Chapter 4

Effects of a Gaussian Size Distribution on the Absorption Spectra of III-V Semiconductor Quantum Dots
Chapter 4

EFFECTS OF A GAUSSIAN SIZE DISTRIBUTION ON THE ABSORPTION SPECTRA OF III-V SEMICONDUCTOR QUANTUM DOTS

4.1 Introduction

Quantum dots (QDs), also called zero-dimensional quantum boxes (QB), of III-V compound semiconductors are being progressively used in the fabrication of optoelectronic devices, such as lasers and detectors, for higher efficiencies and lower threshold currents, taking advantage of the modified density of states in particular. The absorption spectra of QDs are expected to be a series of $\delta$-function-like discrete lines due to the nature of the density of states. There have been constant efforts to utilize QDs and QD systems for infrared detectors [1–6]. A self-assembled technique using the Stranski-Krastanow growth mode [2] has proven to be an excellent method for fabricating QDs and QD systems. The dot sizes in a QD system are randomly distributed and, consequently, their energy states are also randomly distributed.
4.1.1 Optical absorption in semiconductors

Interaction of electrons and photons in semiconductors forms the basis of technologies such as optical communications, displays and optical memories. In the quantum-mechanical theory, each mode of electromagnetic radiation of frequency $\omega/2\pi$ and wave number $\kappa$ is characterized by particles called photons, having energy $h\omega$ and momentum $h\kappa$. A semiconductor sample kept at a finite temperature $T$, permeated by electromagnetic radiation of all frequencies. Electrons interact with photons associated with this radiation all the time. In some interactions photons are absorbed by the atoms and in others photons are emitted [7]. Through such interactions, a statistical equilibrium is established, in which the photon number associated with a mode per unit volume of phase space becomes

$$n_{p0} = \frac{1}{\exp(h\omega/k_BT) - 1} \quad (4.1)$$

where $k_B$ is the Boltzmann constant. When external radiation is incident on the sample, the photon number increases and the rate of absorption and emission of photons change. A new steady state condition is established in which the number of photons absorbed is larger than the number emitted. Let $-\frac{dn_p}{dt}$ represent the rate of the absorption of the photon. The absorption coefficient, defined as the ratio of the power absorbed per unit length of the sample and the incident power, is then given by

$$\alpha = \frac{-\left(\frac{dn_p}{dt}\right)}{(n_p - n_{p0})} \left(\frac{c}{n_r}\right)^{-1} \quad (4.2)$$

where $c$ is the velocity of light in vacuum, $n_r$ is the refractive index of the medium and $c/n_r$ represents the distance traveled by the wave in unit time. The ratio of $-(dn_p/dt)h\omega$ and $(n_p - n_{p0})h\omega$ represents the ratio of the incident and
absorbed power. Evaluation of the absorption coefficient in the quantum-mechanical theory requires an expression for $\frac{dn}{dt}$. The required expression is obtained by considering the interaction between the electrons and the photons quantum-mechanically. Photons interact with the electrons through the field associated with the radiation. The electron carries a negative charge, which interacts with the electric and magnetic fields of the electromagnetic radiation. The force on the electron due to the electric field is the charge times the field and that due to the magnetic field is the Lorentz force determined by the cross product of the electron velocity and the field. The energy associated with the interaction determines the interaction Hamiltonian that is responsible for electron scattering [8].

![Diagram of interband and intraband transitions for quantum wells, quantum wires (left) and quantum dots (right). The diagrams show a scheme of the band/level structure.](image_url)

**Figure 4.1.** Interband and intraband transitions for quantum wells, quantum wires (left) and quantum dots (right). The diagrams show a scheme of the band/level structure.

Electromagnetic radiation is absorbed in semiconductors through two processes: 'Interband' and 'Intraband' transitions. *Interband* transitions take place between the conduction band and valence band and involve two kinds of
carriers, electrons and holes. The energy of the transition is the bandgap energy plus the confinement energies of the electrons and holes. \textit{Intraband} transitions happen inside either the conduction or the valence band and involve only one type of carrier. In a QD, \textit{intraband} transitions occur between discrete energy levels. In QWs and QWRs there exists subbands inside the conduction or valance band. \textit{Intraband} transitions in these structures between two subbands are called \textit{intersubband} transitions as depicted in Fig. 4.1. Another type of \textit{intraband} transitions may occur which involves the transitions of a carrier from one subband to the same subband with absorption of a photon and emission of a phonon.

