QR and GaAs substrate.

The electron effective mass position dependence is given by:

$$m^*(E, \mathbf{r}) = \begin{cases} m_1^*(E), & \in QR, \\ m_2^*(E), & r \notin QR, \end{cases}$$

where $m_1^*(E)$ is the effective mass in the InAs QR and $m_2^*(E)$ is the effective mass in GaAs substrate. Following Y. Li et. al. [1] approach, the energy dependence of the electron effective mass (non-parabolic effect) is defined by the Kane formula [3] (non-parabolic approximation):

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

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. Inside the QR, E refers to the ground state confinement energy; for the substrate in Eq.(2) E should be replaced by $E - V_0$. Here we took into account the effect of non-paraboly in the QR, as well as in the substrate. We also assumed that QR confinement states are affecting the substrate even at sufficiently large distances from the QR. The equation (1) satisfies the asymptotical boundary conditions: $\Psi(\mathbf{r})|_{r \rightarrow \infty} = 0$. For numerical solution these conditions mean that the displacement from the regions of interest does not significantly affect the energies or wave functions in the regions.

The non-linear Schrödinger equation Eq.(1) was solved by the iteration procedure [2, 4], splitting the solution domain into two subdomains (QR and substrate):

$$\begin{aligned} H(m_i^{*,n-1})\Phi^n &= E^n \Phi^n, \\ m_i^{*,n} &= f_i(E^n), \end{aligned}$$

where n is a number of iteration, i refers to the subdomain of the system ($i=1$ for the QR, and $i=2$ for the substrate), $H(m_i^{*,n})$ is the Hamiltonian (left side) of the Eq.(1), and f_i are the functions defined in Eq.(2). During each step of iterations the problem (1) is reduced to solving the linear Schrödinger equation, in the cylindrical coordinates (ρ, z, ϕ) . Taking into account an axial symmetry of the quantum dot system, it is simplified further to the form:

$$\begin{aligned} &\left\{ \frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} - \frac{l^2}{\rho^2} \right) \right. \\ &\left. - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial z^2} + V(\rho, z) \right\} \Phi(\rho, z) = E \Phi(\rho, z). \end{aligned} \quad (3)$$

The wave function can be written as: $\Psi(\mathbf{r}) = \Phi(z, \rho) \exp(il\phi)$, where $l=0, \pm 1, \pm 2, \dots$ is the electron orbital quantum number. For the ground state one

has to take $l=0$ in Eq. (3). It is assumed that the wave function $\Phi(\rho, z)$ is continuous throughout the subdomain interface.

3. RESULTS AND DISCUSSION

The Schrödinger equation (3) is solved using the finite element method (FEM) by the PDE MATLAB [5] toolbox. Following the model of Y. Li et al [2] for the InAs/GaAs quantum ring, we studied the dependence of the electron ground state and effective mass from geometrical characteristics of the QR. The following experimental values are used for the QR (index 1) and substrate (index 2)

components: $\frac{2m_0P_1^2}{\hbar^2} = 22.4$, $\frac{2m_0P_2^2}{\hbar^2} = 24.6$, $E_{g,1} = 0.42$

eV, $E_{g,2} = 1.52$ eV, $\Delta_1 = 0.34$ eV, $\Delta_2 = 0.49$ eV [1]. The bulk effective masses of InAs and GaAs are chosen as $m_{0,1}^* = 0.024 m_{0,1}^*$ and $m_{0,2}^* = 0.067 m_{0,2}^*$, respectively. The magnitude V_0 of the confinement potential was calculated as $V_0 = 0.7(E_{g,2} - E_{g,1})$ [4]. In Fig.3 the electron ground state energy for the ellipsoidal shape quantum ring is shown as a function of radial width ΔR . Solid lines represent the result of our calculation with non-parabolic approximation. The dotted line is the result of the same approximation by Y. Li et. al. [1]; the dashed line represents our calculation with parabolic approximation.

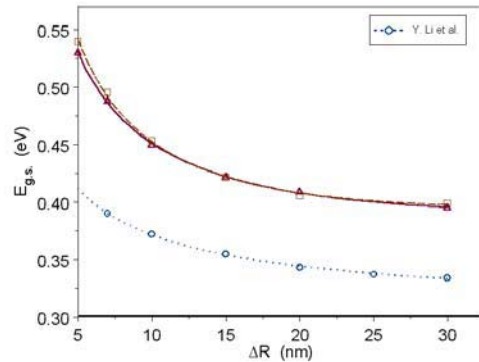


Figure 3. The electron ground state energy for the quantum ring as a function of radial width ΔR . The geometrical parameters of the ring are $R_1 = 24$ nm, $H = 2.4$ nm. The solid line and the dotted line represent the result of the present calculation, and the calculation of Y. Li et. al. [1], respectively, both with non-parabolic approximation; the dashed line corresponds to the present calculation with parabolic approximation.

