Computer Simulation of Electron Energy States for Three-Dimensional InAs/GaAs Semiconductor Quantum Rings

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ABSTRACT

In this article we study the electron energy states for three-dimensional (3D) semiconductor quantum rings. Our model formulation includes: (i) the effective one-band Hamiltonian approximation, (ii) the position and energy dependent quasi-particle effective mass approximation, (iii) the finite hard wall confinement potential, and (iv) the Ben Daniel-Duke boundary conditions. We solve the 3D model by nonlinear iterative algorithm to obtain self-consistent solutions. The model and simulation provide a novel way to calculate the energy levels of nano-scopic semiconductor quantum ring. They are useful to clarify the principal dependencies of quantum ring energy states on material band parameter, ring size and shape.

Keywords: Semiconductor quantum ring, InAs/GaAs, Electronic state, and Computer simulatuion

1 INTRODUCTION

In recent years, the study of semiconductor nano-structures, such as quantum dots, quantum ring, and quantum molecule has been of a great interest from experimental and theoretical points of view [1-10]. The progresses in semiconductor nanostructure fabrication provide us an alternative to construct nano-scopic systems with a wide range of geometries and sizes [1-9]. The micro-scopic and meso-scopic metallic semiconductor quantum rings have been received a considerable attention for the recent decades, but the development in fabrication of nano-scopic semiconductor rings bridges significantly the gap between semiconductor quantum dots and meso-scopic semiconductor ring structures. Unfortunately, most of theoretical quantum ring models so far are only assuming electrons move in a two-dimensional plane with a parabolic confinement potential ([1] and references therein). The above studied models did not consider some important properties of the nano-scopic semiconductor quantum ring, such as (i) effect of the ring's shape, (ii) effect of the radius variation for semiconductor quantum rings, and (iii) effect of the finite hard wall confinement potential.

In this work, we propose a comprehensive model description and simulation methodology for electron energy states in 3D semiconductor small quantum rings (see Fig. 1). The model formulation leads to a 3D nonlinear model problem and is solved with full numerical simulation self-consistently. Based on the effective 3D one band Hamiltonian, the energy (non-parabolic) and position dependent quasi-particle effective mass approximation [4], the finite hard wall confinement potential, and the Ben Daniel-Duke boundary conditions, the studied model is formulated for realistic 3D InAs/GaAs semiconductor quantum rings. To solve the multi-dimensional nonlinear Schrödinger equation, we apply our proposed a nonlinear iterative scheme recently [7-9] to compute the self-consistent solution of the problem [5]. In each iterative loop, the eigenvalue and eigenfunction of the Schrödinger equation are obtained with the central difference method, shifted and balanced QR algorithm, and inverse iteration method. A unified comparison of electron energy states for 2D and 3D models are presented comprehensively.

The dependence of electron ground state energy on the inner radius (R_1) of InAs/GaAs quantum ring as well as ring's height and radial width are presented systematically. We further calculate 2D model (a simplified adiabatic approach), and 3D rectangular and ellipsoidal radial cross sections for rings of height H = 2 nm and radial width ΔR = 20 nm. The result shows the dependence of the electron ground state energy on the outer radial width of the quantum ring. We find a large discrepancy among these results and also find that results for different radial cross shapes (we calculate the rectangular shape [6] and ellipsoidal as a more realistic [1]) are different greatly.

The paper is outline as follows. Sec. 2 presents the 3D quantum ring model and computation algorithms. Sec. 3 demonstrates and discusses the simulation results. Sec. 4 draws the conclusions.

2 MODELING AND SIMULATION

We consider semiconductor quantum rings with the hard-wall confinement potential that is induced by a discontinuity of conduction band edge of the system components. This approach is commonly used to calculate electron energy levels in quantum heterostructures [10].

With this approach, we solve 3D nonlinear Shrödinger equation directly without any additional simplifications and approximations. It is an important point and should be considered that the approximations of material basic parameters in the study of nano-scopic semiconductor quantum rings. For 3D semiconductor quantum structures, the approximated effective electron one band Hamiltonian is as follows

$$H = -\frac{\eta^2}{2}\nabla_r(\frac{1}{m(E,r)})\nabla_r + V(r) \tag{1}$$

where $m(E, r)$ is the electron effective mass that depends on energy and position

$$\frac{1}{m(E,r)} = \frac{P^2}{\eta^2}[\frac{2}{E + E_g(r) - E_c(r)} + \frac{1}{E + E_g(r) + \Delta(r) - E_c(r)}] \tag{2}$$

and $V(r) = E_c(r)$ is the confinement potential of quantum rings. The $E_c(r)$, $E_g(r)$, $\Delta(r)$, and P are the position dependent electron band edge, band gap, spin-orbit splitting in the valance band, and momentum matrix element, respectively [10]. We solve the quantum ring problem with cylindrical coordinate (R, ϕ, z). The quantum ring system is cylindrical symmetry so that the wave function can be written as:

