Physica E 66 (2015) 107–115

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Impurity position effect on optical properties of various quantum dots

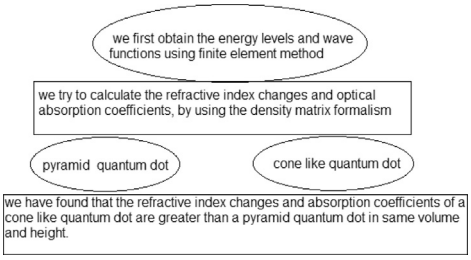
R. Khordad [b], H. Bahramiyan [a,*]

[a] Department of Optics and Laser Engineering, Marvdasht Branch, Islamic Azad University, Marvdasht, Iran
[b] Department of Physics, College of Sciences, Yasouj University, Yasouj 75914-353, Iran

HIGHLIGHTS

- We obtain the energy levels and wave functions using finite element method in the presence of impurity.
- The absorption coefficients and refractive index changes have been obtained.
- The optical properties of a cone like quantum dot are greater than a pyramid quantum dot of same volume and height.
- The impurity location plays an important role in optical properties of a pyramid and a cone like quantum dot.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 17 May 2014
Received in revised form
18 July 2014
Accepted 29 September 2014
Available online 6 October 2014

Keywords:
Binding energy
Optical properties
Quantum dot

ABSTRACT

In this work, we have investigated the effect of impurity position on optical properties of a pyramid and a cone like quantum dot. For this goal, we first obtain the energy levels and wave functions using finite element method (FEM) in the presence of impurity. Then, we have studied the influence of impurity location on refractive index changes and absorption coefficients of the two quantum dots. We found that there is a maximum value for total refractive index changes and absorption coefficients at a special impurity position. Also, we have found that the refractive index changes and absorption coefficients of a cone like quantum dot are greater than a pyramid quantum dot in same volume and height. According to the results, it is deduced that the impurity location plays an important and considerable role in the electronic and optical properties of a pyramid and a cone like quantum dot.

1. Introduction

During the past three decades, the physics of low-dimensional semiconductor structures has become a vital part of present-day research. Low-dimensional structures allow the study of a variety of new mechanical, optical, and transport phenomena [1]. Examples of low-dimensional semiconductor structures are quantum wells, quantum wires, and quantum dots [2–5]. There are several technological progresses in the fabrication of semiconductor structures like chemical lithography, molecular beam epitaxy, and etching [2–4]. Among the nanostructures, quantum dots have become subject of intensive experimental and theoretical studies nowadays. The improvements of the semiconductor growth techniques have offered the possibility to obtain quantum dots with various shapes such as spherical, cylindrical, ellipsoidal, pyramid-like, and cone-like [5–8].

It is clear that the semiconductor structures open new possibilities to tailor the mechanical, electronic, magnetic and optical properties of materials. The optical and transport properties of low-dimensional semiconductor structures have became subject of intensive experimental and theoretical studies in the several last decades [6,9]. These properties are sensitive to external effects such as external electric and

* Corresponding author.
E-mail address: hossein.bahramiyan@gmail.com (H. Bahramiyan).

http://dx.doi.org/10.1016/j.physe.2014.09.021
1386-9477/

magnetic fields, pressure, temperature, and impurity positions. Hitherto, many investigations have been done on optical, electronic and transport properties of low-dimensional semiconductor structures under the external effects [10–17].

The knowledge of the electrical and optical properties of nanostructures associated with shallow-donor impurities is important in semiconducting low-dimensional systems. In this sense, the investigation of impurity-related effects in low-dimensional semiconductor structures can show the number of publications [18–24]. These reports deal with various nanostructures and different physical features such as the influence of quantum wire cross section geometry, application of electric and magnetic fields, hydrostatic pressure and temperature effects.

The problem of shallow donor impurities confined to a semiconductor structure has been studied extensively during the two last decades [25–30]. Study of impurity states is important, not only to understand how such levels differ from the bulk, but also in the fabrication and subsequent working of electronic and optical devices based on such systems. The impurity states have the essential roles in the thermal, optical and electrical properties and also in semiconductor devices. Hitherto, many works have been performed on the impurity states in quantum dots [27–29].

We know that optical properties of semiconductor nanostructures such as quantum wells, quantum wires, and quantum dots have attracted much attention in the past few years. In this regard, much attention has been focused on refractive index changes and absorption coefficients. In the past few years, several works have been done on effect of impurity states on optical properties of various quantum dots.

In this paper, we intend to study effect of impurity location on refractive index changes and absorption coefficient of a pyramid and a cone like quantum dot that is grown on a wet layer in the presence of impurity. For this purpose, we have calculated the energy levels and wave functions in the effective mass approximation numerically by using the finite element method.

