Effects of hydrostatic pressure and temperature on interband optical transitions in InAs/GaAs vertically coupled double quantum dots

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Abstract. We consider the effect of hydrostatic pressure, temperature and the variations of structure’s sizes on interband transition energy and absorption coefficient in InAs/GaAs vertically coupled double quantum dots. The threshold energy of interband optical transitions is examined as a function of hydrostatic pressure and temperature for the different geometries of the structure. We also investigated the dependencies of the interband light absorption coefficient on the incident photon energy.

1. Introduction
Coupled quantum structures, consisting of two smaller band-gap nanomaterials, which are different in band-gap energies and are separated by a thin embedded barrier with a larger band gap, have been receiving considerable attention because of the interest in both investigations of fundamental physics [1-3] and for potential applications in electronic and optoelectronic devices [4-6]. Among the many coupled double quantum structures InAs/GaAs coupled double quantum dots (DQDs) are of current interest because of their promising applications in quantum information storage devices [7] and detectors [8]. M. Bayer, et al. [9] demonstrate coupling and entangling of quantum states in a pair of vertically aligned, self-assembled quantum dots (QDs) by studying the emission of an interacting electron-hole pair in a single dot molecule as a function of the distance between dots. From optical studies of excitons and corresponding calculations authors demonstrated that an electric field on vertically coupled pairs of In0.6Ga0.4As/GaAs QDs controls the mixing of the excitonic states on the two dots and also provides controllable coupling between carriers in the dots [10].

Many works related to the theoretical investigation of electronic and excitonic states of semiconductor DQD have been reported recently [11-15]. In the adiabatic approximation and using an exact diagonalization technique the energy spectrum in vertically coupled DQD is calculated [11]. The effect of the electric field on electronic states in vertically coupled DQD [12] and the effect of the magnetic field on exciton ground-state energy in double and triple vertically coupled QDs have been

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investigated [13,14]. Using the three-dimensional finite-difference method the interband transition energies of InAs/GaAs DQD have been calculated [15]. In this work the photoluminescence (PL) experimental transition energies for InAs/GaAs DQDs, as determined from the temperature-dependent PL spectra, were in reasonable agreement with those of the theoretical interband transition energies calculated by using a finite-difference method taking into account shape-based strain and nonparabolic effects.

Hydrostatic pressure is a thermodynamic variable for the solid state, which provides a powerful tool to control and investigate the electronic states and optical properties of semiconductor materials. In [16] the effect of hydrostatic pressure on the interband optical transitions in InAs/GaAs QDs with lens shape geometry has been investigated.

In this work the effect of hydrostatic pressure and temperature on interband transition energy is investigated in InAs/GaAs vertically coupled DQDs. The threshold energy of interband optical transitions is examined as a function of hydrostatic pressure and temperature for the different geometries of the structure. We also investigate the dependencies of the interband light absorption coefficient on the incident photon energy. The paper is organized as follows: in Section 2 we describe the theoretical framework, Section 3 is dedicated to the results and discussion, and finally, our conclusions are given in Section 4.

2. Theoretical framework

In the effective-mass approximation, the Hamiltonian in cylindrical coordinates for electron (heavy hole) in InAs/GaAs vertically coupled DQDs under the influence of hydrostatic pressure ($P$) and temperature ($T$) is given by

$$
\hat{H}_{e, hh} = -\frac{\hbar^2}{2m_{e(hh)}(P,T)} \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) + V_{e(hh)}(\rho, z, P, T),
$$

(1)

where $m_{e(hh)}(P, T)$ and $V_{e(hh)}(\rho, z, P, T)$ are, respectively, the pressure- and temperature-dependent electron (heavy hole) effective mass and the confining potential. For InAs $m_{e(hh)}(P, T)$ are given by [16,17]:

$$
m_e(P, T) = m_0 \left( 1 + 3.8 \cdot 10^4\text{meV} \left( \frac{3E_g(P, T) + 760\text{meV}}{3E_g(P, T)(E_g(P, T) + 380\text{meV})} \right) \right)^{-1}, \quad \rho_{hh} = m_0 \left( \gamma_1 - 2\gamma_2 \right)^{-1},
$$

(2)

where $\gamma_1 = 20.4$ and $\gamma_2 = 8.37$ [16,17], $m_0$ is the free electron mass, $E_g(P, T)$ is the bulk InAs(GaAs) bandgap.

In figure 1 we present the schematic view of vertically coupled DQDs.

