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Computations of the optical transitions and absorption spectra in a set of realistic, elongated InAs/GaAs quantum boxes having a Gaussian distribution

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InAs/GaAs quantum dots (QDs) grown by various methods do not have the same dimensions in the three axes. This paper reports on expressions for computations of the optical transitions and absorption spectra of InAs/GaAs QDs that have a square base and the variation of the height is Gaussian. The dots were considered to be elongated quantum boxes with square bases having finite potentials at the boundaries. The results are in excellent agreement with reported experimental data of photoluminescence and absorption. The expressions could be successfully applied to short quantum wires. © *2011 American Institute of Physics*. [doi:10.1063/1.3549151]

I. INTRODUCTION

Quantum dots (QDs) of III–V compound semiconductors, also called quasizero-dimensional quantum boxes (QBs), are being progressively used in the fabrication of optoelectronic devices, such as lasers and detectors, for higher efficiencies and lower threshold currents.[1–4] Recent advances in material growth technologies aid the successful growth of self-organized QDs.[5–9] The absorption spectra of ideal QDs are expected to be a series of δ-functionlike discrete lines due to the nature of the density of states. For optimization of the device performance the shapes of QDs and their distribution should be precisely known. The electronic band structures from which transitions take place depend on the shapes and sizes of the dots, whereas the widths of absorption or emission spectra depend on the nature of the distribution.

Reports on QBs having infinite barrier are available in the literature.[10,11] Recently, Kumar and Biswas[12] presented results of realistic $In_{0.66}Ga_{0.33}As/GaAs$ and $In_{0.7}Ga_{0.3}N/GaN$ QBs having finite barrier. The boxes were considered to be of the same dimension on the three axes.

As reported, QDs grown by various methods do not have the same dimensions in the three axes. For strained QDs the length is much larger than the height and for relaxed QDs the height is much greater than the length.[13] In these cases, the symmetric cubic QB approximation may not lead to the best insights about the QDs. For the InAs/GaAs system, the InAs dots have a typical base size of 10–25 nm and height of 2–10 nm,[14–18] the actual size being dependent upon the growth conditions. These dimensions are small enough that strong quantum effects are observed.

Since the realistic dots are not symmetric, this paper reports an expression for the computation of the absorption spectra of InAs/GaAs QDs that have a square base and the variation of the height is Gaussian.

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The absorption spectra from sets of QDs of various heights and bases have been studied. We have studied different sets of QDs when the volume remains constant and when the base remain constant for various values of the relative standard deviation of the dots. The height has a Gaussian distribution about the average dot height.

All the necessary formulations are presented and have been compared with experimental optical data of QDs. It is seen that the theoretical computations are in excellent agreement with the experimental data.

II. THEORETICAL MODEL

For a 3D rectangular infinite well, the potential is zero inside the box of side length L_i (where $i = 1, 2, 3$) and infinite outside the box. In such a case, the normalized wave function becomes

$$\psi(x) = \sqrt{\frac{8}{L_1 L_2 L_3}} \sin(k_1 x_1) \sin(k_2 x_2) \sin(k_3 x_3) \qquad (1)$$

where $k_j = \pi n_j / L_i$ ($n_j = \pm 1, \pm 2, \ldots$) is the wave vector along x_j direction. For a rectangular box with square base, we consider base as $L_1 = L_2 = L_b$ and height as $L_3 = L$, Equation (1) reduces to

$$\psi(x) = \sqrt{\frac{8}{L_b^2 L}} \sin(k_1 x_1) \sin(k_2 x_2) \sin(k_3 x_3). \qquad (2)$$

