Optical transitions in quantum dots

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Abstract

The analysis of the electronic states of a quantum dot of InAs grown on a GaAs substrate has been studied for different geometries. We did the calculation with each type of geometry we based on the Schrödinger equation for stationary particle and we used "Comsol" for calculations. We calculated energy values as a function of each of the parameters: length, width and thickness of the wetting layer where other parameters are held constant.

Keywords: hétérostructures InAs / GaAs, the Schrödinger equation, simulation, COMSOL.

1. Introduction

There are several ways to make quantum dots among these techniques include the method known as Stranski-Krastanov, which is the one used for the growth of quantum dots. An important point is that this growth process results in the formation of a two-dimensional layer of InAs based uppermost islets called wetting layer, and acting as a reservoir of electrons scattered over a continuum of power levels.[1, 2, 3]. The objective of this work is to grow hetero structure from two semiconductor materials (InAs/ GaAs). We make calculations by "Comsol" with each type of geometry (rectangular, sphericaland conical) at the same height and the same radius. To get a better idea of how energy changes indicates that we vary one of the parameters of the function (3). The energy level values obtained are listed in the table (01).

2. Method

We detail the theoretical model that we used to determine the wave functions and energy Eigen statesof electrons and holes through the resolution of the Schrödinger equation [1,2]

$$E \Psi = H \Psi \qquad (1)$$

$$i \frac{h}{2\pi} \frac{\partial \Psi}{\partial t} = H \Psi \qquad (2)$$

The equation can be simplified to a stationary Schrödinger equation:

The parameters of the equation are:
- h ($\approx 6{,}626.10^{-34}$ J.s) is Planck's constant.
- μ is the reduced mass.
- V is the potential energy.
- E is the valueofenergy.
- Ψ is the quantum mechanical wave function.

$$-\nabla.\left(\frac{h^2}{8\mu\pi^2} \nabla\Psi \right) + V\Psi = E\Psi \qquad (3)$$

results in the modification of some parameters such as the radius, quantum dot height and thickness of the wetting layer. Indeed, the solutions of equation (3) where $I = 0$, which are transition energies depicted in Figures (4, 5 and 6). The energy electron-heavy hole transition is written by:

$$\Delta E_{e\text{-}hh} = E_e + E_{hh} + Eg_{InAs} \qquad (4)$$

To resolve this problem, use the form PDE interface coefficient. The model solves for an eigenvalue / eigenvector. Electronvolt is used as an energy and nanometer length units of the geometry unit.

3. Result and discussion:

3.1. The electronic states of a quantum dot InAs with each type of geometry:

The first step we choose is the realization of three different geometric structures shown in Figure

(1),(2)and (3).We make calculations with Comsol each type of geometry with the same dimensions (height, radius, and thickness of the layer of wetting. The energy levels are listed in Table 01, and we see that the highest energy states are obtained for the conical quantum dot; we find that the energy is inversely proportional to the size of quantum dot.

geometry types	E_0 (eV)
conical	1.05
elliptic	0.95
rectangular	0.91

Table 01: The energy levels for each geometry in the ground state E_0 (eV)

Figure 01: The energy values for conical structure (E=1.05 eV)

Figure 02: The energy values for elliptical structure (E=0.95 eV)
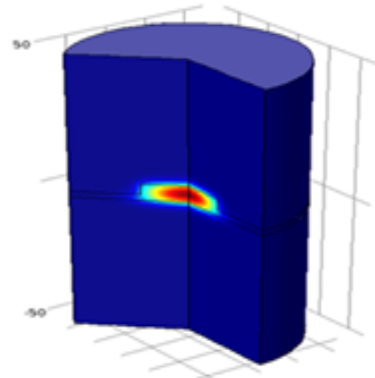

Figure 03: The energy values for conical structure (E=0.91 eV)

3.2. Changes in the parameters of the quantum dot:

Among the three geometries, we have chosen the conical structure and we have made changes on the radius of the quantum dot "r" between (50A° and 250A°), the thickness and layer wettingand we obtained the results shown in the figures (4,5 and 6) respectively which correspond to energy levels of optical transition. The analysis of these figures shows that the transition energy is strongly dependent on the size of the quantum dot. Indeed, these energies are inversely proportional to the dimensions of the dot and to the thickness of the wetting layer.
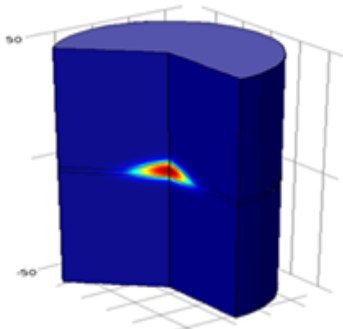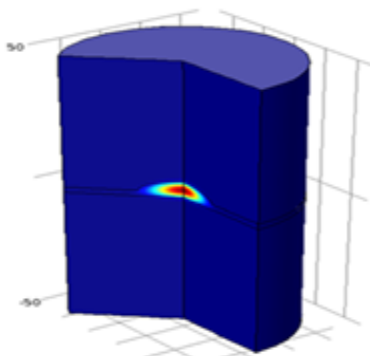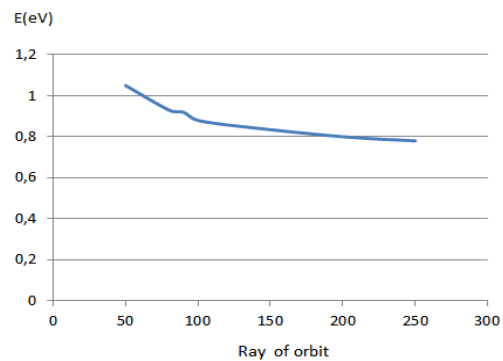

Figure 04: The energy values for changes in the ray of orbit

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confinement energy hen reduces the size of the structures [4, 5].

4. Conclusion:

Our results obtained by studying a single quantum dot, were we use Comsol softwareand by simulation of elliptic, conical and rectangular nano-crystalsInAs shows that the energy associated with the ground level depends on the shape and volume of quantum dots.
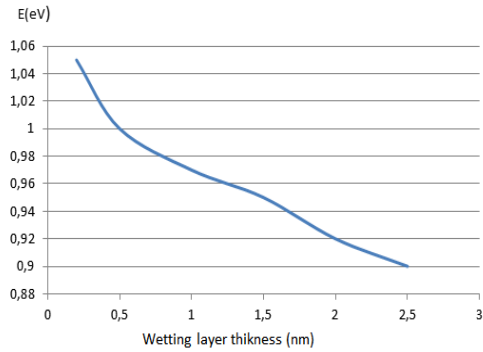

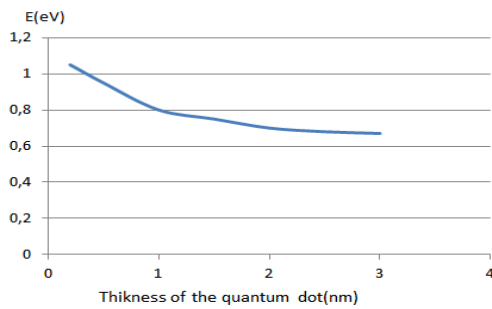*Figure 05:* The energy values for Changes in thickness of the quantum dot.

Figure 06: The energy values for Changes in the witting layer thickness.

There is an offset of the energy of transitions to higher energies because of the change in the

References:

[1]COMSOL Multiphysics Model Library copyright 1998–2008 by COMSOL AB. All rights reserved.
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