

P-2-1
Effect of Shape and Size on Electron Transition Energies of InAs Semiconductor Quantum Dots

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1. Introduction

Recent advances in the fabrication of semiconductor quantum dots generated a huge quantity of experimental and theoretical data (see [1,2] and references therein). The three-dimensional (3D) confinement of charge carriers in those structures allows very rich optical and magnetic characteristics that potentially may have very important device applications. The spectral broadening [1,3] in semiconductor quantum dots caused by the nonuniformity in the size and shape is of the primary concern for practical laser applications

The shape of quantum dots is debated intensively in theoretical works, since an accurate calculation (and explanation) of the electronic structure obviously depends on the dot shape. A wide range of shapes and sizes was used in the theoretical models to simulate InAs dot properties. The diversity in the theoretical model and approach makes it difficult to compare the theoretical results of different authors and to verify the models on the basis of experimental results. To the best of our knowledge, a comprehensive analysis of the influence of the dot size and shape on the electron energy states by using a unified model of the semiconductor band structure has not been done yet.

In this study we calculate and compare the electron energy state systems for 3D small InAs/GaAs quantum dots of four different shapes: disk (DI), ellipsoidal lens (EL), cut sphere lens (CL), and conical (CO). All of them are cylindrically symmetric (with the circular top view cross section). We use a unified approach, the effective 3D one electronic band Hamiltonian, the energy (non-parabolic) and position dependent electron effective mass approximation, and the Ben Daniel-Duke boundary conditions. The energy states and wave functions are solved numerically with the finite difference, balanced QR, and inverse iteration methods.

2. Theoretical Model and Method of Calculation

We consider quantum dot structures in the one-band envelope-function formalism in which the effective Hamiltonian is given by [4]

$$\hat{H}_0 = -\frac{\hbar^2}{2} \nabla_{\mathbf{r}} \frac{1}{m(E, \mathbf{r})} \nabla_{\mathbf{r}} + V(\mathbf{r}), \quad (1)$$

where $\nabla_{\mathbf{r}}$ stands for the spatial gradient, $m(E, \mathbf{r})$ in Eq. (1) is energy and position dependent electron effective mass

$$\frac{1}{m(E, \mathbf{r})} = \frac{2P^2}{3\hbar^2} \left(\frac{2}{E + E_g(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E + E_g(\mathbf{r}) - V(\mathbf{r}) + \Delta(\mathbf{r})} \right), \quad (2)$$

where $V(\mathbf{r})$ is the position dependent confinement potential. In (2), inside the dot $V(\mathbf{r})$ is zero and it equals V_0 for all \mathbf{r} outside the dot. The $E_g(\mathbf{r})$, $\Delta(\mathbf{r})$, and P stand for position dependent band gap, the spin-orbit splitting in the valence band, and the momentum matrix element, respectively.

We investigate various shapes of the dot: DI, EL, CL, and CO (see Fig. 1). Those all are cylindrically symmetric with the base radius R_0 and height z_0 in the cylindrical (R, ϕ, z) coordinate. Since the system is cylindrically symmetric, the wave function can be represented as

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

where $l = 0, \pm 1, \pm 2, \dots$ is the electron orbital quantum number and the problem remains 2D in (R, z) coordinates with the boundary conditions of the form

$$\begin{aligned} \Phi_{in}(R, z) = \Phi_{out}(R, z), \quad z = f_s(R), \\ \frac{1}{m_{in}} \left(\frac{\partial \Phi_{in}(R, z)}{\partial R} + \frac{df_s(R)}{dR} \frac{\partial \Phi_{in}(R, z)}{\partial z} \right) \Bigg|_{z=f_s(R)} = \\ \frac{1}{m_{out}} \left(\frac{\partial \Phi_{out}(R, z)}{\partial R} + \frac{df_s(R)}{dR} \frac{\partial \Phi_{out}(R, z)}{\partial z} \right) \Bigg|_{z=f_s(R)}, \end{aligned} \quad (4)$$

where $z = f_s(R)$ ($s = \text{DI, EL, CL, or CO}$) is the contour of the structure's cross section on the $\{R, z\}$ plane. The structure shape is generated by the rotation of this contour around the z axis.