It is evident from Fig.3 that there is a significant difference between our calculations and the corresponding results of Y. Li et. al. [1]. The reason for that, in our opinion, is that the formula (2) in [1] was not applied correctly. This assumption is confirmed by the fact that the asymptotic

($\Delta R \rightarrow \infty$, $R_1 = 2.4$ nm, $H = 2.4$ nm) value of the effective electron mass m_1^*/m_0 estimated from [1] is 0.076, whereas our calculation produce $m_1^*/m_0 = 0.045$. We consider the latter value to be more realistic, since for InAs/GaAs QR $m_{InAs}^* \leq m_1^* \leq m_{GaAs}^*$ [6], where $m_{InAs}^*/m_0 = 0.024$, and $m_{GaAs}^*/m_0 = 0.067$ [1]. Comparing the results of the calculations in parabolic and non-parabolic approximation (Fig.3), one can conclude that when the height of the RQ is less than its width ($H/\Delta R < 1$), the contribution of the non-paraboly is minimal. On the other hand, a similar study conducted for the cylindrical shape QD with the base radius R and the height z , reveals a significant influence of the non-parabolic effect on the electron ground state energy, when ($z/R < 1$). This is shown in Fig.4, where the solid and dashed lines represent calculations within non-parabolic and parabolic approximations, respectively.

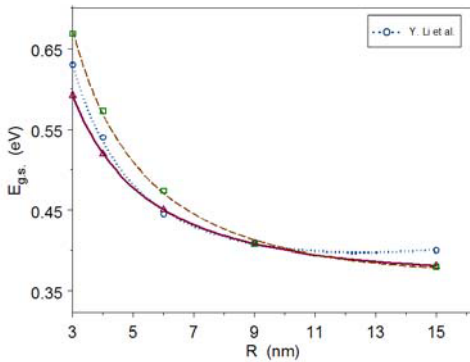


Figure 4. The electron ground state energy for the cylindrical shape InAs/GaAs QD with the height $z=2.5$ nm as a function of radius R . The notations are the same as in Fig. 3.

The calculation of Y. Li et. al. for the parabolic approximation [4] is depicted with a dotted line. It is in a good agreement with our calculations. Fig. 5 shows the results of calculations of the electron ground state energy and effective mass as functions of the QR height. For the ground state energy a contribution of the non-parabolic effect is even less than in Fig. 3. The two curves for non-parabolic and parabolic solutions in Fig. 5 practically coincide. At the same time the electron effective mass for both QR and substrate varies significantly. The graphs $m^*(H)$ for both QR and the substrate tend towards joining at $H \rightarrow 0$ (Fig. 5), since as it follows from (2), when the energy of the “confinement state” is approaching its maximum value (0.067), then the effective mass for the QR and the substrate carriers will approach the bulk value of m_{GaAs}^* .

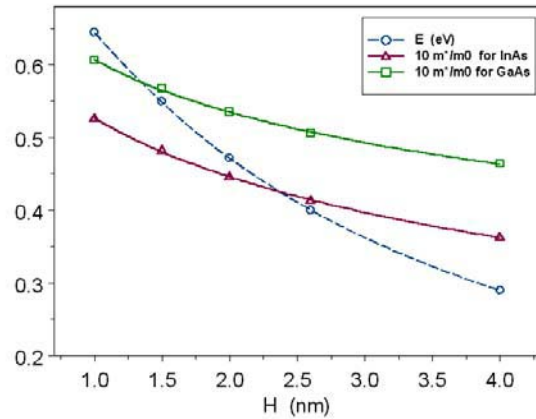


Figure 5. Electron ground state energy in eV (dashed line) and normalized effective masses (solid lines) of the QR and substrate as a function of height H . The radial width $\Delta R = 15$ nm, and the inner radius $R_1 = 24$ nm.

It is appropriate to note here that QR electron state is practically independent from the variation of the inner radius R_1 ($3 \text{ nm} \leq R_1 \leq 24 \text{ nm}$), which agrees with the calculations [1]. Thus a change in volume of QR due to the variation of R_1 is not followed by the change in the electron state. This means that for the 3D structure of interest the cross-section area $S = H \cdot \Delta R$ has a role of a spatial parameter similar to the width of the potential hole in the one-dimension case.

