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Impact of Electronic States of Conical Shape of Indium Arsenide/Gallium Arsenide Semiconductor Quantum Dots

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Abstract

Semiconductor quantum dots (QDs) have unique atom-like properties. In this work, the electronic states of InAs quantum dot grown on a GaAs substrate has been studied. The analytical expressions of electron wave function for cone-like quantum dot on the semiconductor surface has been obtained and the governing eigen value equation has been solved, thereby obtaining the dependence of ground state energy on radius and height of the cone-shaped nano-dots. In addition, the energy of eigenvalues is computed for various length and thickness of the wetting layer (WL). We discovered that the eigen functions and energies are nearly associated with the GaAs potential.

Keywords: Conical quantum dots; Eigenvalue problem; Schrödinger equation; Energy level; Quantum number

MSC 2020 No.: 35B05, 35Q40, 35Q55, 81Q80

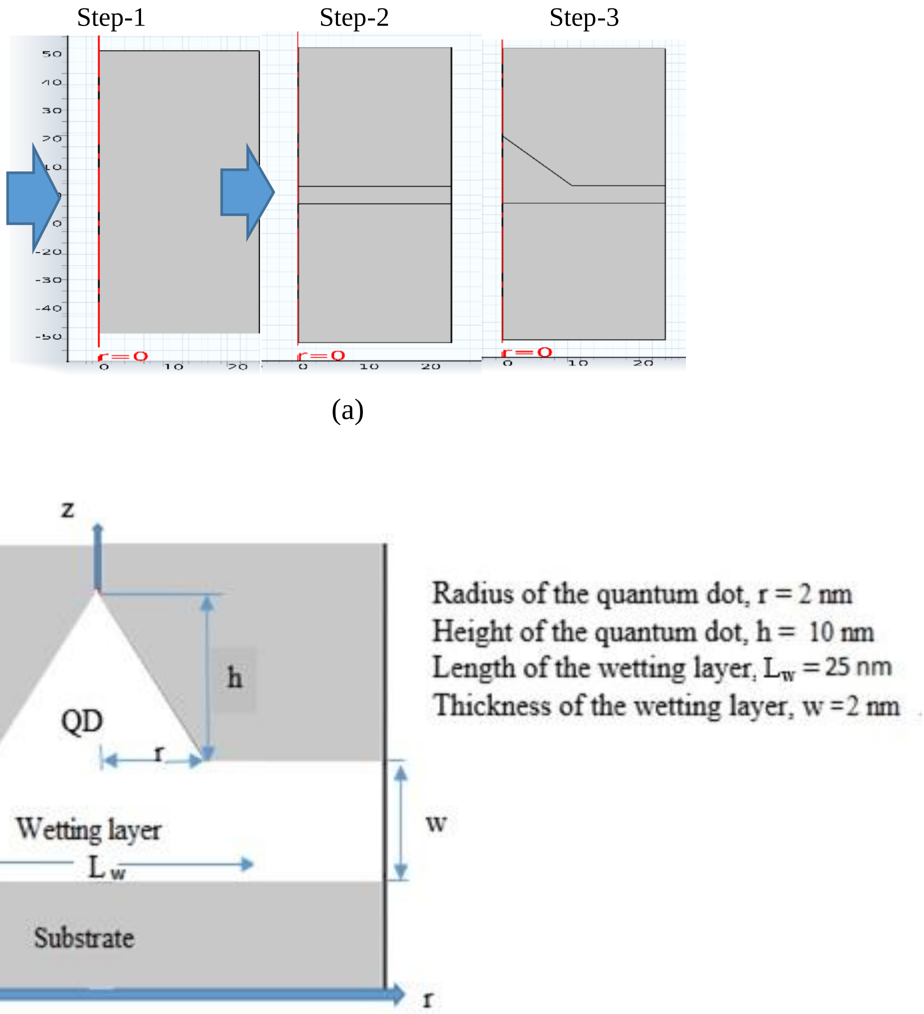
1. Introduction

In recent years, the study of semiconductor quantum dots (QD) have been of great interest because of the extremely useful applications in micro and nano-optoelectronics such as in solar cell, infrared detectors etc. Semiconductor structures growth allow realizing QD of different shapes and geometry (Kappenberger et al. (2018)). For example, Indium Arsenide (InAs) nanostructures on Gallium Arsenide (GaAs) can form conical and cylindrical quantum dots. InAs is well known for its high electron mobility and narrow bandgap. It is extensively used as a terahertz radiation source as it is a photo-dember emitter. The presence of size quantization in all three directions makes the energy of the charge carrier atom-like and strongly dependent on the geometry of the sample (Heinrichsdorff et al. (1998)). This allows a substantial mathematical analysis of the relevant solution of Schrödinger equation, as well as the nature of the energy of electron states (Benahmed et al. (2014)). In InAs nanostructures on GaAs, the variation carriers are sufficiently restricted to enable the quantification of those energy levels of a system (Imran et al. (2018)). Considering the confinement potential of conical QD relatively simple, assuming that an electron is in an impenetrable QD amidst zero potential energy inwardly, it is possible to achieve a number of numerical results for the wave functions and the energy of QDs electron states (Yiming et al. (2001)). Molecular ray epitaxy has grown indium self-assembled plasmonic nanostructures (Gibson & Gehl (2015)). Band structures of conical quantum dots including wetting layer's nanotechnology can be found in (Melnik & Willatzen (2004)). Discrete transparent frame conditions for a Schrödinger equation on circular regions can be found in (Arnold et al. (2012)), and for semiconductor quantum dot lasers, see (Christensen & Saxe (2013)). A survey of dispersive destinations of (non) linear Schrödinger -type equations can be found in (Gasser et al. (2000)). For some interesting and related papers, we referee the readers to (Alam and Tunç (2020a, 2020b, 2020c)), (Islam et al. (2021)) and the references of these papers.