\textbf{4.1.2 A brief review on the effects of dot size variation on the spectral response of quantum dot detectors}

The spectral response of the detectors utilizing QD systems is subject to change due to the variation of the dot size \cite{2,6,9}. Kang \textit{et al} \cite{2} studied the size distribution of QD in quantum dot infrared photodetectors (QDIPs) with the temperature dependent dark current and photocurrent spectra. They introduced a method to measure the distribution of electron states of QDs and, further, explained the photocurrent spectrum with the distribution of extracted activation energies from the temperature dependent dark currents.

Apalkov \textit{et al} \cite{6} investigated the effects of interdot coupling on the properties of QDIPs. In their work, the group addressed the splitting of the optical absorption of coupled quantum dots due to electron hopping between the dots. The group proposed that the splitting depends on the size of the dots and the interdot distance and it can be observed only for small dots, less than 20 nm. They studied the system numerically within the effective mass approximation.
Pattada et al [9] employed Fourier-transform infrared spectroscopy technique to investigate the optical absorption coefficient of intersubband transitions in Si-doped In$_{0.3}$Ga$_{0.7}$As/GaAs multiple QD structures. They fabricated waveguides with 45° polished facets from molecular beam epitaxy grown wafers with different quantum dot size. They found that the measured maximum optical absorption coefficient was in the order of $1.103 \times 10^4$ cm$^{-3}$ and the peak position energy of the intersubband transition shifted towards lower energy when the quantum dot size was increased. The group also measured the photoluminescence (PL) spectra for different samples with different quantum dot size.

There are reports [10,11] on the effect of a Gaussian distribution of the dot size on the optical absorption spectra. In such investigations, the dots were approximated as cubic or spherical structures having infinite potential barriers at the boundaries. Wu et al [10] calculated the interband optical absorption of a nonuniform semiconductor QD system and estimated the effect of dot size variation on the resolvability of the absorption peaks. They assumed the dots to be cubic with infinite potential barriers at the boundaries and having a size distribution described by a Gaussian function. They showed that the total absorption spectrum of such a dot system depends strongly on the dot size distribution.

Ferreira et al [11] calculated the optical absorption coefficient of an inhomogeneous quantum dot system analytically and numerically. They approximated the QDs as spheres whose surfaces constitute infinite potential barriers, with a size distribution described by a Gaussian function. The group analyzed the effects of size nonuniformity on the optical absorption spectrum of quantum dot systems and studied the effects of shape through the comparison of their results to those relating to cubic quantum dots [10]. They showed that the optical absorption spectrum of spherical quantum dots depends

"Studies on some important properties of III-V Nanostructures"
strongly on the dot size distribution and that, although the curves obtained for cubic and spherical quantum dots with comparable volumes were similar, there were differences in the relative energy positions and relative intensities of the optical absorption peaks.

There are reports on electron and hole confinement in QBs [12–18]. Fabricated QDs may be typically circular or lens like structures rather than square. In some investigations these dots are approximated as thin quantum boxes [15,16]. Shape effects are minimal for structures with the same cross sectional area [15]. Further to this, QDs have been previously analyzed with the help of infinite potential barriers [19–21], realistic semiconductor QDs having finite potential barriers have not been widely discussed or analyzed.

In this chapter we present an investigation on the optical absorption spectra of realistic semiconductor QD systems with a non uniform size distribution described by a Gaussian function. We have approximated the QD as a QB with finite potential barriers which may be helpful for proper analysis of the optical properties of realistic semiconductor QD systems. A comparative study of the ideal and realistic dots was carried out. It is found that the absorption spectra of different realistic III-V compound semiconductor QDs depend strongly on the dot size distribution described by the parameter $\xi$[10], the ratio of the standard deviation of the dot size to the average dot size of the system. The results were compared with the ideal dots where we find that the spectra of the realistic dots seem to be red-shifted and the line width decreases. Further studies on the absorption spectra corresponding to different values of $\xi$ were carried out and it was found that the resolvability of the absorption peaks depend on $\xi$. After statement of the exact nature of the problem and the aim, the chapter is to narrate clearly the modification of formulae that had to be done as necessary, computational methodologies and the results in detail, along with necessary discussions.
4.2 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 resulting normalized wave function becomes [16, 22]

\[
\psi(x) = \frac{8}{L_1 L_2 L_3} \sin(k_1 x_1) \sin(k_2 x_2) \sin(k_3 x_3)
\]  