The confinement energies of the electron, $E_e(n^2)$, and that of the hole, $E_h(n^2)$ (in units of $\hbar^2/mL^2$) for a finite well can be approximated as[19]

$$E_e(n^2) = \frac{2P_e^2}{(P_e+1)^2} \left[\left(\frac{n\pi}{2}\right)^2 - \frac{1}{3(P_e+1)^3} \left(\frac{n\pi}{2}\right)^4 - \frac{27P_e - 8}{180(P_e+1)^6} \left(\frac{n\pi}{2}\right)^6 \right], \qquad (3)$$

$$E_h(n^2) = \frac{2P_h^2}{(P_h+1)^2}\left[\left(\frac{n\pi}{2}\right)^2 - \frac{1}{3(P_h+1)^3}\left(\frac{n\pi}{2}\right)^4 - \frac{27P_h-8}{180(P_h+1)^6}\left(\frac{n\pi}{2}\right)^6\right], \quad (4)$$

where P_e and P_h are the well strength parameters defined as $P_e = (\sqrt{2m_0 m_e^* V_0}/\hbar)L/2$ and $P_h = (\sqrt{2m_0 m_h^* V_0}/\hbar)L/2$, where V_0 is the height of the well (conduction/valance band) and L is the well width. m_0, m_e^*, and m_h* are the rest mass and effective masses of electrons and holes, respectively.

The resonance energy of a realistic QD, having finite potential barriers, is defined as the photon energy needed for the creation of electron-hole pair. This may be represented as

$$\hbar\omega_{\text{real}} = E_g + E_e(l^2, m^2, n^2) + E_h(l^2, m^2, n^2), \quad (5)$$

where E_g is the bandgap of the semiconductor material and l, m, n are integers having their usual meanings.

The optical absorption constant is defined as the ratio of the energy removed from the incident beam per unit time and unit volume to the incident flux.[10] The energy flux is interpreted as the product of the energy density and the speed of flow. Using this definition, the optical absorption coefficient of a realistic rectangular QD with height L and base length L_b is calculated as

$$\alpha_{\text{real}} = \frac{A_{\text{real}}}{L_b^2 L}\sum_{(l^2,m^2,n^2)} g(l^2,m^2,n^2) \times \delta[\hbar\omega_{\text{real}} - \{E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\}]. \quad (6)$$

The aspect ratio is defined as $\gamma = \text{Height}(L)/\text{Base}(L_b)$; thus Eq. (6) takes the form

$$\alpha_{\text{real}} = \frac{\gamma^2 A_{\text{real}}}{L^3}\sum_{(l^2,m^2,n^2)} g(l^2,m^2,n^2)\delta[\hbar\omega_{\text{real}} - \{E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\}], \quad (7)$$

where $g\ (l^2, m^2, n^2)$ is the degeneracy of the energy level determined by (l, m, n). A_{real} is a constant in terms of the momentum matrix P_n so that[10]

$$A_{\text{real}} = \frac{2\pi e^2 |P_n|^2}{m_0^2 \varepsilon_r^{1/2} \varepsilon_0 c\, \omega_{\text{real}}}, \quad (8)$$

where e is the fundamental charge, ε_0 is the permittivity of free space, ε_r the host material, c is the speed of light and ω_{real} is the photon frequency. The interband absorption of a QD is characterized by a series of discrete lines at photon energies given by Eq. (5). As mentioned by Wu *et al.*, the absorption spectra is the superimposition of the contribution from each individual dot, the overall behavior is modeled by considering a Gaussian distribution of the dot height L, which can be represented as[10]:

$$P(L) = \left(\frac{1}{D}\right)\left(\frac{1}{\sqrt{2\pi}}\right)\exp\left[-\frac{(L-L_0)^2}{2D^2}\right] \quad (9)$$

where L_0 is the average dot height of the system and D is the standard deviation. Let ξ be the relative standard deviation of the dot given by

$$\xi = D/L_0 \quad (10)$$

$$\therefore P(L) = \frac{1}{\xi L_0}\cdot\frac{1}{\sqrt{2\pi}}\exp\left[-\left(\frac{L}{L_0}-1\right)^2 / 2\xi^2\right]. \quad (11)$$