To the best of the researcher's inspection, it seems that no analysis has been compiled of the impact of electronic states of the conical shape of Indium Arsenide/Gallium Arsenide semiconductor quantum dots. They are not together tackled by researchers. This effort aims to examine the electronic states in a conical QD from two semiconductor materials (InAs/GaAs) in terms of wave function and energy.

2. Problem Design

In order to construct the geometry for simulating QD, a rectangle of 100 nm×25 nm area was drawn on 2D axisymmetric model wizard, representing GaAs. A second rectangle having dimension of 2 nm×25 nm was drawn in the middle of the first rectangle, representing InAs wetting layer. Finally, a triangle of 2 nm radius and 10 nm height, representing the QD dimension, was drawn. The computation domain consist of 10 nm height and 2 nm radius axisymmetric conical InAs QD grown on a 2 nm thick InAs wetting layer (WL) on a 100 nm multiplying by 25 nm GaAs matrix. By changing the dimension of the quantum dot and potential barrier of the QD, we obtained the desired data set.



(a)

(b)

Figure 1. a) Construction of 2D geometry in COMSOL multiphysics for simulating InAs QD system on GaAs. All length units are in nm. The QD dimensions will be varied and so will the computation field (CF),
b) A closer look of a quantum dot where Indium Arsenide domain (InAs) acts as interior domain and Gallium Arsenide (GaAs) as an exterior domain

3. Mathematical Model and Numerical Procedure

Interestingly quantum dots demonstrate the same physical behavior as artificial atoms and are governed by Schrdinger equation similar to that of atoms. Therefore, electron states and eigen values are calculated through one band Schrödinger equation:

$$-\frac{h^2}{8\pi^2}\nabla.\left(\frac{1}{m_e(z,r)}\nabla\psi(r)\right)+V(r)\psi(z,r)=E\psi(z,r), \tag{1}$$

where $h, m_e(z,r), V(z,r), E$ and $\psi(z,r)$ stand for the reduced Planck's constant, the position dependent electron effective mass, the potential energy, the electron energy and the wave function of the electron.

Since the wave function is separable, then we can write $\psi = \chi(z,r)(\Phi)$, where Φ is the azimuthal angle. Then rewrite the Schrödinger equation in cylindrical coordinates as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e(z,r)}\frac{\partial \chi(z,r)}{\partial z}\right)+\frac{\partial}{\partial r}\left(\frac{r}{m_e(z,r)}\frac{\partial \chi}{\partial r}\right)\right]\Theta(\Phi)-\frac{h^2}{8\pi^2}\frac{\chi(z,r)}{m_e(z,r)r^2}\frac{d^2\Theta(\Phi)}{d\Theta^2} \tag{2}$$

$$+V\chi(z,r)\Theta(\Phi)=E\,\chi(z,r)\Theta(\Phi).$$

We can rearrange Equation (2) in order to get following two independent equations:

