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Investigation of potential profile effects in quantum dot and onion-like quantum dot-quantum well on optical properties

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ABSTRACT

This paper investigates GaAs/AlGaAs modified quantum dot nanocrystal and GaAs/AlGaAs/GaAs/AlGaAs quantum dot-quantum well heteronanocrystal. These quantum dots have been analyzed by the finite element numerical methods. Simulations carried out for state $n=1$, $l=0$, and $m=0$ which are original, orbital, and magnetic state of quantum numbers. The effects of variation in radius layers such as total radius, GaAs core, shell and AlGaAs barriers radius on the wavelength and emission coefficient are studied. For the best time, it has also investigated the effect of mole fraction on emission coefficient. Meanwhile, one of the problems in biological applications is alteration of the emission wavelength of a quantum dot by changing in its dimension. This problem will be resolved by changing in potential profile.

1. Introduction

The research which is described in this article focuses on the characterization of electronic and optical properties of modified Quantum dot (MQD) GaAs/AlGaAs and Quantum dot-quantum well (QDQW) GaAs/AlGaAs/GaAs/AlGaAs semiconductor nanocrystal as function of size and shape. The most striking property of semiconductor Quantum dots (QDs) is their ability to change the optical properties by controlling their size. When the size of a bulk semiconductor crystal is reduced, the surface area to volume ratio increases and surface structure strongly affects on optical and electronic properties. Furthermore, the electronic properties of crystal stop behaving as a bulk structure. This behavior is a result of quantum confinement effects that is due to the spatial restrictions.

Two important classes of QDs are known MQD and QDQW [1–4]. In this paper, the emission coefficient of MQD and QDQW structures in the GaAs/AlGaAs materials has been compared. MQD and QDQW structures are schematically shown in Fig. 1(a, b).

It is clean that the changing in dimension is one of the common methods to alter the emission wavelength of a QD. This change in dimension is not always applied method for ever. For example in biological applications, the dimensional limitation is an essential limitation [5–7]. Therefore in this article, the effect of changing in potential profile of QD on shift in wave length has been investigated which can resolve dimensional limitations in many applications. For analyzing, the Poisson–Schrödinger equation is worked out by the Finite element method (FEM). The FEM is a procedure of numerical methods that is used to find approximate numerical solutions to partial differential equations (PDEs), which can handle irregular boundaries in the same way as regular boundaries. To introduce structures, we have probed their electronic properties such as energy estate, wave functions and optical properties such as emission coefficient.

2. Mathematical b+ackground and operation principle

In this section, the mathematical and calculation model for description of electrical and optical properties of the MQD and QDQW nanostructures is presented. In order to calculate Eigenvalues, wave functions, and related quantities, the effective mass equation is used. The Schrödinger and Hamiltonian for the QDs are

$$H\psi = E\psi \tag{1}$$

$$H = \frac{-\hbar^2}{(2\times m^*(r))}\nabla^2 - \frac{e^2}{\varepsilon(r)\times r} + V(r) \tag{2}$$

where $m^*(r)$ and $\varepsilon(r)$ are electronic effective mass and dielectric constant of the MQD and QDQW materials, respectively. In principle, the interaction between electrons and holes in the MQD and QDQW should include the screened electrons and holes, coulomb attraction, and interaction with polarization charge at the dielectric interface. Therefore, for simplicity, we used coulombic potential with an average dielectric constant. The confinement potential and the effective mass $V(r)$, $m^*(r)$ are taken to be spherically symmetric in the present work:

$$V(r)_{QD} = \begin{cases} V_0(r) & 0 < r < R_C \\ V_1(r) & R_C < r < R_{C_1} \end{cases} \tag{3}$$

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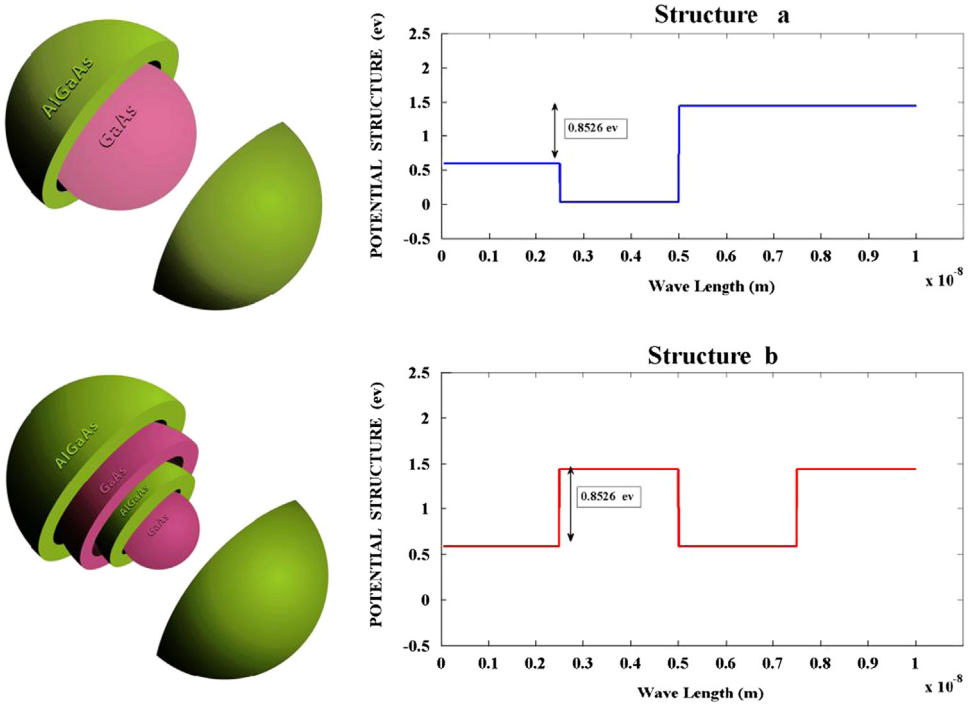

