The effect of Woods–Saxon potential on envelope function, intersubband dispersion curves and group velocity of InAs/GaAs quantum dots with wetting layer

Ali Khaledi-Nasab a,b,c,⁎, M. Sabaeian b, M. Sahrai c, V. Fallahi a, M. Mohammad-Rezaee b

⁎ Corresponding author at: University of Tabriz, Research Institute for Applied Physics and Astronomy, East Azerbaijan, Tabriz 51665163, Iran. Mobile: +98 916 992 6029.
E-mail address: Ali.khaledi1989@gmail.com (A. Khaledi-Nasab).

Abstract

In this study, one band Schrödinger equation for InAs/GaAs quantum dots coupled to their wetting layer was solved numerically by using a finite element method (FEM). We have carried out the conduction of the Woods–Saxon (WS) potential in the quantum dots (QDs) as well as a constant finite barrier between InAs quantum dot/wetting layer and GaAs matrix is considered for comparison. It is found by WS potential that the envelope functions never become completely localized inside the dot; therefore this delocalization leads to strong alternations in absorption and dispersion profiles which is not negligible. Also, it is found that group velocity is affected by the WS potential and reveals remarkable blue-shift in comparison to the constant finite potential.

Article info

Article history:
Received 16 August 2013
Received in revised form 27 January 2014
Accepted 28 January 2014
Available online 4 February 2014

Keywords:
InAs/GaAs quantum dot
Woods–Saxon potential
Wetting layer

1. Introduction

Over the last decade, progress in nanofabrication has been the center of attention due to its contribution in practical and conceptual areas such as physical, chemical and biological researches. Recent scientific reports have emphasized on the tremendous potentials of semiconductor nanoparticles, the so called quantum dots (QDs). In QDs, the dimensions of the confinement are less than de Broglie wavelength of carriers, or equivalently, the nanocrystal diameter has to be less than twice the Bohr radius excitons in the bulk materials [1]. Owning to marvelous characteristics, QDs have found numerous applications in a vast variety of fields such as cell biology (i.e. ability to be conjugated to proteins) [2–5], nanoscale emitters [6,7], QD solar...
cells [8,9], and quantum information processing [10,11]. Moreover, it is revealed that QDs are proper labels for single-molecule experiments in live cells [12]. Mainly, QD probes were promoted for their signature optical spectrum, the so-called wide absorbance, narrow, and symmetric emission with size-dependent peak positions [3]; moreover the size tunable spectra are other interesting features of QDs [9,10].

With respect to new advantages on nanotechnology, the self-assembled QDs can be formed during the epitaxial growth by using a vapor phase like molecular beam epitaxy (MBE) [13], metal organic chemical vapor deposition (MOVPE) [14], Stranski–Karstavan (SK) method [15], and chemical synthesis like colloidal chemistry or electrochemistry [16]. QDs can be synthesized at interface steps of thin quantum wells [17,18] or by self-assembly in the SK growth mode during MBE [19,20]. Afterward the process is being driven by the strain resulting from the smaller lattice parameter of the matrix (barrier) compared to that of the dots; for instance in our case it is 7% for InAs dots in GaAs. The InAs samples used for optical spectroscopy are then covered by the barrier material which is GaAs. In experiment the InAs dots contain a remarkable amount of fraction x of Ga, leading to the formation of In$_{1-x}$Ga$_x$As dots. The SK is applicable to a large variety of III–V and II–VI compounds [21]. A fascinating alternative for fabricating GaAs or InAs QDs is provided by a technique which is not strain driven, called molecular droplet epitaxy (MPE) [22]. The high optical quality of GaAs droplet dots owing to new achievements has allowed investigations of carrier and nuclear spin dynamics [23,24]. Because of the carrier confinement potentials which are between tens and hundreds of meV, the samples elaborated with the above techniques are suitable for various optical applications like optical spin manipulation [21].