**Figure 1.** Schematic image of vertically coupled DQDs. H is the height of QD, R is the radius of QD, W is the thickness of wetting layers and D is the spacer thickness.
\[ E_g(P,T) = E_g^0 + \alpha P - \beta T^2 (T + c)^{-1}, \]  

\[ E_g^0 = 533 \text{meV} \quad (E_g^0 = 1519 \text{meV}) \] is the energy gap at \( P = 0 \text{kbar} \) and \( T = 4 \text{K} \), \( \alpha = 7.7 \text{meV/kbar} \) and \( \beta = 0.276 \text{meV/K} \) are the pressure coefficients and \( c = 83 \text{K} \) is the temperature coefficient [16].

In equation (1) \( V_{\text{el}}(\rho,z,P,T) \) is the pressure and temperature dependent confining potential for electron (heavy hole):

\[ V_{\text{el}}(\rho,z,P,T) = \begin{cases} G_{G\text{aAs}} \left( E_g^{\text{GalAs}}(P,T) - E_g^{\text{InAs}}(P,T) \right) & \text{outside QD}, \\ 0 & \text{inside QD}, \end{cases} \]

where \( G_{G\text{aAs}} \) and \( G_{\text{InAs}} \) are band offsets for conductance (0.54) and valence (0.46) bands respectively [20].

Since the height of each QD is much smaller than their radii the motion along the \( z \) axis is strongly confined. Taking this into account the Schrödinger equation with Hamiltonian (1) can be solved using the adiabatic approximation [11, 12, 19]. So, the wave functions of electron and heavy hole can be given by:

\[ \Psi(\rho,\varphi,z) = (2\pi)^{-1/2} e^{i\varphi} g^{e/\mathbf{h}}(z) f^{e/\mathbf{h}}(\rho), \]

where \( g^{e/\mathbf{h}}(z) \) is the wave function in \( z \) direction, \( f^{e/\mathbf{h}}(\rho) \) is the radial wave function [11], \( \mu = 0, \pm 1, \pm 2, \ldots \) is the magnetic quantum number and \( \nu \) is the subband number.

For calculating the absorption coefficient we employ the known expression [20]

\[ \alpha(\omega,P,T) = \frac{4\pi^2 e^2}{ncm V_0^2 \omega} \sum |\tilde{\rho}|^2 \delta \left( E_j(P,T) - E_i(P,T) - \hbar \omega \right) \left[ f(E_j(P,T)) - f(E_i(P,T)) \right] \]

where \( e \) is the electron charge, \( c \) is the speed of light, \( V_0 \) is the normalized volume of the sample, \( n \) is the refraction index, \( \omega \) is the frequency of light, \( \tilde{\rho} \) is the light wave polarization vector, summation is carried out over all initial \( (i) \) and final \( (f) \) states, and \( f(E) \) is the Fermi - Dirac distribution function.

For interband transitions in equation (5) the momentum matrix element is\( \tilde{\rho}_{ij}^{Q} = \langle u_i^\varphi | \hat{p} | u_j^\varphi \rangle \), where \( u_i^\varphi \) and \( u_j^\varphi \) are the Bloch amplitudes at the centre of the Brillouin zone, \( Q \) is the overlab integral, and \( \varphi_i \) and \( \varphi_j \) are the envelope functions of final and initial states, respectively. For interband transitions, we obtain selection rule \( \mu = \mu' \). Under the condition of the conduction band being practically empty (low temperatures), for the absorption coefficient we obtain:

\[ \alpha(\omega,P,T) = \frac{4\pi^2 e^2}{ncm V_0^2 \omega} \sum |\tilde{\rho}|^2 \delta \left( E_{j(0)}^{e/\mathbf{h}}(P,T) - E_{i(0)}^{e/\mathbf{h}}(P,T) - \hbar \omega \right) \left[ f(E_{j(0)}^{e/\mathbf{h}}(P,T)) - f(E_{i(0)}^{e/\mathbf{h}}(P,T)) \right] \times \]

\[ \frac{\Gamma}{(\hbar \omega - \Delta_{\mu\nu\varphi})^2 + \Gamma^2}, \]

where \( I_{z}^{(1)} \) and \( I_{z}^{(2)} \) are the overlap integrals of wave functions in \( z \) direction when \( 0 < \rho < R(P) \) and \( \rho > R(P) \) respectively, \( R(P) \) is the pressure dependent radius of QD, \( \Gamma \) \((= 4\text{meV})\) is the Lorentzian parameter and \( \Delta_{\mu\nu\varphi} = E_{e,\mu}^{e,\mu}(P,T) + E_{h,\mu}^{e,\mu}(P,T) + E_g^{\text{InAs}}(P,T) \) is the threshold energy.
3. Results and discussion
The calculations are performed only for the first allowed interband transitions from the heavy hole ground (symmetric) states with \( \nu = 1, \mu = 0 \) to the electron ground states with \( \nu' = 1, \mu' = 0 \). In all figures of this section we have used 5.4Å value for wetting layer thickness \( W(0) \).