Fig. 1. (a) 3-D Schematic of MQD (ev) and (b) 3-D Schematic of QDQW nanostructure (ev) versus radius (m).

$$V(r)_{QDQW}=\begin{cases}V_0(r) & 0<r<R_C\\ V_1(r) & R_C<r<R_{C_1}\\ V_2(r) & R_{C_1}<r<R_{C_2}\\ V_3(r) & R_{C_2}<r<R_{C_3}\end{cases} \tag{4}$$

$$m^*(r)_{QD}=\begin{cases}m_{GaAs} & 0<r<R_C\\ m_{AlGaAs} & R_C<r<R_{C1}\end{cases} \tag{5}$$

$$m^*(r)_{QDQW}=\begin{cases}m_{GaAs} & 0<r<R_C\\ m_{AlGaAs} & R_C<r<R_{C1}\\ m_{GaAs} & R_{C1}<r<R_{C2}\\ m_{AlGaAs} & R_C2<r<R_{C3}\end{cases} \tag{6}$$

where R_C, R_{C1}, R_{C2}, $V_0(r)$, $V_1(r)$, $V_2(r)$, $V_3(r)$, m_{GaAs}, m_{AlGaAs} are the GaAs core radius, AlGaAs barrier radius, GaAs shell radius, AlGaAs second barrier layer radius, corresponding potentials, effective mass for each region of MQD and QDQW, respectively. For Eigen-states of Hamiltonian, the wave function is written in the form of

$$\psi(r,\theta,\varphi)=R(r)\times Y_{lm}(\theta,\varphi) \tag{7}$$

where $R(r)$ and $Y_{lm}(\theta,\varphi)$ are radial and spherical harmonic wave functions, respectively. The result of above the Eigen-equation of Hamiltonian is

$$H(R(r)\times Y_{lm}(\theta,\varphi))=E(n,l)\times(R(r)\times Y_{lm}(\theta,\varphi)) \tag{8}$$

We find the Schrödinger equation in spherical coordinates that is satisfied by the $R(r)$:

$$r^2\frac{d^2R(r)}{dr}+2r\frac{dR(r)}{dr}+[(E(n,l)-V(r))Ar^2+Br-l(l+1)]\times R(r)=0 \tag{9}$$

where $A=2m^*/\hbar^2$, $B=2e^2/\varepsilon(r)$ and E, e, n, and l are Eigen-value, electron charge, principle quantum number, and orbital angular quantum number, respectively.

The associated wave function solution must satisfy the continuity condition at all boundaries of heteronanocrystal layers introduced in Eqs. (10)–(12). Since there are three discontinuities in this structure, the following boundary conditions could be used to determine the Eigen-energies:

For $r=R_C$:

$$\begin{cases}R_{0<r<R_C}(R_C)=R_{R_C<r<R_{C1}}(R_C) & \text{and}\\ \frac{1}{m^*_{GaAs}}\frac{dR_{0<r<R_C}}{dr}|_{r=R_C}=\frac{1}{m^*_{AlGaAs}}\frac{dR_{R_C<r<R_{C1}}}{dr}|_{r=R_C}\end{cases} \tag{10}$$

For $r=R_{c1}$:

$$\begin{cases}R_{R_C<r<R_{C1}}(R_{C_1})=R_{R_{C1}<r<R_{C2}}(R_{C1}) & \text{and}\\ \frac{1}{m^*_{AlGaAs}}\frac{dR_{R_C<r<R_{C1}}}{dr}|_{r=R_{C1}}=\frac{1}{m^*_{GaAs}}\frac{dR_{R_{C1}<r<R_{C2}}}{dr}|_{r=R_{C1}}\end{cases} \tag{11}$$

For $r=R_{C2}$:

$$\begin{cases}R_{R_{C1}<r<R_{C2}}(R_{C2})=R_{R_{C2}<r<R_{C3}}(R_{C2}) & \text{and}\\ \frac{1}{m^*_{GaAs}}\frac{dR_{R_{C1}<r<R_{C2}}}{dr}|_{r=R_{C2}}=\frac{1}{m^*_{AlGaAs}}\frac{dR_{R_{C2}<r<R_{C3}}}{dr}|_{r=R_{C2}}\end{cases} \tag{12}$$

To determine the method of the Galerkin approach to Eigen-value FEM problems, we will consider the case of torsional vibrations of a uniform circular cross-section. The differential equations and boundary conditions required for determining shape modes and natural frequencies are shown in Eqs. (9) and (10) for MQD and (9)–(12) for QDQW, to apply the Galerkin method. We multiply Eq. (9) by a test function ϕ and integrate it by parts:

$$\int_0^l\left\{\left(r^2\frac{d^2R(r)}{dr^2}+2r\frac{dR(r)}{dr}\right)+[(E(n,l)-V(r))Ar^2+Br-l(l+1)]R(r)\right\}\times\phi\,dr=0 \tag{13}$$

Therefore, with consideration of the initial and boundary conditions, we obtained modified forms of Galerkin approach:

$$-\int_0^l r^2\frac{d\phi}{dr}\frac{dR(r)}{dr}dr-\int_0^l 2rR(r)\frac{d\phi}{dr}dr+\int_0^l[(E-V(r))Ar^2+Br-l(l+1)]R(r)\phi\,dr=0 \tag{14}$$

In this equation, l is the length of FEM element and the next step is to implement FEM approximation using a set of basic