Visual Evolutions during Quantum Dots

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Abstract

The power levels can then be modeled by means of the element in a box model in which the force of dissimilar states is reliant on the extent of the box. Quantum dots are supposed to be in the 'weak imprisonment regime' if their radii are on the arrange of the exciton Bohr radius; the investigation of the electronic states of a quantum dot of InAs developed on a GaAs substrate has been deliberate for unusual geometries. We did the computation with each type of geometry we based on the Schrödinger equation for inactive element and we used "Comsol" for calculations. We considered energy values as a purpose of each of the parameters: duration, width and thickness of the wetting layer where supplementary parameters are held invariable. Wherever the quantum internment affects are entirely dominant and the energy levels opening up to the degree that the energy spectrum is approximately permanent, thus emitting white light.

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

I. INTRODUCTION

There are numerous ways to make quantum dots surrounded by these techniques consist of the technique known as Stranski-Krastanov, which is the one worn for the enlargement of quantum dots. Stranski-Krastanov growth is one of the three most important modes by which thin films grow epitaxial at a crystal facade or boundary. In addition known as 'layerplus-island growth', the SK mode follows a two step procedure: originally, absolute films of adsorbates, up to quite a few monolayers thick, grow in a layer-bylayer method on a crystal substrate. Beyond a critical coating breadth, which depends on damage and the chemical potential of the deposited film, growth continues through the nucleation and coalescence of adsorbates 'islands'. A quantum dot (QD) is a nanocrystal complete of semiconductor materials that is undersized enough to exhibit quantum mechanical properties. Particularly, its excitons are restricted in all three spatial dimensions. The electronic properties of these materials are transitional connecting those of bulk semiconductors and of separate molecules.

The required condition for the accomplishment of a good course hétérostructures is that the two materials have the same hand of a crystalline structure and other parameters of bordering mesh. A significant point is that this development process results in the formation of a two-dimensional layer of InAs based uppermost islets called wetting layer, and performing as a reservoir of electrons scattered over a variety of power levels. InAs nanostructures may pose a possible for electronic imprisonment in combination with many semiconductors III-V as GaAs. In these nanostructures, the charge carriers are then adequately restricted to allow the quantification of the energy levels of the arrangement. The purpose of this work is to grow hetero arrangement from two semiconductor equipment (InAs / GaAs). The hole in the InAs / GaAs scheme is low satisfactory so that the consequent optical transitions are in the perceptible or near infrared. We make calculations by "Comsol" with each type of geometry at the same altitude and the matching radius. To get a better idea of how energy changes indicates that we vary one of the parameters of the significance. The energy level principles obtained are listed in the Table 1.

| Geometry types | E ₀ (eV) |
|----------------|---------------------|
| Conical | 2.05 |
| Elliptic | 1.95 |
| Rectangular | 1.91 |

 Table 1. The Energy Levels For Each Geometry in the Ground State E0 (Ev)

II. METHODOLOGY

We detail the theoretical model that we used to determine the wave functions and energy Eigen states of electrons and holes through the resolution of the Schrödinger equation

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

$$i\frac{h}{2\pi}\frac{\partial\Psi}{\partial t} = H\Psi \tag{2}$$

The equation can be simplified to a stationary Schrödinger equation:

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

The parameters of the equation are:

- ✓ h (\approx 6,626.10-34 J.s) is Planck's constant.
- \checkmark µ is the reduced mass.
- \checkmark V is the potential energy.
- \checkmark E is the value of energy.
- \checkmark Ψ is the quantum mechanical wave function.

Where the periodicity situation implies that the primary quantum number must be an integer. It residue to solve the equation 3, it is an occurrence of a PDE on the form factor, we will revise as:

$$\nabla . (-c\nabla - \alpha + \gamma) + \alpha + \beta . \nabla = d_a \lambda.$$

- ✓ d_a is a damping coefficient or a mass coefficient.
- \checkmark c is the diffusion coefficient.
- $\checkmark \alpha$ is the conservative flux convection coefficient.
- \checkmark β is the convection coefficient.
- \checkmark a is the absorption coefficient.
- \checkmark γ is the conservative flux source term.