In figures 2 (a) - (c) we present the threshold energy of interband transitions in InAs/GaAs vertically coupled DQDs as a function of hydrostatic pressure. Several values of the spacer thickness \( D \) (figure 2 (a)), height \( H \) (figure 2 (b)) and radius \( R \) of QDs have been considered. For complete range of hydrostatic pressure considered, the following effects are observed: 1) the height of confining potential is an increasing function of hydrostatic pressure (because of the difference of pressure coefficients of InAs and GaAs), which itself increases the threshold energy; 2) the energy gap of InAs material is an increasing function of hydrostatic pressure, which itself increases the threshold energy; 3) the dimensions of the structure are decreasing functions of hydrostatic pressure and they force the threshold energy to increase; 4) the electron-effective mass is an increasing function of hydrostatic pressure, which itself decreases the threshold energy. Since, the first three factors are stronger than the last one, the threshold energy is an increasing function of hydrostatic pressure. From

![Figure 2](image-url)

**Figure 2.** The threshold energy of the interband optical transitions in vertically coupled InAs/GaAs DQDs as a function of hydrostatic pressure. Several values of spacer thickness \( D(0) = 50Å, R(0) = 120Å – (a) \), height \( H(0) = 30Å, R(0) = 120Å – (b) \) and radius \( R(0) = 50Å, H(0) = 30Å – (c) \) of QDs have been considered at \( T = 4K \).

![Figure 3](image-url)

**Figure 3.** The threshold energy of the interband optical transitions in vertically coupled InAs/GaAs DQDs as a function of temperature. Several values of spacer thickness \( D(0) = 50Å, R(0) = 120Å – (a) \), height \( H(0) = 30Å, R(0) = 120Å – (b) \) and radius \( R(0) = 50Å, H(0) = 30Å – (c) \) of QDs have been considered for \( P = 0 \).
figure 2 (a) it is clear that with the increase of the spacer thickness the threshold energy increases, which is caused by the increase of distance between the energy levels of symmetric states of electron and hole. With the increase of the heights (figure 2 (b)) and radii (figure 2 (c)) of QDs the size quantization of electron and hole weakens and threshold energy decreases.

The effect of temperature on threshold energy of interband transitions in InAs/GaAs vertically coupled DQDs is presented in figure 3. The effect of temperature leads to the following variations of parameters: 1) the height of confining potential is a decreasing function of temperature (because of the difference of temperature coefficients of InAs and GaAs), which itself decreases the threshold energy; 2) the energy gap of InAs material is an decreasing function of temperature, which itself decreases the threshold energy; 3) the effective mass of electron is a decreasing function of temperature, which itself increases the threshold energy. Since the first two factors are stronger than the last one, the threshold energy is a decreasing function of temperature. The effect of variations of structure’s dimensions on threshold energy is the same as in previous case.

In figure 4, the dependences of the absorption coefficient caused by interband transitions from the heavy hole ground states with ν = 1, μ = 0 to the electron ground states with ν = 1, μ = 0 on incident photon energy for different values of the spacer thickness (figure 4 (a)), height (figure 4 (b)), radius (figure 4 (c)) of QDs and hydrostatic pressure (figure 4 (d)) have been considered. Figure 4 (a) and (d) show that with the increase of the spacer thickness and hydrostatic pressure respectively, the peak position of the absorption coefficient is shifted to the high energy region (“blue shift”). Such a behavior caused by the increase of the threshold energy between initial and final states. From figure 4 (b) and (c) it is clear that with the increase of heights and radii of QDs the peak position of the absorption coefficient is shifted to the low energy region (“red shift”). In all cases the maximum value of the absorption coefficient moves to the higher energy range.
of the absorption coefficient is greater for the smaller values of incident photon energy. The reason of this result is the decrease of the energy distance between initial and final states which leads to the increase of overlap integrals.

4. Conclusions
The effects of hydrostatic pressure, temperature and variation of the structure’s sizes on interband transition energy and absorption coefficient are investigated in InAs/GaAs vertically coupled DQDs. The threshold energy of interband optical transitions is examined as a function of hydrostatic pressure and temperature for the different geometries of the structure. We also investigated the dependencies of the interband light absorption coefficient on the incident photon energy. The main findings can be summarized as follows: 1) the threshold energy of interband transition is an increasing function of hydrostatic pressure, 2) the threshold energy of the interband transitions is a decreasing function of temperature, 3) the “blue shift” is observed in the interband absorption spectrum with the increase of spacer thickness of DQDs and hydrostatic pressure, 4) the “red shift” is observed in the interband absorption spectrum with the increase of heights and radii of DQDs.

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