The electronic and optical properties of QDs were illustrated by many authors in the literature both theoretically and experimentally. The effect of size and wetting layer on intersubband electronic and linear and nonlinear optical properties of InAs/GaAs QDs were investigated by numerous works both theoretically and experimentally [25–27]. Sandall et al. [28] took advantage of In(Ga)As QDs grown on a silicon substrate as a photo-detector. They measured dark currents in In(Ga)As on Si photodetectors three orders of magnitude lower than in Ge on Si. Terahertz emission with size-dependent peak positions [3]; moreover adjusting the WS potential parameters has significant impact on the optical properties [52]. The WS potential also is being applied to solve the Duffin–Kemmer–Petiau (DKP) equation which is the first order relativistic wave equation and represents spin-0 (scalar) and spin-1 (vectorial) particles [53].

Recent studies [54–57] have been carried out on the effects of WS potential in solving 1D position-dependent mass Schrödinger equation, which calculated the function, transmission and reflection coefficients. Costa et al. [58] simulated the spatial confinement; their methodology enables the study on a wide range of systems and confinement regimes by using variational methods to investigate WS potential in a QD/atom system by varying two parameters in the model potential. Investigation of two electrons confined in a QD with the WS potential by using a numerical diagonalization method of the Hamiltonian matrix within the effective mass framework was performed by Xie [54]. The scattering solutions of the 1D Schrödinger equation for WS potential within the position-dependent mass formalism were carried out by Arda et al. [57], and they obtained the function, transmission and reflection coefficients in terms of Heun’s function. Lu et al. [55] studied the effects of intense laser fields on intersubband nonlinear properties of donor impurities in a GaAs/AlGaAs QD with WS potential with effective mass approximation. They have showed the dependence of linear and third order susceptibility on laser intensity and a few values for dot radius, as well as barrier height and confinement barrier slope. Recently, Aytekin et al. [60] studied the effects of an applied electric field on the refractive index changes, optical rectification, and second and third harmonic generation in two dimensional QDs with WS potential in the framework of density matrix. It is demonstrated that optical rectification susceptibility is strongly dependent on the electric field. The applied electric field value also causes the second harmonic generation susceptibility to shift the peak position. Moreover, their calculations showed an increase in the third harmonic generation susceptibility by increasing the applied electric field.

WS potential has been used to explain the effect of interdiffusion on electronic states and light absorption [21–23].
excitonic states [24], and impurity states [25] in QDs, and electronic states of semiconductor super-lattices [26].

In this communication, the Schrödinger equation for dome-shaped InAs/GaAs QDs coupled to their wetting layer is solved numerically. Both constant and WS potentials have been investigated by performing a comparison. Using envelope function and density matrix approach, the linear susceptibility and group velocity of InAs/GaAs QDs will be explored.

2. Theory and Model

InAs QDs and wetting layer grown on GaAs matrices are the workhorse system for optical simulations. InAs grows on GaAs initially layer-by-layer, but after just 1.5 monolayers InAs QDs form and the QDs are subsequently capped by GaAs [59]. The envelope function in single QDs was calculated by solving Schrödinger equation within the effective mass approximation using a finite element method (FEM). Throughout this work, the InAs QDs are embedded on InAs wetting layer in a large GaAs matrix, as well as the GaAs cap covering the QDs according to the SEM images of real grown QDs [59]. In the following, a model procedure will be presented that allows us to determine energy eigenvalue and associated envelope function of any cylindrically symmetric QDs structure. The starting point is the 1-band Schrödinger equation in the effective mass approximation

\[
-\frac{\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \psi}{\partial z^2} \right) + V_{\psi}(\mathbf{x}) \psi = E \psi,
\]

where \( \hbar \) is the well-known Planck’s constant, \( m^* \) is the electron effective mass, \( \psi(\mathbf{x}) \) is the electronic envelope function, \( E \) is the eigenenergy, and \( V_{\psi}(\mathbf{x}) \) is the potential energy. Using cylindrical symmetry for dome-shaped QD, the envelope function can be separated. Thus the envelope function will consist of a part with coordinate dependence \( r \) and \( z \) in addition to another angular-dependent \( \phi \) unit. In cylindrical coordinates \( \mathbf{X} = (z, r, \phi) \), \( V_{\psi}(\mathbf{x}) = V_{\psi}(z, r) \) where \( z \) and \( r \) are the axial and radial coordinates, and \( \phi \) is the azimuthal angle ranging from 0 to \( 2\pi \). Cylindrical symmetry allows us to use the separation of variables technique as follows for the envelope function:

\[
\psi(\mathbf{x}) = \chi(z, r) \phi(\phi). \tag{2}
\]