(4.3)

where \(k_j = \frac{n_j \pi}{L_j} \) (\(n_j = \pm 1, \pm 2, \ldots\)) is the wave vector along \(x_j\) direction. For a cubic box of side \(L\), Eq. (4.3) reduces to [10]

\[
\psi(x) = \left( \frac{2}{L} \right)^{3/2} \sin(k_1 x_1) \sin(k_2 x_2) \sin(k_3 x_3)
\]  

(4.4)

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 [23]

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

(4.5)

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

(4.6)

\[
n^2 = \sum n_j^2, j = 1,2,3
\]  

(4.7)

where \(P_e\) and \(P_h\) are the well strength parameters defined as \(P_e = (\sqrt{2m_0m_e^*V_0}/\hbar)L/2\) and \(P_h = (\sqrt{2m_0m_h^*V_0}/\hbar)L/2\), 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 lowest state corresponds to \(n^2 = 3\). For an infinite deep...
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potential well, \( P \to \infty \) and Eqs. (4.5) and (4.6) reduces to the well known result

\[
\lim_{P \to \infty} E_e(n^2) = \frac{\pi^2 \hbar^2 n^2}{2m_0m_e^* L^2} \tag{4.8}
\]

and

\[
\lim_{P \to \infty} E_h(n^2) = \frac{\pi^2 \hbar^2 n^2}{2m_0m_h^* L^2} \tag{4.9}
\]

Let us now define the resonance energy of a realistic QD, having finite potential barriers, as the photon energy needed for the creation of electron-hole pair. This may be represented as [10]

\[
\hbar \omega_{\text{real}} = E_g + E_e(n^2) + E_h(n^2) \tag{4.10}
\]

where \( E_g \) is the band gap of the semiconductor material. The resonance energy of an ideal dot having infinite potential barriers, \( \hbar \omega_{\text{ideal}} \), can be expressed as [10]:

\[
\hbar \omega_{\text{ideal}} = \lim_{P \to \infty} \hbar \omega_{\text{real}} = E_g + \frac{\pi^2 \hbar^2}{2L^2} \left[ \frac{1}{m_0m_e^*} + \frac{1}{m_0m_h^*} \right] n^2 = E_g + \frac{\pi^2 \hbar^2 n^2}{2\mu L^2} \tag{4.11}
\]

where \( 1/\mu = 1/(m_0m_e^*) + 1/(m_0m_h^*) \). 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 [11]. 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 cubic dot with length \( L \) is calculated as [10]

\[
\alpha_{\text{real}} = \frac{A_{\text{real}}}{L^3} \sum_{\langle n^2 \rangle} g(n^2) \delta \left[ \hbar \omega_{\text{real}} - \left( E_g + E_e(n^2) + E_h(n^2) \right) \right] \tag{4.12}
\]

where \( g(n^2) \) is the degeneracy of the energy level determined by \( n^2 = \sum n_j^2 \). Only \( \Delta n=0 \) transitions are considered allowed.
\( A_{\text{real}} \) is a constant in terms of the momentum matrix \( P_n \) so that [10]

\[
A_{\text{real}} = \frac{2\pi e^2 |P_n|^2}{m_0 \varepsilon_r \varepsilon_0 c \omega_{\text{real}}} \tag{4.13}
\]

where \( e \) is the fundamental charge, \( \varepsilon_0 \) is the permittivity of free space, \( \varepsilon_r \) the host material, \( c \) is the speed of light and \( \omega_{\text{real}} \) is the photon frequency. Similarly for an ideal QD system, the optical absorption coefficient can be expressed as [10]

\[
\alpha_{\text{ideal}} = \frac{A_{\text{ideal}}}{L^3} \sum_{(n^2)} g(n^2) \delta [\hbar \omega_{\text{ideal}} - (E_g + \frac{n^2 \hbar^2}{2mL^2} n^2)] \tag{4.14}
\]

where

\[
A_{\text{ideal}} = \frac{2\pi e^2 |P_n|^2}{m_0 \varepsilon_r \varepsilon_0 c \omega_{\text{ideal}}} \tag{4.15}
\]