Combining Eqs. (7) and (11), the total absorption spectra of an ideal QD system due to the nonuniform dot size distribution is represented as

$$\alpha_{\text{real}} = \frac{\gamma^2 A_{\text{real}}}{\xi L_0}\cdot\frac{1}{\sqrt{2\pi}}\sum_{(l^2,m^2,n^2)} g(l^2,m^2,n^2) \times \int_0^\infty \frac{1}{L^3} e^{-(\frac{L}{L_0}-1)^2/2\xi^2} \times \delta[\hbar\omega_{\text{real}} - (E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\}]dL. \quad (12)$$

We know from the properties of Dirac delta function

$$\int_{-a}^{b} H(x)\delta(g(x))dx = \sum_{i=1}^{N}\frac{H(x_i)}{g'(x_i)},$$

where x_i are the solutions to $g(x) = 0$, in the range $a < x < b$. Using this relation Eq. (12) becomes

$$\alpha_{\text{real}} = \frac{\gamma^2 A_{\text{real}}}{\xi L_0}\cdot\frac{1}{\sqrt{2\pi}}\sum_{(l^2,m^2,n^2)} g(l^2,m^2,n^2) \times \sum_{i=1}^{N}\frac{(1/L_r^3)e^{-[(L_r/L_0)-1]^2/2\xi^2}}{|[\hbar\omega_{\text{real}} - (E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\}]'|_{L=L_r}}. \quad (13)$$

where L_r is the root of the function and 'N' denotes the number of roots of the function

$$g(x) = \hbar\omega_{\text{real}} - \{E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\} = 0. \quad (14)$$

We define a dimensionless term

$$\beta_{\text{real}} = \frac{A_{\text{real}}}{\sqrt{2\pi}} \times \frac{\mu}{\pi^2\hbar^2} \quad (15)$$

where μ is reduced effective mass.

Thus the relative absorption coefficient is defined as

$$\frac{\alpha_{\text{real}}}{\beta_{\text{real}}} = \frac{\gamma^2}{\xi} \times \frac{\pi^2\hbar^2}{\mu L_0}\sum_{(l^2,m^2,n^2)} g(l^2,m^2,n^2) \times \sum_{i=1}^{N}\frac{(1/L_r^3)e^{-[(L_r/L_0)-1]^2/2\xi^2}}{|[\hbar\omega_{\text{real}} - (E_g + E_e(l^2,m^2,n^2) + E_h(l^2,m^2,n^2)\}]'|_{L=L_r}} \quad (16)$$

III. RESULTS AND DISCUSSION

The results of computations of the absorption spectra of InAs/GaAs QD systems are shown in Figs. 1–3. The electron effective mass was taken to be $0.027m_0$ and for holes $0.4m_0$ for InAs. The band-offset ratio was considered to be 60:40.[20] For 3D rectangular QDs, the heights of wells in the conduction and valance band in the three directions are 0.57 and 0.38 eV, respectively.

The horizontal axis is the photon energy corresponding to real dots defined by Eq. (5) and the vertical axis is the relative absorption of the realistic dots defined as$(\alpha_{real}/\beta_{real})$ according to Eq. (16).

Figure 1 shows the plot of the lowest absorption peak $(l, m, n) = (1, 1, 1)$ for three sets of the InAs/GaAs QD system of same volume with $\xi = 0.05$.In these computations the volume of the QBs are kept constant, equal to the volume of a symmetric cubic QB of average dot height of 8 nm having a Gaussian distribution. The other two sets studied are rectangular QBs of the same volume having average heights of 4 and 12 nm, respectively. It is observed from Fig. 1 that the absorption peaks for these two rectangular QBs are blueshifted with the changing aspect ratio. The increase in the intensity with decreasing average dot height is justified from Eq. (16). It is shown that the relative optical absorption coefficient depends inversely on the average dot height.