After some mathematical treatment Eq. (1) will be reformulated as

\[
\frac{-\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \phi}{\partial z^2} \right) + \frac{\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \phi}{\partial r^2} \right) \phi + \frac{\hbar^2}{2m^*} \frac{\partial^2 \phi}{\partial \phi^2} + V_{\psi}(z, r) \chi(z, r) \phi = E \chi(z, r) \phi \tag{3}
\]

Here we divide Eq. (3) by \( \phi \chi(z, r)/m^* r^2 \); therefore Eq. (3) is rearranged as

\[
\frac{m^* r^2}{\chi(z, r)} \left(\frac{-\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \phi}{\partial z^2} \right) + \frac{\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \phi}{\partial r^2} \right) \phi \right) + V_{\psi}(z, r) - E = \frac{-\hbar^2}{2m^*} \frac{\partial^2 \phi}{\partial \phi^2} \phi = -\frac{\hbar^2}{2} \frac{\partial^2 \phi}{\partial \phi^2} \tag{4}
\]

It is straightforward to say that the solution of Eq. (4) could be proposed as

\[
\phi(\phi) = e^{il\phi}, \tag{5}
\]

where \( l \) is a separation constant. The envelope function must be single-valued under \( 2\pi \) rotation. In our modeling \( l \) can takes values of \( l = 0, \pm 1, \pm 2, \ldots \):

\[
-\frac{\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \chi}{\partial z^2} \right) + \frac{\hbar^2}{2m^*} \left(\frac{1}{m^*} \frac{\partial^2 \chi}{\partial r^2} \right) + \frac{\hbar^2}{2m^* r^2} + V_{\psi}(z, r) \chi = E \chi \tag{6}
\]

Due to existence of two different materials in the Schrödinger equation (in simplified or original form), there are discontinuous coefficients under spatial derivative operators; hence physically, in the modeling procedure the following boundary condition must be satisfied:

\[
\psi \in C(Q), \quad \left(\frac{-\hbar^2}{m^*} \frac{\partial \psi(z, r)}{\partial r} \right)_{\text{QD/wetting layer}} = \left. \frac{-\hbar^2}{m^*} \frac{\partial \psi(z, r)}{\partial r} \right|_{\text{QD/wetting layer}} \tag{7}
\]

where \( C \) is the class of continuous function, \( Q \) is the spatial \((z, r)\) domain of interest, and \( n \) is the outward normal vector. The envelope function solution for a stepwise constant effective mass potential is given by

\[
\psi_{nl}(z, r, \phi) = A_{nl} Z_{nk}(2J_{nl} z) e^{l\phi} \tag{8}
\]

\( Z_{nk} \) is acquired from the solution of

\[
\frac{\partial}{\partial \phi} \left( \frac{1}{m^*_k} \frac{\partial Z_{nk}}{\partial \phi} \right) + \frac{2}{\hbar^2} \left( E - V(z) - \frac{\hbar^2 k^2}{2m^*_k(z)} \right) Z_{nk} = 0 \tag{9}
\]

\( \psi_{nl} \) must satisfy the following condition:

\[
\frac{\partial \psi_{nl}(z, r, \phi)}{\partial \phi} \bigg|_{r=r_{in}} - \frac{\partial \psi_{nl}(z, r, \phi)}{\partial \phi} \bigg|_{r=r_{out}} = 0, \quad \text{if} \quad J_{nl}(r_{in}) \neq 0 \tag{10}
\]

Because

\[
J_{n-1}(y) - J_{n+1}(y) = \frac{2}{\hbar^2} \frac{dJ_{nl}(y)}{dy} \tag{11}
\]

As it is obvious, the 3D Schrödinger equation was simplified to 2D equation. In this regard, we considered an electron confined in a two-dimensional QD and replaced \( V(r) \) by \( V_{\text{WS}}(r) \) as

[diagram of a 3D structure with labeled parts]
WS-potential and given by
\[
V_{WS}(r) = \frac{V_0}{1+\exp(R_0-r/\gamma)}
\] (12)

where \(V_0\) is the potential depth with specific value for each material, \(R_0\) is the radius of QD, and \(\gamma\) denotes the confinement barrier slope [60].