The constant \( A_{\text{ideal}} \) and the photon frequency \( \omega_{\text{ideal}} \) corresponds to that of an ideal dot having infinite potential barriers. The interband absorption of a QD is characterized by a series of discrete lines at photon energies given by Eqs. (4.10) and (4.11). As mentioned by Wu et al [10], 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 size of side length \( L \) which can be represented as [10]:

\[
P(L) = \left( \frac{1}{D \sqrt{2\pi}} \right) \exp \left[ -\frac{(L - L_0)^2}{2D^2} \right] \tag{4.16}
\]

where \( L_0 \) is the average dot size of the system and \( D \) is the standard deviation. Let \( \xi \) be the relative standard deviation of the dot given by

\[
\xi = D/L_0 \tag{4.17}
\]


\[
P(L) = \frac{1}{\xi L_0} \cdot \frac{1}{\sqrt{2\pi}} \exp \left[ -\left( \frac{L}{L_0} - 1 \right)^2 / 2 \xi^2 \right]
\] (4.18)

Let us now define two dimensionless parameters: the reduced photon energies \( \chi_\text{real} \) and \( \chi_\text{ideal} \) for a realistic and ideal QD system respectively, represented as

\[
\chi_\text{real} = \frac{\hbar \omega - E_g}{[E_e(n^2)_{L=L_0} + E_h(n^2)_{L=L_0}] / n^2}
\] (4.19)

and

\[
\chi_\text{ideal} = \frac{\hbar \omega - E_g}{\pi^2 \hbar^2 / 2 \mu L_0^2}
\] (4.20)

\( E_e(n^2)_{L=L_0} \) and \( E_h(n^2)_{L=L_0} \) are the values of \( E_e(n^2) \) and \( E_h(n^2) \) for \( L = L_0 \). Now combining Eqs. (4.14) and (4.16), the total absorption spectra of an ideal QD system due to the non uniform dot size distribution is represented as [10]

\[
\alpha_\text{ideal} = \frac{\Lambda_\text{ideal} \cdot 1}{\sqrt{2\pi}} \sum g(n^2) \int_0^\infty \frac{1}{L^3} e^{-[0-L_0]2/2\xi^2} \times \delta[\hbar \omega - (E_g + \frac{n^2 \hbar^2}{2 \mu L_0^2})] dL
\] (4.21)

Integrating Eq. (4.21) and utilizing Eq. (4.17)

\[
\alpha_\text{ideal} = \frac{\beta_\text{ideal} \cdot 1}{21 \times 3} \sum g(n^2) \exp \left[ -\left( \frac{n}{\chi_\text{ideal}} - 1 \right)^2 / 2 \xi^2 \right]
\] (4.22)

where \( \beta_\text{ideal} = \frac{(1/\sqrt{2\pi}) \Lambda_\text{ideal}}{\pi^2 \hbar^2 / 2 \mu L_0^2} \) (4.23)

Now we model the optical absorption spectra of a realistic cubic dot of finite potential barrier at the boundaries as

\[
\alpha_\text{real} = \frac{\beta_\text{real} \cdot 1}{21 \times 3} \sum g(n^2) \exp \left[ -\left( \frac{n}{\chi_\text{real}} - 1 \right)^2 / 2 \xi^2 \right]
\] (4.24)
where \( \beta_{\text{real}} = \frac{(1/\sqrt{2\pi})A_{\text{real}}}{[E_e(n^2)_{L=L_0} + E_h(n^2)_{L=L_0}]/n^2} \)  \( (4.25) \)

In the realm of an ideal cubic QD system, \( P_e, P_h \rightarrow \infty \) and the photon frequency, \( \omega = \omega_{\text{ideal}} \) such that

\[
\lim_{P_e, P_h \rightarrow \infty} \beta_{\text{real}} = \frac{(1/\sqrt{2\pi})A_{\text{ideal}}}{\pi^2 \hbar^2 / 2\mu L_0^2} = \beta_{\text{ideal}} \quad (4.26)
\]