$$\Phi(r) = \Phi(R,z)\exp(il\phi), \tag{3}$$

where $l = 0,\pm1,\pm2,...$ is the electron orbital quantum number and the model is

$$-\frac{\eta^2}{2m_i(E)}(\frac{\partial^2}{\partial R^2} + \frac{\partial}{R\partial R} + \frac{\partial^2}{\partial z^2} - \frac{l^2}{R^2})\Phi_i(R,z) + V_i(R,z)\Phi_i(R,z) = E\Phi_i(R,z) \tag{4}$$

where $V_{i=1}(R, z) = 0$ is inside the ring and $V_{i=2}(R, z) = V_0$ is outside the ring. The boundary conditions are

$$\Phi_1 = \Phi_2 \text{ and}$$
$$\frac{1}{m_1(E)}\{\frac{\partial\Phi_1}{\partial R} + \frac{df_s}{dR}\frac{\partial\Phi_1}{\partial z}\} = \frac{1}{m_2(E)}\{\frac{\partial\Phi_2}{\partial R} + \frac{df_s}{dR}\frac{\partial\Phi_2}{\partial z}\} \tag{5}$$

where $z = f_s(R, z)$ is a contour generator of the cross section of quantum rings structure in (R, z) plane. The 3D structures are generated by the rotation of this contour around the z-axis.

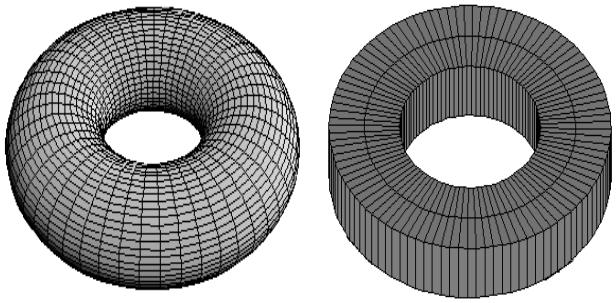

Fig. 1. An illustration of 3D semiconductor quantum rings. The right plot shows a quantum ring with the rectangular shape cross section. The left one shows a more realistic (ellipsoidal shape cross section) quantum ring from the fabrication point of view.

The electron effective mass is a spatial and energy dependent function; therefore the derived Schrödinger equation leads to a nonlinear equation in energy. To obtain a self-consistent solution to the model efficiently, we apply our proposed [7-9] nonlinear iterative algorithm recently (see Fig. 2).

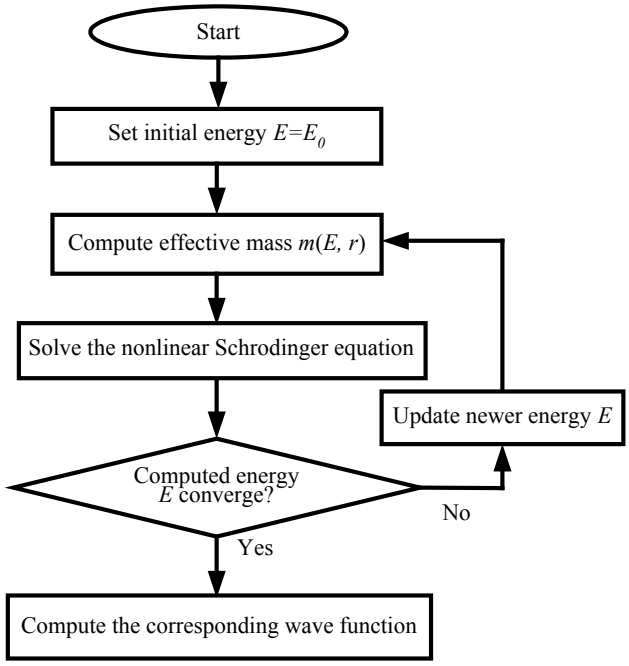

Fig. 2. Computer simulation method for quantum ring problem. This algorithm has been applied to solve semiconductor quantum dot problems by us earlier.

This feedback iteration scheme consists of (i) setting an initial energy E_0, (ii) computing effective mass m, (iii) solving the Schrödinger equation with its boundary conditions for energy E, and (iv) returning to step (ii). The iteration loop terminates when a specified stopping criterion is reached. To solve the Schrödinger equation in step (iii), the Schrödinger equation is discretized with nonuniform mesh central difference method, and the corresponding matrix eigenvalue problem is solved with the balanced and shifted QR method, and the inverse iteration method. The dominant method for solving matrix eigenvalue problem in semiconductor nanostructure simulation is the QR algorithm. In our simulation experience, convergence (the maximum norm error in energy < 10^{-8} eV) is reached by taking only 9-10 iterations.