2. Theory and model

In the effective mass approximation, the Hamiltonian of a hydrogenic donor impurity located at the position $\mathbf{r}_0$in a quantum dot is given by

$$H = H_0 - \frac{e^2}{\varepsilon|\mathbf{r}-\mathbf{r}_0|}, \tag{1}$$

where e and ε are the electron charge and medium permittivity, respectively. The Hamiltonian without impurity can be written as

$$H_0 = -\frac{\hbar^2}{2m^*}\nabla^2 + V(x,y,z). \tag{2}$$

Here, m^* is the effective mass of the electron. In this present work, we have considered two various quantum dots, pyramid and cone like, with finite confining potential. The confining potential $V(x, y, z)$ is given by

$$V(x,y,z) = \begin{cases} 0 & \text{inside} \\ V_0 & \text{outside} \end{cases}. \tag{3}$$

where V_0 is the potential height between GaAs and $Ga_{0.5}In_{0.5}As$. It is clear that due to the complicated form of the quantum dot shapes, the calculation of energy levels and wave functions, analytically, is a nontrivial task. Therefore, we are interested in using the finite element method (FEM) to find wave functions and energy levels of the systems [31]. In the following, we briefly present the FEM to solve the Schrodinger equation in the Cartesian coordinates.

The finite element method (FEM), sometimes referred to as finite element analysis (FEA), is a computational technique used to obtain approximate solutions of boundary value problems in engineering and basic sciences [32,33]. Simply stated, a boundary value problem is a mathematical problem in which one or more dependent variables must satisfy a differential equation everywhere within a known domain of independent variables and satisfy specific conditions on the boundary of the domain. The field is the domain of interest and most often represents a physical structure. The field variables are the dependent variables of interest governed by the differential equation. The boundary conditions are the specified values of the field variables (or related variables such as derivatives) on the boundaries of the field. Depending on the type of physical problem being analyzed, the field variables may include physical displacement, temperature, heat flux, and fluid velocity to name only a few.

We consider a volume of some material or materials having known physical properties. The volume represents the domain of a boundary value problem to be solved. We construct a grid in real space using a discrete number of points. The eigenenergies and eigenstates of the electrons confined in a quantum dot are evaluated solving the three-dimensional Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z) + (V(x,y,z)+V^{int}(x,y,z))\varphi(x,y,z) = E\varphi(x,y,z) \tag{4}$$

The operator ∇^2 is properly discretized using the standard three-point finite difference approximation. The confinement volume is represented by a three-dimensional mesh of (x_i, y_i, z_i) points.

In order to carry out simulation numerically, one needs to discretize Eq. (4). The spatial derivative is approximated for all discretized space except on boundaries and given by

$$\begin{aligned}
&\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}+V(x,y,z)+V^{int}(x,y,z)\right]\varphi^{(int,out)}(x,y,z) \\
&\approx \frac{1}{\Delta x^2}[\varphi^{(int,out)}(i+1,j,k) - 2\varphi^{(int,out)}(i,j,k) + \varphi^{(int,out)}(i-1,j,k)] \\
&+ \frac{1}{\Delta y^2}[\varphi^{(int,out)}(i,j+1,k) - 2\varphi^{(int,out)}(i,j,k) + \varphi^{(int,out)}(i,j-1,k)] \\
&+ \frac{1}{\Delta z^2}[\varphi^{(int,out)}(i,j,k+1) - 2\varphi^{(int,out)}(i,j,k) + \varphi^{(int,out)}(i,j,k-1)] \\
&+ \left[V(i,j,k)+V^{int}(i,j,k)\right]\varphi^{(int,out)}(i,j,k)
\end{aligned} \tag{5}$$

where $V^{int}(x,y,z) = -e^2/(\varepsilon|r-r_0|)$.

The notations $\varphi^{(int,out)}(i,j,k)$ are used as $\varphi^{(int,out)}(i\Delta x, j\Delta y, k\Delta z)$ where Δx, Δy and Δz are spatial spacing. Also, the superscriptions "int" and "out" represents the wave function inside and outside the dot.

The continuity of the wave function on the quantum dot boundary is defined as

$$\varphi^{int}(x,y,z)|_{in\ the\ boundary} = \varphi^{out}(x,y,z)|_{in\ the\ boundary} \tag{6}$$

Also, derivative of wave function on the quantum dot boundary is defined as:

$$\frac{1}{m_{in}}\hat{n}.\vec{\nabla}\varphi^{int}\Big|_{in\ the\ boundary} = \frac{1}{m_{out}}\hat{n}.\vec{\nabla}\varphi^{out}\Big|_{in\ the\ boundary}, \tag{7}$$