This agrees with the choice of our denominator of Eq. (4.25). Eqs. (4.22) and (4.24) represent a set of Gaussian absorption peaks with peak photon energies determined by the average dot size \( L_0 \) and represented in Eqs. (4.10) and (4.11). The linewidths of the \( n^2 \) absorption peak of the ideal and realistic dot, \( W_{\text{ideal}} \) [10] and \( W_{\text{real}} \) are given by

\[
W_{\text{ideal}} = \frac{4.71\xi}{(1-3.9\xi^2)^2} [n^2\pi^2\hbar^2 / 2\mu L_0^2] \quad (4.27)
\]

\[
W_{\text{real}} = \frac{4.71\xi}{(1-3.9\xi^2)^2} [E_e(n^2)_{L=L_0} + E_h(n^2)_{L=L_0}] \quad (4.28)
\]

and \( W_{\text{reduction}} = W_{\text{ideal}} - W_{\text{real}} \)  \( (4.29) \)

where \( W_{\text{reduction}} \) represents the difference in the linewidths of the \( n^2 \) absorption peak of the ideal and realistic dots. It could be inferred from Eqs. (4.27) and (4.28) that the linewidth is proportional to the size deviation \( \xi \) and approaches zero when \( \xi \rightarrow 0 \). Also the linewidth is larger for higher transition energy levels.
4.3 Results and Discussion

Figure 4.2. Absorption spectra of the lowest transition of In$_{0.7}$Ga$_{0.3}$N/GaN QD system corresponding to both real and ideal dots for relative standard deviation $\xi = 0.02$, 0.05, 0.10 and 0.20, as specified. The solid and dotted curves correspond to the realistic and ideal QD systems respectively. The photon energy for real and ideal dots is defined by Eqs. (4.10) and (4.11). The relative absorption of the ideal and realistic dots defined as $\alpha_{\text{ideal}} / (\beta_{\text{real}}/2L\sigma^2)$ and $\alpha_{\text{ideal}} / (\beta_{\text{ideal}}/2L\sigma^2)$ from Eqs. (4.22) and (4.24) respectively.

The results of computations of the absorption spectra of In$_{0.7}$Ga$_{0.3}$N/GaN and In$_{0.66}$Ga$_{0.33}$As/GaAs QD systems are shown in Figs. 4.2, 4.3 and 4.4. In each of these figures, the spectra of the realistic and ideal QD system are shown in the same plot. Figure 4.2 shows the plot of the lowest absorption peak ($n^2 = 3$) for In$_{0.7}$Ga$_{0.3}$N/GaN QD system with $\xi = 0.02$, 0.04, 0.10 and 0.20. The absorption spectra for the realistic and ideal dots are denoted by solid and dotted lines respectively. The horizontal axis is the photon energy corresponding to real and ideal dots defined by Eqs. (4.10) and (4.11) respectively. The vertical axis is the relative absorption of the ideal and
realistic dots defined as $\alpha_{\text{real}} / (\beta_{\text{real}}/2L_0^3)$ and $\alpha_{\text{ideal}} / (\beta_{\text{ideal}}/2L_0^3)$ according to Eqs. (4.22) and (4.24).

Figure 4.3. Absorption spectra of the lowest four transitions of In$_x$Ga$_{1-x}$N/GaN QD system corresponding to both real and ideal dots. In each of these plots, the solid and dotted lines represent the individual absorption peaks of real and ideal dots respectively, while the closed and open circle curves correspond to their superposition. The photon energy for real and ideal dots is defined by Eqs. (4.10) and (4.11). The relative absorption of the ideal and realistic dots defined as $\alpha_{\text{real}} / (\beta_{\text{real}}/2L_0^3)$ and $\alpha_{\text{ideal}} / (\beta_{\text{ideal}}/2L_0^3)$ from Eqs. (4.22) and (4.24) respectively.
For In$_{0.7}$Ga$_{0.3}$N/GaN QD system, the energy band gap of In$_x$Ga$_{1-x}$N, $E_g$, was calculated from the equation [24]:

$$E_g(x) = (1 - x)E_{g\text{GaN}} + x E_{g\text{InN}} - bx(1 - x)$$  \hspace{1cm} (4.28)