Figure 2 shows the lowest four available absorption peaks for InAs/GaAs QD system with $\xi = 0.02$, 0.05, 0.10 for average dot height of the QD considered to be 8 nm and the aspect ratio: $\gamma = 0.67$. From the trend of the curves it is observed that as the value of ξ decreases the linewidth of the absorption spectra decreases. In case of homogeneous growth, with ξ extremely small the spectra will be a series of Dirac delta functions.

In Fig. 3 the height of the QD varies for a constant base length $L_b = 8$ nm and constant value of $\xi = 0.1$. It is observed from Fig. 3 that as the height of the dot increases the number

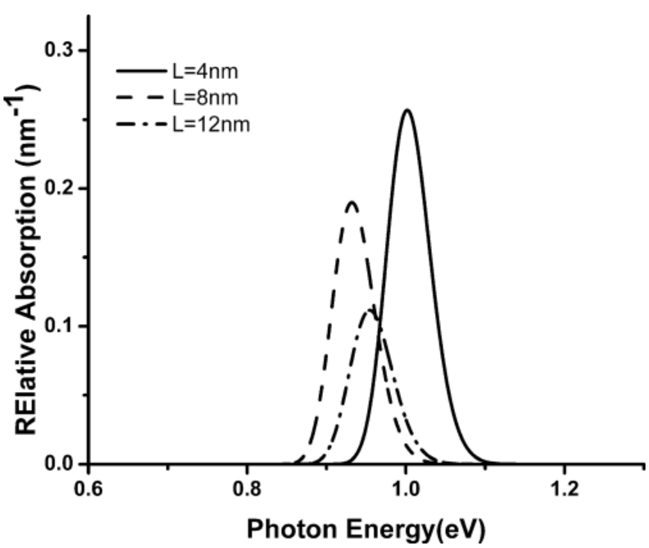

FIG. 1. Absorption spectra of the lowest transition of the InAs/GaAs QD system of similar volume of different average dot height having a Gaussian distribution.The photon energy of the real dots is defined by Eq. (5) and relative absorption coefficient is defined as $(\alpha_{real}/\beta_{real})$ from Eq. (16).

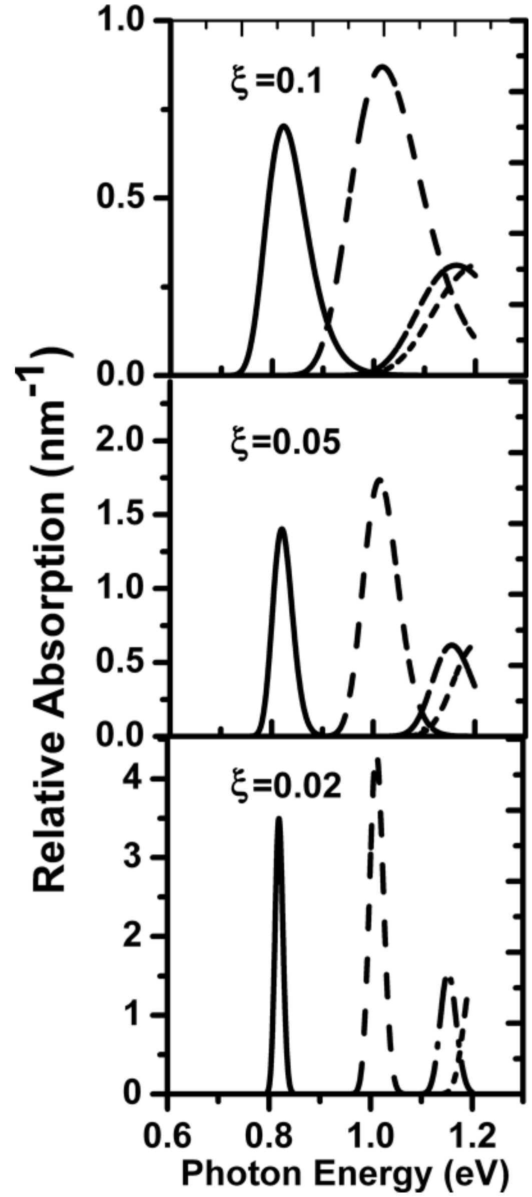

FIG. 2. Absorption spectra of lowest four transitions of the InAs/GaAs QDs of base length 12 nm and average dot height 8 nm for different relative standard deviation ξ.

of higher order transitions increases and the peak energies undergo a redshift.