Where the non-zero coefficients are:

$$c = h^{2} / (8\pi^{2}m_{e}) \qquad a = [h^{2} / (8\pi^{2}m_{e})]l^{2}/r^{2} + V$$

$$\beta_{r} = -h^{2} / (8\pi^{2}m_{e}).l/r \qquad d_{a} = 1$$

And $\lambda = El.$

We can model the generally structure in 2D as exposed in Figure 1 below: Whenever we will vary the values of the "wet "is the wetting layer thickness, "r" is the radius and "z "is the height of the QD. Then, we nearby the consequences obtained from the numerical assessment used while interpreting these results in the adaptation of some parameters such as the radius, quantum dot height and thickness of the wetting coating. Certainly, the solutions of equation (3) where l = 0, which are evolution energies depicted in Figure 5, Figure 6 and Figure 7. The appearance of the transition energy is printed as follows:

$$E_{tr} = E_g + E_e + E_h \tag{4}$$

Where Ee is the quantization power of the electrons, Eh is the quantization energy of the holes and Eg is the energy gap.



Figure 1. Geometry 2D of a Quantum Dot and a Wetting Layer

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

III. RESULT AND DISCUSS

A. The Electronic States of a Quantum Dot in as With Each Type Of Geometry

The first step we choose is the realization of three different geometric structures shown in Figure 2, Figure 3 and Figure 4.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 2, 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.

| Name | Expression | Description |
|-------|-----------------|---|
| me1 | 0.067*m0 | The electron mass coefficient for GaAs |
| me2 | 0.023*m0 | The electron mass coefficient for InAs |
| mv1 | 0.51*m0 | The hole mass coefficient mass for GaAs |
| mv2 | 0.41*m0 | The hole mass coefficient for InAs |
| m0 | 9.1e-31 | Electron mass |
| Vc1 | 0.697 | Potential barrier, GaAs (ev) |
| Vc2 | 0 | Potential barrier, InAs (ev) |
| h-bar | 1.05459*10^(34) | Planck's constant |
| L | 0 | Principal quantum number |

Table 2. All parameters used in the Calculation



Figure 2. The Energy Values for conical Structure (E=2.05eV)



Figure 3. The Energy Values for Elliptical Structure (E=1.95 eV)



Figure 4. The Energy Values for Rectangular Structure (E=1.91 eV)

B. Changes in the Parameters of the Quantum Dot

Amongst the three geometries, we have selected the conical structure and we have made changes on the radius of the quantum dot "r" connecting ($50A^{\circ}$ and $250A^{\circ}$), the thickness and layer wetting and we obtained the outcome shown in the Figure 5, Figure 6 and Figure 7 correspondingly which communicate to energy levels of optical conversion. The investigation of these figures shows that the transition energy is powerfully dependent on the size of the quantum dot. Undeniably, these energies are inversely comparative to the dimensions of the dot and to the depth of the wetting coating.



Figure 5. The Energy Values for Changes in the QD Radius



Figure 6. The Energy Values for Changes in the Thickness of the Quantum Dot



Figure 7. The Energy Values for Changes in the Witting Layer Thickness

In present is an offset of the energy of transitions to advanced energies for the reason that of the change in the internment energy hen reduces the size of the structures.

IV. CONCLUSIONS

We have presented a review on the mid infrared properties of InAs/GaAs semiconductor self – assembled quantum dots. Our results obtained by studying a single quantum dot, were we use Comsol software and by simulation of elliptic, conical and rectangular nano-crystals InAs shows that the energy associated with the ground level depends on the shape and volume of quantum dots. Wherever the quantum internment affects are entirely dominant and the energy levels opening up to the degree that the energy spectrum is approximately permanent, thus emitting white light.

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