where, $x$ is the mole fraction of indium, $E_{g\text{GaN}}$ and $E_{g\text{InN}}$ are the energy band gaps of GaN and InN respectively, and $b$ is the bowing parameter (vide Fig. 5.5 of chapter 5). In our calculation $E_{g\text{GaN}}, E_{g\text{InN}}, 'x'$ and 'b' was assumed to be 3.4 eV, 2 eV, 0.7 and 1.4 respectively. Considering $x = 0.7$, the band gap $E_{g\text{InGaN}}$ comes out to be 2.126 eV. For finite potential barriers, considering the band offset ratio to be 55 : 45 [25], the conduction and valance band heights were found to be 0.701 eV and 0.573 eV. The average dot size was considered to be 7.25 nm. The effective masses are assumed to be 0.2$m_0$ for electrons [24] and 1.56$m_0$ for heavy holes [26]. The computed absorption spectra of In$_{0.7}$Ga$_{0.3}$N/GaN QD system is shown in Fig. 4.3.

There are reports on the growth of In$_{0.66}$Ga$_{0.33}$As/GaAs QDs [27]. The computed absorption spectra of such QD ensemble is shown in Fig. 4.4. The band gap, $E_{g\text{InGaAs}}$, of In$_x$Ga$_{1-x}$As is determined from the empirical relation [28]

$$E_{g\text{InGaAs}} = 1.516 - 1.214x + 0.264x^2$$  \hspace{1cm} (4.29)

where $x$ is the concentration of indium. The effective masses [29] were taken to be 0.041$m_0$ for electrons and 0.417$m_0$ for holes, which were obtained through a linear extrapolation between the effective masses of InAs and GaAs. $E_{g\text{InGaAs}}$ and the band offset ratio were considered to be 0.830 eV and 60 : 40 respectively. For realistic dots, the well height of the conduction and valance bands were found to be 0.412 eV and 0.274 eV. The average dot size was considered to be 9 nm.
Figure 4.4. Absorption spectra of the lowest four transitions of In$_{0.66}$Ga$_{0.33}$As/GaAs QD system corresponding to both real and ideal dots. In each of these plots, the solid and dotted lines represent the individual absorption peaks of real and ideal dots respectively, while the closed and open circle curves correspond to their superposition. The photon energy for real and ideal dots is defined by Eqs. (4.10) and (4.11). The relative absorption of the ideal and realistic dots defined as $\alpha_{\text{real}} / (\beta_{\text{real}}/2L_0^3)$ and $\alpha_{\text{ideal}} / (\beta_{\text{ideal}}/2L_0^3)$ from Eqs. (4.22) and (4.24) respectively.

The range of photon energies in Figs. 4.3 and 4.4 were so chosen so as to accommodate the lowest four transitions. The solid line and the filled circles
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represent the individual absorption peaks and their superposition of the realistic dots respectively, while for ideal dots it is represented by dotted line and open circles. In both the cases, with ξ=0.02, all the peaks could be resolved. As ξ increases, the resolvability decreases. It should be noted at this juncture that for In$_{0.66}$Ga$_{0.33}$As/GaAs QD system the curves could not be extended beyond a certain energy (1.302 eV) since the confinement energies exceeded the height of the well, and only the lowest two transitions could be observed, as shown in Fig. 4.4. This problem is not encountered in case of In$_{0.7}$Ga$_{0.3}$N/GaN QD system and the lowest four transitions could be accommodated, as depicted in Fig. 4.3.

It is observed that for realistic dots there is red shift of the absorption peaks and there is a decrease in the linewidth as compared to the ideal QD system for the same size deviation. The photon energies corresponding to the Gaussian absorption peaks depend on the band gap of the semiconductor material and the confinement energies of the conduction and the valance bands. For realistic dots having finite potential barrier, the confinement energies are less as compared to ideal dots having infinite potential barriers. As a result, the absorption peaks suffer from a red shift.