To establish the reliability of the formulations and computations we compared the theoretically obtained data with the reported experimental values for a set of InAs/GaAs QD systems. Available photoluminescence (PL) and absorption data were matched assuming negligible Stokes shift in InAs/GaAs QD system.[21] As reported by Cusack *et al.*,[22] the optical emission from the ground state has energy around 1.1 eV. The present theoretical model shows energy at 1.075 eV from InAs/GaAs QD of height 2.5 nm and aspect ratio 4 [considering $me^* = 0.04m_0$ and $mh^* = 0.59m_0$ (Ref. 22)]. This is in close agreement with the experimental optical data of Marzin *et al.*[15] and the ground state PL spectra of 1 eV recently reported by Sun *et al.*,[23] the latter being within ~2.6% error of the value of 0.974 eV calculated in the present paper for the same dot dimensions and $\xi = 0.1$.

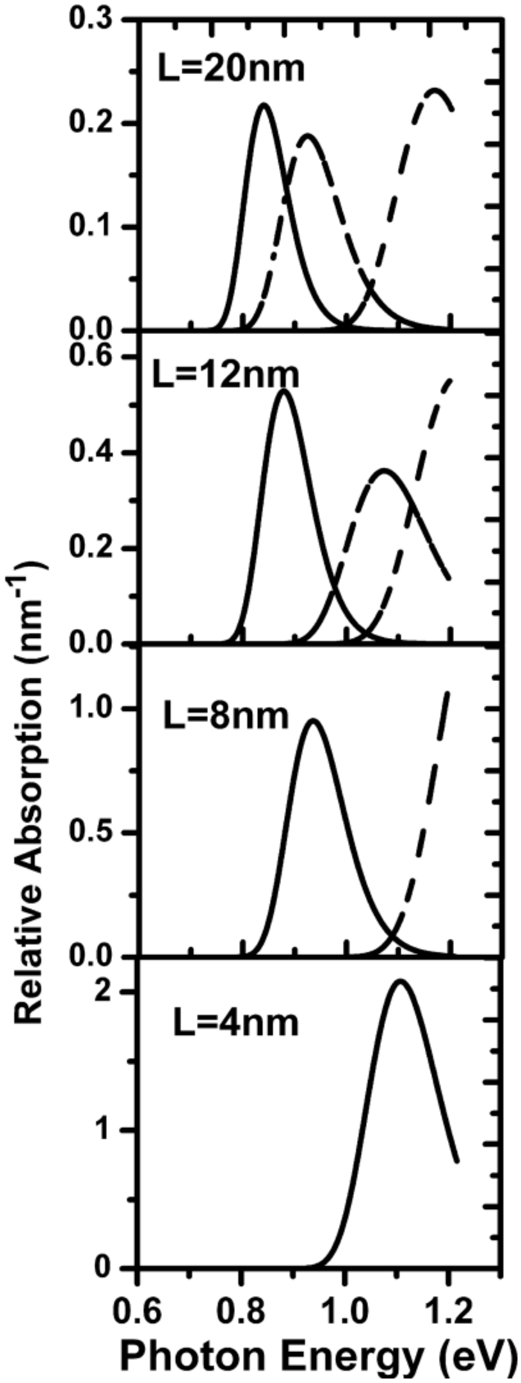

FIG. 3. Absorption spectra of the lowest four transitions of the InAs/GaAs QD system with constant base at 8 nm and varying the average dot height.