2.1. Boundary condition

In order to present more realistic solution, appropriate boundary conditions must be taken under consideration. Fig. 1 shows the geometry, numbered boundaries as well as the dimensions of dome-shaped InAs/GaAs QDs.

The confined electronic states are the main interest; hence, the Dirichlet boundary condition \((\psi = 0)\) is imposed for boundaries 1 and 3. In order to satisfy the continuity condition \((-1/m_r \nabla \psi \mid_{x_i} = (\nabla \psi \mid_{x_i})_{GaAs}\) (Eq. (8)) is applied for boundaries 5, 6, 7, and 8.

With attention to the symmetry of the problem the computational area could be divided into two equal parts by line 2; therefore, boundary 2 will be replaced by 2' (dashed-dotted vertical line in Fig. 1). It is obvious for \(l \geq 1\) the Dirichlet boundary condition must be considered, and the reason is to guarantee that the expression \(\hbar^2/2m_r \frac{\partial^2 \psi}{\partial x_i^2}\) will not diverge at \(r = 0\). On the other hand, in special case, when \(l = 0\), to ensure the presence of \(\nabla \psi\) at \(r = 0\), the Neumann boundary condition must be imposed. In our computational approach we will consider \(l = 1\); hence we will apply the Dirichlet boundary condition. For relatively large values of \(r\), the envelope function for InAs QDs/wetting layer and GaAs matrices, asymptotically approaches, either, the envelope function for the pure wetting layer problem or, zero if the state is true QD state; consequently Eq. (10) could be considered for boundary number 4. Finally based on mentioned symmetry we only take half of Fig. 1 under consideration; in the other words Fig. 1 is divided by 2 and the simulation carried out for this geometry.

Using a density matrix approach and perturbation theory, the linear susceptibility for two-level system will be derived as [25,61]
\[
\chi^{(1)}(\omega) = \frac{N}{\epsilon_0 \hbar} \left\{ M_{21}^2 \left[ \frac{1}{\omega_{21} - \omega - i\gamma_{21}} + \frac{1}{\omega_{21} + \omega + i\gamma_{21}} \right] + M_{22}^2 \left[ \frac{1}{\omega_{22} - \omega - i\gamma_{22}} + \frac{1}{\omega_{22} + \omega + i\gamma_{22}} \right] \right\}
\] (13)

With respect to the probe frequency, the derivative of the dispersion has a major role in calculation of the group velocity. For sufficiently short propagation distances, pulse distortion is not too severe, and the motion of the pulse can be described by \(v_g\) given by \(v_g = c/n_g\), where \(n_g = n + \omega \frac{dn}{d\omega}\). Therefore, the group
The velocity $v_g$ is expressed as [61–63]

$$v_g = \frac{C}{1 + \chi(\omega) + \alpha \frac{d\chi(\omega)}{d\omega}} \quad (14)$$

As Eq. (6) implies, for a negligible real part of susceptibility, the group velocity can be significantly reduced via a steep positive dispersion [62,64,65]. Strong negative dispersion, on the other hand, can lead to an increase in the group velocity and even a negative group velocity [66].

In real experiments, it is easier to measure the delay time which is given by

$$\Delta T = \frac{L}{v_g} = \frac{L}{c} (n_f - 1) \frac{C}{L} \quad (15)$$

where $L$ is the length of optical medium and $C$ is speed of light. We will work with $n_f - 1$ which has direct correspondence to delay time.