The variation of the energy of the sub-bands with change in the size of the dots is much more pronounced in the case of infinite wells as compared to finite wells. Hence larger deviation in the absorption energies for a particular ξ is expected in the case of infinite wells and hence the absorption spectra become broader. Moreover in a narrow finite well less number of levels will be available for transitions which will make the spectrum narrow. The computed values of the difference in the linewidth of ideal and realistic In$_{0.7}$Ga$_{0.3}$N/GaN and In$_{0.66}$Ga$_{0.33}$As/GaAs QD systems for the lowest three transitions are depicted in table 4.1.
TABLE 4.1. Difference in the linewidth, $W_{\text{reduction}}$, of the $n^2$ absorption peak of ideal and realistic $\text{In}_{0.7}\text{Ga}_{0.3}\text{N}/\text{GaN}$ and $\text{In}_{0.66}\text{Ga}_{0.33}\text{As}/\text{GaAs}$ QD systems computed from Eq. (4.29) for $\xi=0.02$ and $\xi=0.05$.

<table>
<thead>
<tr>
<th>Transition</th>
<th>$\xi=0.02$ (in eV)</th>
<th>$\xi=0.05$ (in eV)</th>
<th>$\xi=0.02$ (in eV)</th>
<th>$\xi=0.05$ (in eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1^{\text{st}}$ ($n^2=3$)</td>
<td>0.002</td>
<td>0.007</td>
<td>0.015</td>
<td>0.039</td>
</tr>
<tr>
<td>$2^{\text{nd}}$ ($n^2=6$)</td>
<td>0.005</td>
<td>0.013</td>
<td>0.033</td>
<td>0.083</td>
</tr>
<tr>
<td>$3^{\text{rd}}$ ($n^2=9$)</td>
<td>0.008</td>
<td>0.030</td>
<td>----</td>
<td>----</td>
</tr>
</tbody>
</table>

Figure 4.5. Variation of the energy difference of the absorption peak of the ideal and realistic dots with average dot size. Results of computations are presented for both $\text{In}_{0.7}\text{Ga}_{0.3}\text{N}/\text{GaN}$ and $\text{In}_{0.66}\text{Ga}_{0.33}\text{As}/\text{GaAs}$ QD systems for the lowest two transitions.
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Figure 4.6. Variation of the linewidth of realistic QD systems on the average dot size for $\xi = 0.02$ and 0.05. The linewidth is defined by Eq. (4.28) and the results of computations are presented for both In$_{1-x}$Ga$_x$N/GaN and In$_{0.66}$Ga$_{0.33}$As/GaAs realistic QD systems for the lowest transition.

For In$_{0.66}$Ga$_{0.33}$As/GaAs QD system, the data corresponding to the lowest two transitions could only be computed since the absorption spectra corresponding to the higher order transitions were found to be absent, as shown in Fig. 4.4. It is also observed that the red shift is more pronounced for smaller average dot size, as shown in Fig. 4.5. In Fig. 4.5, the red shift corresponds to the energy difference of the absorption peak of the ideal and realistic dots. Computations were carried out for $\xi = 0.05$, where the lowest two transitions could be well resolved. In case of In$_{0.7}$Ga$_{0.3}$N/GaN QD system, due to the relatively small well height, the red shift corresponding to the second transition level could be obtained only after a certain average dot size.
Figure 4.6 shows the dependence of the linewidth of realistic dots on the average dot size for \( \xi = 0.02 \) and 0.05 respectively. The linewidth is defined by Eq. (4.28) and the results of computations are presented for both In\(_{0.7}\)Ga\(_{0.3}\)N/GaN and In\(_{0.66}\)Ga\(_{0.33}\)As/GaAs realistic QD systems for the lowest transition. It is observed that the linewidth falls rapidly in case of smaller average dot size and seem to saturate as the average dot size increases.

### 4.4 Summary

In this work a model has been formulated to investigate the interband optical absorption of realistic QD systems having finite potentials at the boundaries. Considering the Gaussian distribution of the dot size, the absorption spectra of In\(_{0.7}\)Ga\(_{0.3}\)N/GaN and In\(_{0.66}\)Ga\(_{0.33}\)As/GaAs QD systems have been calculated, where it is observed that for realistic dots there is red shift of the absorption peak and the linewidth decreases as compared to that of the ideal QD system for the same size deviation. The formulations developed in this chapter can be used for analysis of stacked QDs, which are recently used as active elements of semiconductor solar cells.

This work has been published in:


### 4.5 References


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"Studies on some important properties of III-V Nanostructures"
[22] For example, see David J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, 2004, 2nd ed.).