$$\frac{1}{\Theta(\Phi)}\frac{d^2\Theta(\Phi)}{d\Theta^2}=-l^2, \tag{3}$$

$$-m_e r^2\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e(z,r)}\frac{\partial \chi_l(z,r)}{\partial z}\right)\frac{1}{\chi_l(z,r)}+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e(z,r)}\frac{\partial \chi_l(z,r)}{\partial r}\right)\frac{1}{\chi_l(z,r)}\right] \tag{4}$$

$$+m_e r^2\left[V-E\right]=\frac{h^2}{8\pi}l^2.$$

Equation (3) has the solution of the form $\Theta=\exp\left[il\Phi\right]$, where the periodicity condition $\Theta(\Phi+2\pi)=\Theta(\Phi)$ implies that *l*, the principal quantum number, must be an integer. Equation (4) can be rewritten as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e(z,r)}\frac{\partial \chi_l(z,r)}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e(z,r)}\frac{\partial \chi_l(z,r)}{\partial r}\right)\right] \tag{5}$$

$$+\left(\frac{h^2}{8\pi\, m_e(z,r)r^2}l^2+V\right)\chi_l(z,r)\nu=E_l\chi_l\ \left(l\in Z\right).$$

The coefficient form of Partial Differential Equation (PDE), Equation (5), can be stated as:

$$\lambda^2 e_a u-\lambda d_a u+\nabla.\left(-c\nabla u-\alpha u+\Upsilon\right)+\beta.\nabla u+\alpha u=f,$$

where $\nabla=\frac{\partial}{\partial r}\vec{r}+\frac{\partial}{\partial z}\vec{z}$, d_a is a damping coefficient, c is the diffusion coefficient, α is the conservative flux convection coefficient, β is the convection coefficient, a is the absorption coefficient, Υ is the conservative flux source term, e_a the mass coefficient, f is the source term. Here, we take $e_a=0$ and $d_a=f=1$. So, the expression becomes

$$\nabla.\left(-c\nabla u-\alpha u+\Upsilon\right)+\beta.\nabla u+\alpha u=\lambda u,$$

where

$$c=\frac{h^2}{8\pi^2 m_e\left(z,r\right)},\alpha=\frac{h^2}{8\pi^2 m_e\left(z,r\right)}\frac{l^2}{r^2},\beta=\frac{h^2}{8\pi^2 m_e\left(z,r\right)}\frac{1}{r},\quad \lambda=E_1.$$

There are basically two domains that we will be considering the composite QD/WL(wetting layer) domain and the exterior. Wetting Layer is the substrate upon which the quantum dots are grown; The composite QD/WL is made up of InAs resulting in equal potential energyof Indium Arsenide (V_{In}) of electron throught the composite. The QD/WL composite is surrounded by GaAs having potential V_{Ga} higher than V_{In}. As a result the electron tends to reside in the QD/WL domain. For some detailed dicussions, see Table 1.