Based on the fact that the electron effective mass is a spatial and energy dependent function, so the Schrödinger equation is a nonlinear equation in energy. A computational

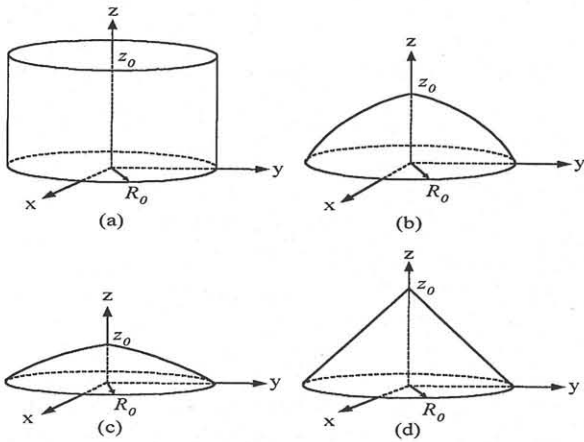


Fig. 1 Schematic diagrams for quantum dots of four different shapes: (a) DI, (b) EL, (c) CL, and (d) CO.

method for such nonlinear problem has been proposed and successfully implemented for the spin-splitting quantum dot problem by us [5] recently. Due to the energy dependence of the electron effective mass, our calculation consists of iteration loops to reach a "self-consistent" energy solution. In the iteration we use a central difference method with nonuniform mesh technique to discretize the 2D Schrödinger equation. The discretized Schrödinger equation together with its boundary conditions (4) leads to an eigenvalue problem

$$AX = \lambda X, \quad (5)$$

where A is the matrix rising from the discretized Schrödinger equation and boundary conditions, X and λ are the corresponding eigenvectors (wave functions) and the eigenvalues (energy states). Because the matrix A is an energy dependent, five diagonal and nonsymmetric matrix, we perform a balancing algorithm to reduce the sensitivity of eigenvalues of the matrix A to small changes in the matrix elements. Then the matrix A is transformed into a simpler upper Hessenberg form. The eigenvalues of the upper Hessenberg matrix are directly computed with QR method. When the eigenvalues are found, we solve the corresponding eigenvectors with the inverse iteration method. In our calculation experience, the proposed computational method converges monotonically and a strict convergence criteria on energies (the maximum norm error less than 10^{-12} eV can be reached by only 12-15 feedback nonlinear iterative loops.

3. Calculation Results and Conclusions

In Fig. 2 we present the calculated electron energy levels for InAs/GaAs quantum dots as functions of the dot volume. The results are plotted relative to the InAs conduction band edge. The ground ($l=0$) and first excited ($l=1$) electron energy levels are illustrated, respectively, where the base radius, R_0 , is taken as 10.0 nm for all shapes.

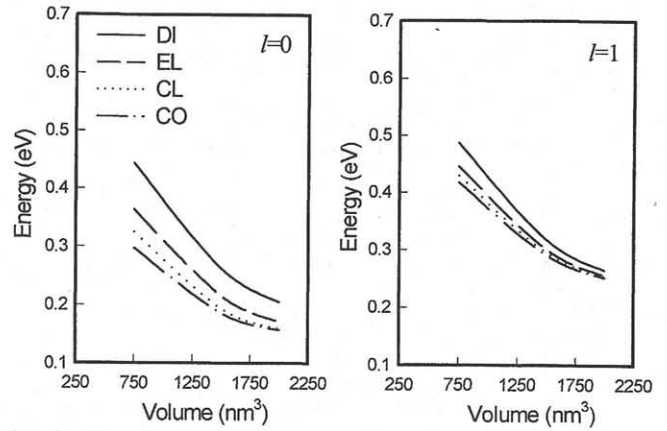


Fig. 2 The electron energy states for InAs/GaAs quantum dots versus the dot volume.

The proposed model predicts rather different electron energy dependences on the volume for dots of different shapes. When the dot volume increases the energy states of different shapes converge. The most sensitive to the dot volume variation is the quantum disks and the least is that of the conical shape dots. The first excited state demonstrates a weaker sensitivity to the dot shape and volume. This is no surprise since the electron wave function is the best confined for the disk geometry when the volume and radius are fixed. The wave function shape confirms weaker confinement for conical shaped dots.

We also calculate volume dependence on the transition energies between hole and electron states for dots with $R_0 = 10.0$ nm. Furthermore, to present the electron energy level dependence on the dot volume V more generally we fitted the energy dependence $E \sim V^\gamma$ to our calculated results. We found that γ parameter is rather different for different dot shapes and can vary widely within a region $0.12 \sim 0.76$ (commonly quoted value is $2/3$). Different volume dependence on different dot shape can be useful in tuning the intersublevel energy spacing when we prepare the quantum dots with different sizes and shapes.

Acknowledgments

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