### 3. Result and discussion

In order to carry out the numerical solution, $V_0$ was set to 0 and 0.697 eV for InAs and GaAs, respectively, and the electron effective mass was set to 0.023 $m_e$ for InAs and 0.069 $m_e$ for GaAs [67]. In WS potential the confinement barrier slope $\gamma$ is set to 30 Å [55]. In this study, the values of $R_0 = 8, 13, 16$ and 20 nm on WS potential are used. To obtain the numerical results for $\chi(\omega)$ and group index, the following parameters have been used: carrier density $N = 3 \times 10^{22}$ atoms/cm$^2$ [25], vacuum permittivity $\varepsilon_0 = 8.85 \times 10^{-12}$, relaxation rate $\gamma_{21} = 5 \times 10^{12}$ s$^{-1}$ [25], speed of light in vacuum $c = 3 \times 10^8$, transition frequencies $\hbar \omega_{21} = E_2 - E_1$ (as output of numerical simulation taken from Table 1), and transition dipole moments $M_{21} = \langle \psi_1 \mid e_r | \psi_1 \rangle$ which is calculated by using numerical envelope function and homemade codes of the Simpson integration method written in MATLAB.

Table 1 presents the result of energy eigenvalues, dipole moments for both constant potential (CP) and WS potential (WSP). These data obtained directly from the numerical treatment for InAs/GaAs QDs by FEM solution for simplified form of Schrödinger equation (Eq. (6)). According to Table 1 the energy eigenvalues for ground and first excited states take relatively smaller values for WS potential in comparison to constant potential, while the transition dipole moment gets greater absolute values.

Fig. 2 illustrates the ground state envelope function. Fig. 2(a) and (b) shows the envelope function with constant potential ($V(r) = V_0$) and Fig. 2(c) and (d) shows the envelope function with WS potential ($V(r) = V_{WS}(r)$) for $R = 8$ and 13 nm, respectively. The envelope function for ground state moves slightly toward the GaAs matrix for WS potential, while in the upper radii, the amount of leakage envelope function stays relatively the same as a constant potential. In the better words, in the ground state for both WS potential and constant potential at $R = 8$ nm, we have shared quantum well (wetting layer) and QD states; nevertheless for $R = 13$ nm the only pure QD state remains on the envelope function profile. The effect of WS potential is small, leading the envelope function to take slightly bigger peak than constant potential.

Fig. 3 shows the distribution of first excited state envelope function for the constant potential (Fig. 3(a)–(d)) and WS potential (Fig. 3(e)–(h)). Fig. 3(a) shows that for $R = 8$ nm the envelope

![Fig. 3](image-url)
function is distributed in wetting layer and QD. In the other words the envelope function consists of a quantum well state, which is a valley, located wetting layer, and a confined QD state which is a peak on QD region. According to Fig. 3(b) at $R=13$ nm the QD state changes its phase from peak to valley, also the quantum well state moves toward QD region and one can say that we have shared state between QD and wetting layer. As Fig. 3(c) and (d) shows the envelope function leaves the wetting layer and it is localized inside the dot for $R=16$ and 20 nm. The phase of both lobes reverses to become peak for the top lobe and valley for bottom one. According to Fig. 3(e) with WS potential, the distribution of envelope function is almost the same as constant potential; however, the first lobe shows a leakage to GaAs matrix albeit it is very slight and negligible. According to Fig. 3(f), at $R=13$ nm both lobes are inside the dot with considerable tail-shaped leakage toward the GaAs matrix. Moreover in comparison to the same dimension with constant potential, first of all there is no quantum well state but only couple of QD states, secondly, the top and bottom lobes of envelope function are peak and valley respectively while they were vice versa for constant potential, and finally the envelope function is not entirely confined inside the QD region owing to leakage to matrixes. Fig. 3(g) and (h) explains that for $R=16$ and 20 nm by increasing the radius of QD, the leakage of envelope function leakage becomes stronger and namely the delocalization increases dramatically. While in constant potential upper radii correspond to more localization of envelope function inside the QD. Fig. 3(g) indicates that the overall profile of envelope wave function is similar to its mutual dimension with constant potential but with significant amount of leakage. Furthermore as Fig. 3(h) shows, the envelope function again experiences sudden changes in the location of peaks (red area) and valley (blue area) in comparison to its same radius (Fig. 3(d)) constant potential. In other words in constant potential the red peak and blue valley were localized at the top and bottom of QD respectively; nevertheless it would be vice versa for the same QD with WS potential.