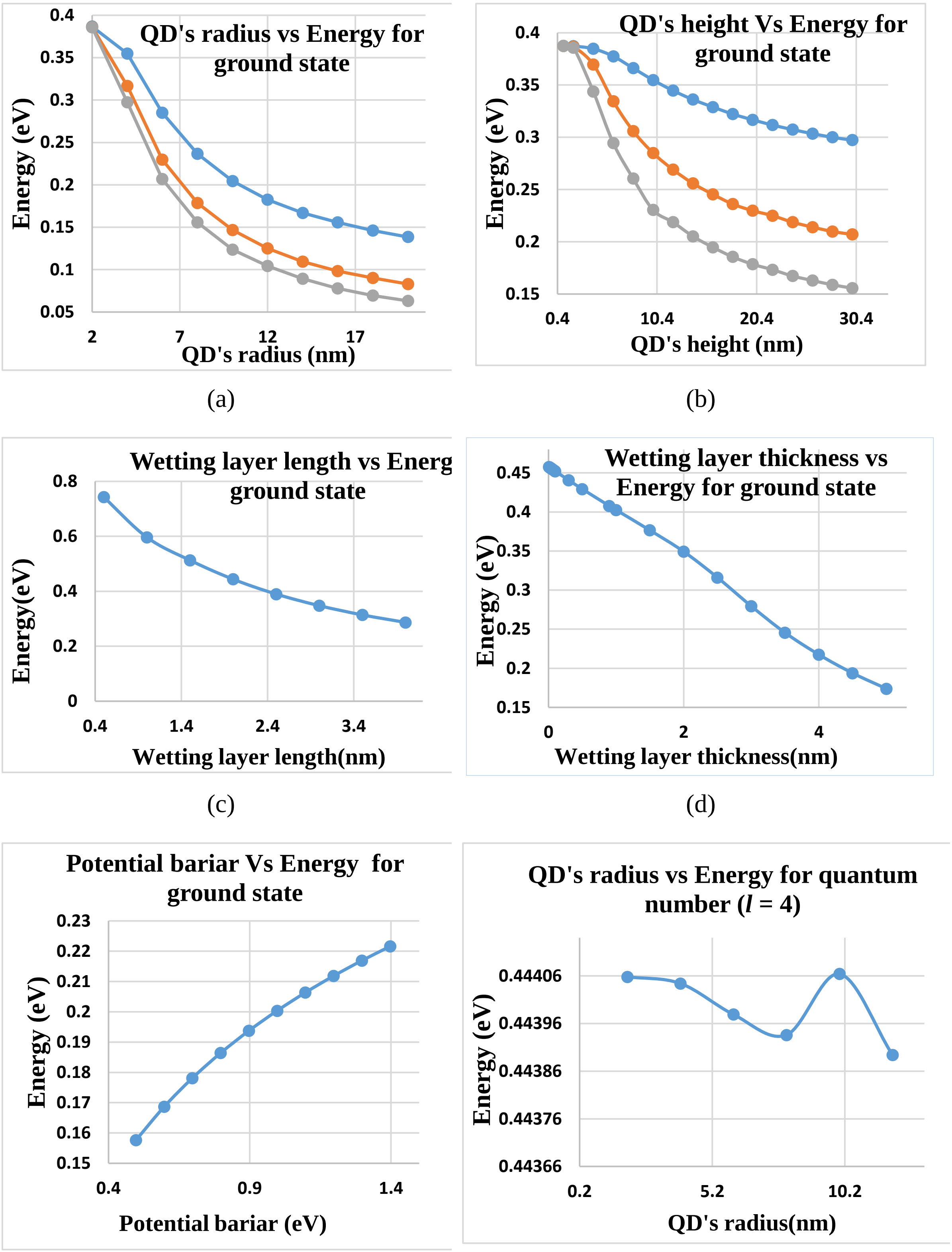
Table 1. This table shows the values and descriptions of m, Hbar, V_{In}, V_{Ga}, c_{In}, c_{Ga} and *L*, respectively

NAME	VALUE	DESCRIPTION
m	5.6856E-12	Electron mass (eV/c^2)
Hbar	6.5821E-16	Reduced Planck constant (eV*s)
V_{In}	0	Potential barrier, InAs (eV)
V_{Ga}	0.69700	Potential barrier, GaAs (eV)
c_{In}	1.6565E-18	c coefficient, InAs
c_{Ga}	5.6856E-19	c coefficient, GaAs
L	0	Principal quantum number

For obtaining a stable and reliable numerical model there are three types of boundary conditions we will apply Dirichlet boundary conditions $\chi = 0$; Neumann conditions, $\frac{\partial\chi}{\partial z}=0$ (*z* denotes the normal to the boundary); and periodic boundary conditions to internal boundaries. The final step of preparing the model for computation mesh is built upon the conical quantum dot geometry with a specific mesh fineness.

4. Result and Discussion

In this work electron properties of cone-shaped quantum dots and the form of wave functions have been obtained by varying one particular dimension at a time while keeping other dimension constant. For example, for 10 nm height of the canonical quantum dot, the ground state (*l* =0) eigen energy has been computed for varying width (i.e. base radius) of the QD in the range 2 nm-20 nm. Figure 2(a) demonstrating that eigen-energy is inversely proportional to QD width.