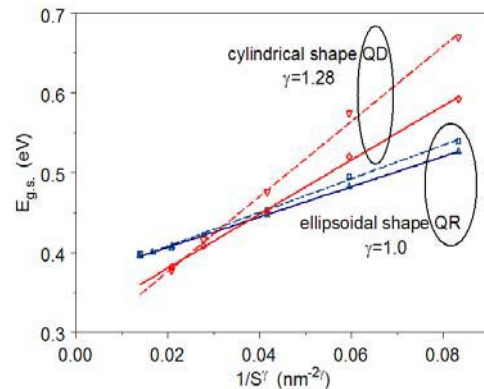


Figure 6. Electron ground state energy as a function of $S = H\Delta R$ for the ellipsoidal shape QR ($R_1 = 24$ nm), and $S = zR$ for the cylindrical shape QD in non-parabolic (solid lines) and parabolic (dashed lines) approximations.

Electron ground state energy dependence on S is shown in Fig. 6. It can be seen, that in the case of QR the non-parabolic effect for QR is sufficiently less prominent, than for QD with the same value of S .

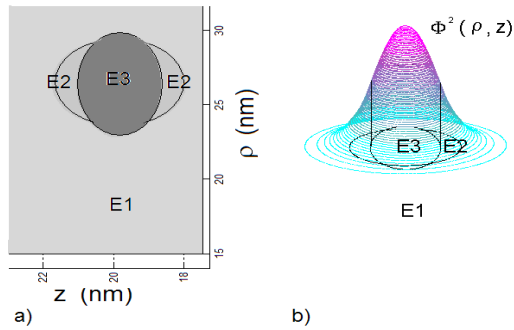


Figure 7. a) InAs/GaAs quantum ring (E3) and substrate domains (E1, E2) cross-section. The E1 domain effective mass is not changed. The E2 domain effective mass depends on the QR confinement energy, b) square of wave function for electron ground state of the InAs/GaAs quantum ring.

Let us consider an assumption of the model of Y. Li et. al. [1], about a strong influence of the QR electron confinement state on the substrate. The obvious way to consider this effect is to calculate a spatial base of the probability density function $\Phi^2(z, \rho)$ for this state. The results of such calculations for the QR having parameters of $H=2.4$ nm, $R_1=24$ nm, and $\Delta R=7$ nm, are depicted in Fig. 7 b). One can see that the function $\Phi^2(z, \rho)$ rapidly decreases when the distance from the QR increases, and only a “tail” of this function spreads beyond the boundaries of the QR. Thus, the area of influence of QR confinement state of electron on the substrate is limited to the range in the order of the width of the QR. The correct account of a spatial dependence of the QR effect on the substrate should lead to another nonlinearity in the Schrödinger equation (1). This concept was tested, and the results of the calculations are shown in Fig. 8. Our model assumes that the geometrical size of the area of influence of the QR is slightly smaller than the characteristic size of the area where $\Phi^2(z, \rho)$ is still nonzero. The calculated value of ground state energy E , marked by the “x”, is within the range between the values of E modeled by a non-parabolic (solid line) and a parabolic (dashed line) approximation for the substrate. We conclude that a consistent model of the QR with an energy dependent effective mass should include a spatial effect of the QR electron state on the substrate.

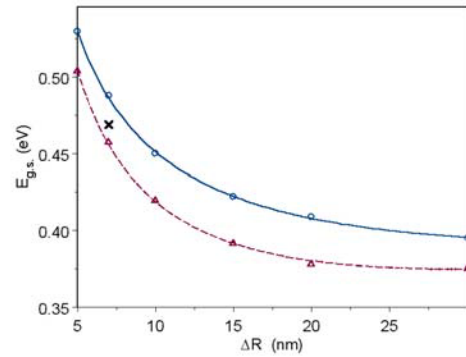


Figure 8. The electron ground state energy for the QR of an ellipsoidal shape as a function of radial width ΔR ; the inner radius $R_1=24$ nm and height $H=2.4$ nm. Solid lines correspond to calculation with non-parabolic approximation taken into account for the GaAs substrate; dashed line is the result with parabolic approximation for the GaAs substrate; the “x” corresponds to the test calculation (Fig. 7).

4. CONCLUSION

The confined energy problem for InAs/GaAs quantum ring was solved with energy dependent effective-mass approximation, applying the finite element method. We have found that for the narrow QR non-parabolic effect does not considerably affect electron states, however, the effective electron mass in both QR and substrate changes significantly. In order to correctly account for the QR impact on the substrate, the model of [1] has to be modified to include additional assumptions about the range and magnitude of such effect.

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