Fig. 4 shows both real part and imaginary part of linear susceptibility versus the probe field frequency for (a) $R=8$ nm and (b) $R=13$ nm, with constant and WS potential. According to Fig. 4(a), the absorption and dispersion for constant potential reveal the bigger peaks in comparison to WS potential. For $R=8$ nm around $10 \times 10^{12}$ Hz movement on the position of the peaks occurs. The amplitude of the peaks is relatively 0.005 smaller in WS potential. Fig. 4(b) shows a big shift in amplitude of the peaks between constant and WS potentials. As it has been clearly observed in Fig. 3(a) and (f), at $R=13$ nm for constant potential, the envelope function has shared states in QD and wetting layer, while it has couple if QD states with leakage in WS potential. At $R=13$ nm the peaks take relatively remarkable reduction when overall profile of linear susceptibility appears. The amplitude of the peaks becomes around 1/4 of its value on constant potential, and also around $20 \times 10^{12}$ Hz movement in the position of the peaks shows up.

Fig. 5 shows the absorption and dispersion profiles for (a) $R=16$ nm and (b) $R=20$ nm. It is obvious that the dissimilarity between the WS and constant potentials is relatively less than $R=13$ nm. Fig. 5 indicates that by rising the dimension of QD from 16 nm (Fig. 5(a)) to 20 nm (Fig. 5(b)) the whole profile of linear susceptibility moves toward lower frequencies. The resonance frequency of the peaks for WS is $40 \times 10^{12}$ Hz bigger than constant potential. Indeed in both constant and WS potentials, the peak takes higher absolute values by increasing the radius.

One of the important parameter which has direct association with linear susceptibility is group velocity and its mutual parameter group index. Fig. 6 depicts a comparison between group indices for $R=8$ nm. Both curves for WS and constant potentials are subjected to negative delay time and consequently superluminal light propagation. Obviously, the peak of constant potential occurs in higher frequencies than that of WS potential. The movement is about $10 \times 10^{12}$ Hz toward higher frequencies.

Fig. 7 illustrates the group velocity for (a) constant and (b) WS potentials for $R=13$, 16, and 20 nm. According to Fig. 7(a) with increasing the dot radius, blue-shift takes place. A blue-shift is around $40 \times 10^{12}$ Hz between the resonance peaks. On the other hand, the amplitude of superluminal peaks tends to have slight smaller values by size escalation.

Fig. 7(b) shows that for $R=13$ nm, the superluminal peak takes relatively half of the amplitude value at $25 \times 10^{12}$ Hz higher frequency of its corresponding peak on constant potential. Surprisingly at $R=16$ nm and $R=20$ nm the group index takes almost the same values but in upper frequencies for WS potential. Moreover in WS potential the amplitude of group index is the same for $R=16$ nm and $R=20$ nm, with red-shift for upper radii.

4. Conclusion

In this work, the effects of Wood–Saxon (WS) potential on dispersion curves and group velocity of a dome-shaped InAs/GaAs QD with its wetting layer were investigated. The single band
Schrodinger equation in effective mass approximation was used to explore the envelope function and energy eigenvalues. A finite element method (FEM) was used to solve Schrodinger equation. It is found that WS potential causes a delocalization in the envelope function for radius upper than $R = 13$ nm. In constant potential, the envelope function is completely inside the wetting layer and QD region; while by employing the WS potential, tail-shaped leakage of envelope function appears. This leakage significantly appears in the first excited state. It is also concluded that the localization of envelope function on constant potential leads to higher absolute values of absorption/dispersion curves in all studied models. For WS potential, the peak occurs at higher frequencies than those of constant potential. Consequently, the WS potential causes blue-shift in the whole profile of linear susceptibility and group index. In addition to blue-shift on group velocity, it is found that for $R = 13$ nm, the negative superluminal peaks take relatively smaller values than those in WS potential. Having reduced absorption is beneficial in slow/fast light applications. The overall results of this study show that the WS potential can be employed to reduce the absolute values of the peaks. Moreover engineering the optical properties of QDs is possible by employing the WS potential.

Acknowledgment

The first author would like to appreciate the helpful discussion of Mr. Mehdi Kashisaz (Department of Chemical & Process
Engineering, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Malaysia) in preparing the manuscript of this paper.

References