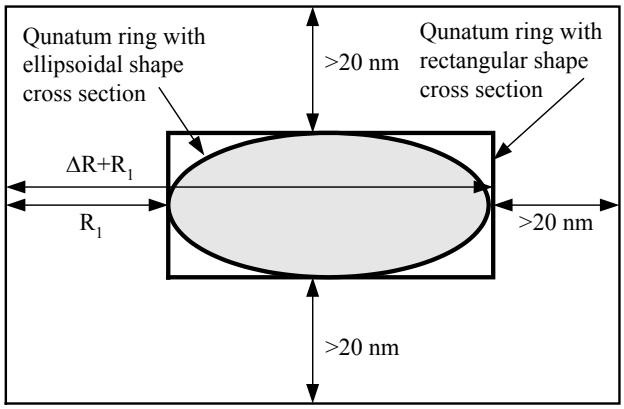

Fig. 3. A schematic diagram of cross section view for 3D semiconductor quantum rings.

3 RESULTS AND DISCUSSIONS

We focus here the discussions on our simulation results for InAs/GaAs quantum rings with the material parameters [10]. To clarify the simulation domain of the quantum ring with different shapes, we plot the cross sections as shown in Fig. 3. For InAs, the energy gap E_{1g} is 0.42 eV, Δ_1 is 0.38 eV, and $m_1(0) = 0.024m_0$. For GaAs we choose: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, and $m_2(0) = 0.067m_0$. The band offset parameter is taken as $V_0 = 0.77$ eV.

Here we present our calculation results for a quantum ring with height $H = 2.0$ nm and radial width $\Delta R = 20.0$ nm. Firstly, we compare the calculated ground state energy for various quantum rings at zero external magnetic field $\boldsymbol{B}$ with the same material parameters and sizes. The ground state energies are computed with three different models: (a) a simple 2D model (so-called adiabatic approach) [5], (b) a 3D model with rectangular shape quantum ring [6]; (c) a 3D model with ellipsoid shape quantum ring.

Fig. 4 shows the ground energy state dependence on the inner radius (R_1) of the ring. It is clearly that we can see that there is a large discrepancy between these two- and three- dimensional approaches. The difference in energy is drastically increased when the ring size is decreased. This is a direct result that the effective confinement increases from approach (a) to (c). To model the energy states for nanoscopic semiconductor quantum rings, our calculation results suggest it is necessary to choose a proper 3D quantum ring simulation and the ring shape. The most realistic ring shape from the fabrication point of view is the 3D ellipsoid shape model [1].

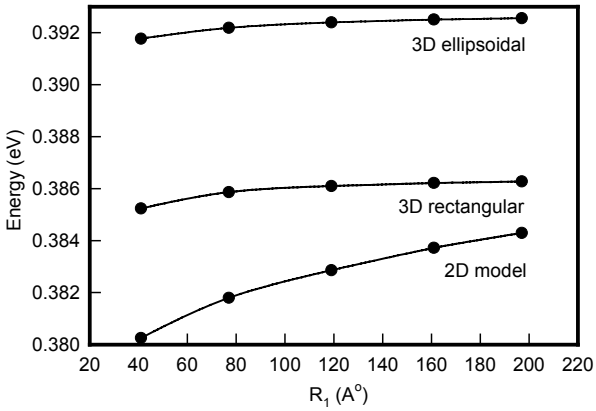

Fig. 4. The dependence of electron ground state energy on the inner radius (R_1) for InAs/GaAs quantum rings. Comparison of 2D (a simplified adiabatic approach) and 3D models (rectangular and ellipsoidal radial cross sections) for quantum rings with having height $H = 2$ nm and radial width $\Delta R = 20$ nm.

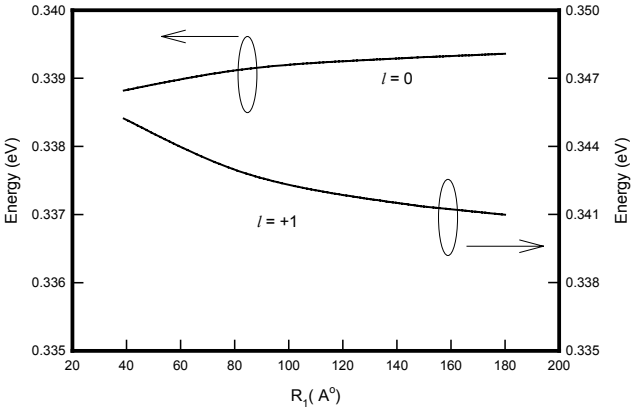

Fig. 5. Energy of quantum rings for $l = 0$ and $l = +1$. The ring has height $H = 2.4$ nm and radial width $\Delta R = 24$ nm.