(a) (b)

(c) (d)

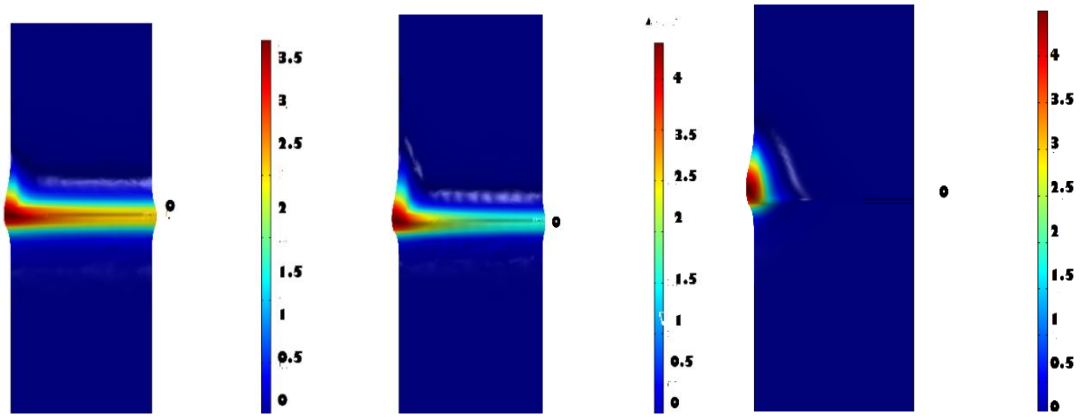
(e) (f)

Figure 2. (a) Variation of eigen energy (for ground state) as a function of radius of the conical quantum dot when other dimension and barrier potential are constant,

(b) Variation of eigen energy (for ground state) as a function of height of the conical quantum dot when other dimension and barrier potential constant,

(c) Variation of eigen energy for (for ground state) as a function of length of the wetting layer of the conical quantum dot when other dimension and barrier potential are constant,
(d) Variation of eigen energy for (for ground state) as a function of thickness of the wetting layer of the conical quantum dot when other dimension and barrier potential are constant,
(e) Variation of eigen energy for (for ground state) as a function of potential barrier of the conical quantum dot for h =10 , r = 4nm , L_w = 2nm, w = 25nm,
(f) Variation of eigen energy (l = 4) as a function of radius of the conical quantum dot when other dimension and barrier potential were constant

This result is compatible with previous computed eigenvalues reported by Gasser et al. (2000) and Benahmed et al. (2014). Furthermore, we observe that, different constant height (such as h = 20 nm and h = 30nm) produces a shifted curve of eigen-energy as a function of radius of QD. In fact, increase in the constant height demonstrates overall decrease in eigen-energy ($E_{h=30} < E_{h=20} < E_{h=10}$). In general, Figure 2(a) demonstrates that higher radius (>7nm) of the canonical quantum dot leads to lower energies. QD's height vs Energy graph (Figure 2(a)) demonstrates that ground state energy is inversely proportional to the QD's height, similar to radius vs energy graph in Figure 2(b). The eigen energy increases almost linearly with the potential barrier of GaAs as (Figure 2(c)) whereas it decreases almost linearly with wetting length (Figure 2(d)) and variation of eigen energy is given by Figure 2(e) and Figure 2(f). Finally, at the following, the visualization of numerical solution of $\chi(z, r)$ for (l = 0) from Comsol simulation are given by Figure 3(a), Figure 3(b) and Figure 3(d), respectively.



(a)

r = 4 nm,
h = 10 nm
L_w = 2nm
w = 25nm
V_{Ga} = 0.697

(b)

r = 4 nm,
h = 10 nm
L_w = 1.2 nm
w = 25nm
V_{Ga} = 1.097 eV

(c)

r = 4nm,
h = 10 nm
L_w = 0.5 nm
w = 25nm
V_{Ga} = 1.497

Figure 3. Visualization of numerical solution of $\chi(z, r)$ for (l = 0) from Comsol simulation. The color bar represents the value of $\chi(z, r)$

For eigen energy corresponding to l = 4 leads to higher energies and therefore represent less confined states. In fact, the excited state like l = 4 becomes confined if the V_{Ga} is increased from the usual 0.697 eV. If V_{Ga} is somehow increased the wave function is repelled additionally from the GaAs making it more likely that the wave function will reside inside the QD's radius and height.

5. Conclusion

We have by studied a single conical quantum InAs quantum dot on GaAs matrix where we used comsol software and presented the eigen-energy and wave function of InAs/GaAs semiconductor quantum dots. Our results obtained Simulation of conical InAs quantum dot shows that the energy associated with the ground level depends on the dimension of quantum dots such as radius, height as well as upon the dimension of the wetting layer. Furthermore, we found that the eigen-energies and functions are closely related to the GaAs potential.

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