We reported the experimental PL data for InAs/GaAs QD system of average dot height of 3 to 4 nm around 1.21 eV when the excitation was 1.4 eV.[24] From this theoretical model for a set of QBs having a base of 5 nm and average height 3.5 nm with a Gaussian distribution and $\xi = 0.02$ [considering $me^* = 0.04m_0$ and $mh^* = 0.59m_0$ (Ref. 22)], the peak was found at 1.19 eV as shown in Figure 4. The mismatch with the experiment is only 2%. It is evident that the dots of larger dimensions within a small ξ were only excited. It is worth noting that the curves are truncated on the higher energy side.

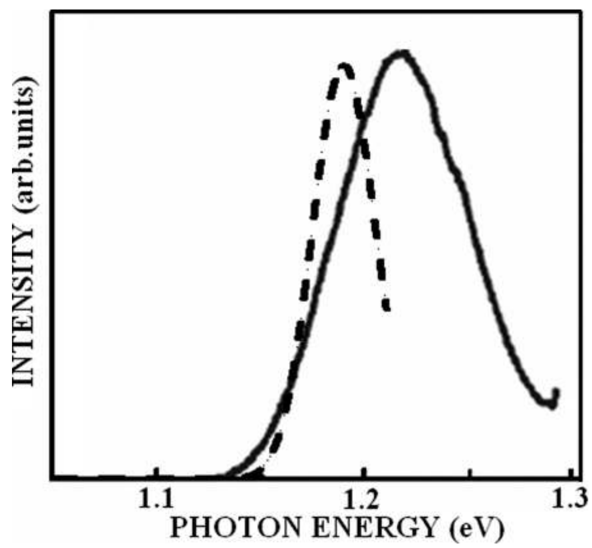

FIG. 4. Available lowest transition of InAs/GaAs QD system of average dot height 3.5 nm and base length 5 nm.The dotted line represents the theoretical and solid line represents the experimental curves.

This model has been applied to short quantum wires.[25] Figure 5 shows experimental and theoretical results of the separation between the ground and first excited state of a set of short quantum wires. The results of the present theoretical computations on wires of similar dimensions matched the experimental results closely.

IV. SUMMARY

To summarize, the paper reports a model for computations of optical transitions and absorption spectra of InAs/GaAs QDs which have square bases and the variation of the height is Gaussian. For proper insight into the properties of the QDs the model of elongated rectangular QBs with finite potentials at boundaries seems to be more appropriate. The

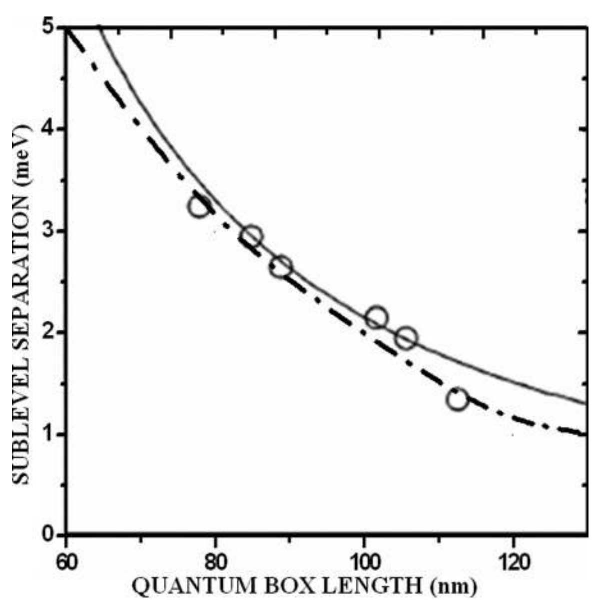

FIG. 5. Separation in energy between the ground state and first excited state as a function of quantum box base length. The experimental data (obtained from Ref. 21) are given by the circles.

calculation in this paper shows that the model may be applied successfully to short quantum wires.

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