The Fig. 5 suggests that the energy variation follows the ring's inner radius for quantum ring with ellipsoid shape cross section view. We found the energy for $l = 0$ increased when the R_1 is increased. In addition, the energy with a decreasing variation for $l = +1$ is corresponding the model theory when the R_1 is increased. However, as shown in Fig. 5, we also found the energy variation has a weak dependence on the inner radius for both of the $l = 0$ and $l =$

+1. It can be observed that the quantum ring has high geometric aspect ratio, ($\Delta R/H > 10$) and hence it decreased the size dependency relation between energy levels and the inner radius of the ring. To make a more clear study on the size effects for quantum ring, we present the dependency relation for other parameters.

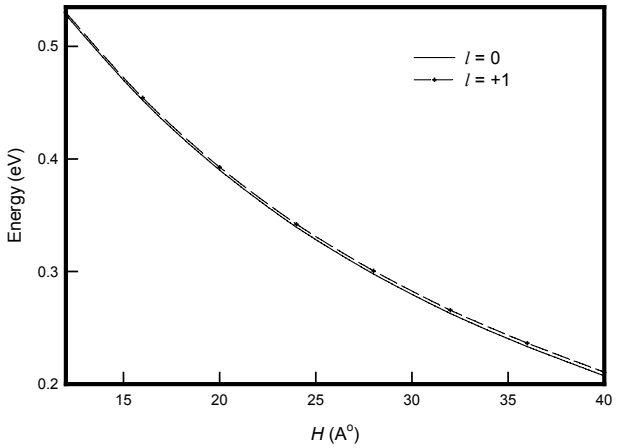

Fig. 6. Energy of quantum rings for $l = 0$ and $l = +1$, where the ring has the inner radius $R_1 = 12$ nm and radial width $\Delta R = 24$ nm.

We further investigate the effect of ring's height for the variation of energy levels. As shown in Fig. 6, we found the ring's height is increased, both the energy levels for $l = 0$ and $l = +1$ are decreased uniformly. It is no surprised since the wave function spreads out the ring along the z-direction is controlled by the ring's height.

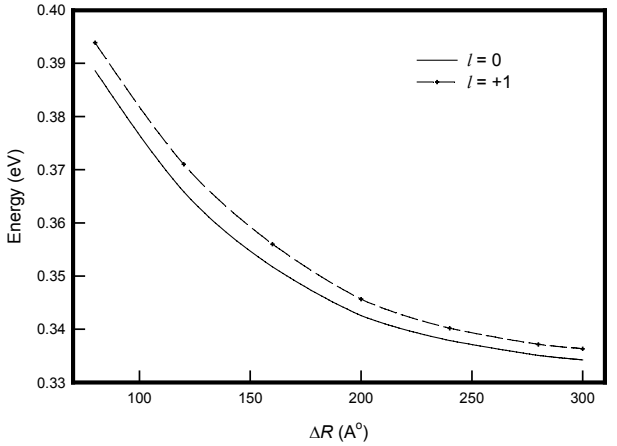

Fig. 7. Energy of the simulated quantum rings for $l = 0$ and $l = +1$, where the ring has height $H = 2.4$ nm and inner radius $R_1 = 24$ nm.

As shown in Fig. 7, we found the radial width ΔR also plays a role in the variation of the energy levels of the quantum ring for $l = 0$ and $l = +1$. Comparison between the Fig. 6 and Fig. 7, it is clearly that the quantum ring's energy levels strongly depend on the ring's height rather than the ring's radial width.

4 CONCLUSIONS

In this work we have comprehensively calculated single electron energy states for realistic three-dimensional model of InAs/GaAs quantum rings with ellipsoid shape. The 3D model has been solved numerically with our proposed nonlinear iterative solution techniques successfully. The simulation results demonstrate a good consistence with experimental measurement and also have been compared comprehensively with those simplified models, such as 1D and 2D models, or 3D model with non-realistic rectangular shape assumption to show the necessity of the realistic 3D model. In the model formulation, we use the effective three-dimensional one band Hamiltonian, the energy (non-parabolic) and position dependent quasi-particle effective mass approximation, and the Ben Daniel-Duke boundary conditions with the finite hard wall confinement potential. In the calculation of the self-consistent solution for the model with various size and shapes, we have successfully applied and implemented our proposed nonlinear iterative scheme earlier in quantum ring electronic state simulation.

The main results demonstrate for those improper model formulations in studying the nano-scopic semiconductor quantum ring will lead to a significant difference in the energy level calculation. From the fabrication point of view, we found the more realistic quantum ring model should be 3D ellipsoidal shape quantum ring. Furthermore, in our study we also found the inner radius, height, and radius width of such nano-scopic semiconductor quantum ring play very important roles in the variation of the energy levels. It will be more complete and interesting study if we take into the effect of magnetic term for the nano-scopic quantum rings.

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