Hydrostatic-pressure-induced $\Gamma$-$X$ mixing in delta-doped $\text{Al}_x\text{Ga}_{1-x}\text{As}$

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Abstract. The mixing between $\Gamma$ and $X$ points in the conduction band is known to manifest in GaAs/Al$_x$Ga$_{1-x}$As heterostructures. Application of hydrostatic pressure leads to the variation of both the $\Gamma$- and $X$-energy gaps in such a way that around $P = 39$ kbar, the GaAs becomes an indirect gap one. Within a narrow interval of $P$ around this value, both minima remain almost energetically aligned. Therefore, it can be expected that some kind of mixing between the states corresponding to the delta-quantum-wells formed at those points should manifest. In this work, we investigate the occurrence of $\Gamma$-$X$ mixing induced by the application of hydrostatic pressure in n-type delta doped Al$_x$Ga$_{1-x}$As, by means of a variational scheme that uses a $2 \times 2$ Hamiltonian with the off-diagonal element being a variational potential energy. Diagonal Schrödinger-like effective mass elements are written with potential functions given by the Thomas-Fermi approximation. The effect of the hydrostatic pressure is incorporated via the dependence on $P$ of the different input parameters in the system: energy gaps, effective masses and dielectric constant. We report the variation of the ground state of the system as a function of $P$.

1. Introduction

Mixing of $\Gamma$ and $X$ conduction band minima has been the subject of study mainly regarding GaAs-AlAs heterostructures [1]-[9]. There are also a significant number of works dealing with the effects of the hydrostatic pressure on the optical and electronic properties in this kind of structures [10]-[15].

The main features of the spectrum of conduction band electrons in Al$_x$Ga$_{1-x}$As n-type delta doped quantum wells (DDQW) were recently investigated [16], within the framework of the one-dimensional local density Thomas-Fermi approximation [17]. Early experimental reports on DDQW in this material can be found in ref. [18]. On the other hand, a theoretical study of the influence of hydrostatic pressure on the electronic states of in GaAs-DDQW has shown the possibility of the formation of a high density two-dimensional electron gas (2DEG) corresponding to the DDQW states at the $X$ minimum of the conduction band in GaAs [19]. Such approach assumed, for instance, that no pressure-induced transition to a semi-insulating state associated to the existence of deep impurity levels is present [20]. The reason for the mixing to occur is the re-accommodation of the ground state for the conduction band electrons due to the displacement of the $\Gamma$ and $X$ energy gaps as functions of $P$. This gives the possibility of having the single
electron ground state formed at $X$ located below the ground level at $\Gamma$, when $P$ goes above of certain value.

This work is aimed at studying the mixing of $\Gamma$- and $X$-related electronic subbands in Al$_x$Ga$_{1-x}$As DDQW, induced by the application of hydrostatic pressure onto the system. Our ansatz considers that within an interval of $P$ there must be a reciprocal influence of $\Gamma$ and $X$ DDQW states given their proximity in the energy scale. That pressure range includes the value for which the positions of the ground state levels, calculated for both minima independently, are aligned. As a consequence, the above mentioned mixing will appear. We will present some preliminary results on this subject. They are derived with the use of a simple variational scheme of calculation.

2. The Model

The electronic states in DDQW can be calculated by means of two main approaches. One of them is the self-consistent solution of coupled effective-mass-Schrödinger and Poisson equations. The second one is the use of an analytical expression for the potential well profile that arises within the formalism of the Thomas-Fermi one-dimensional local density approximation [17]. Then, with this function describing the confining potential, a single band effective mass Schrödinger equation is solved to obtain the subband structure.

In our case, as we are assuming some kind of coupling between the two minima in the conduction band, the Hamiltonian of the system should be written as a $2 \times 2$ matrix. If we use effective atomic units (Bohr radius and Rydberg energy) related with the $\Gamma$ electron effective mass, it has the form:

$$ H = \begin{bmatrix} h_\Gamma & V_{\Gamma X} \\ V_{\Gamma X} & h_X \end{bmatrix} $$

with

$$ h_j = -\frac{\gamma_j}{d^2} + V_j(z), \quad j = \Gamma, X. $$

The parameter $\gamma_j$ is equal to unity when $j = \Gamma$. For the $X$ point $\gamma_X = m_\Gamma/m_X$, where $m_j$ labels the effective masses of both minima along the direction of confinement in the structure, \(z\). The potential functions will be given by the expression:

$$ V_j(z) = E_{Gj} - \frac{a_j^2}{(a_j|z| + z_0j)^4}. $$

These one-dimensional potential functions arise from the Thomas-Fermi approximation [17]. The $E_{Gj}$ are the corresponding energy gaps at both conduction band states. This means that the zero of the scale for the energies is taken at the bulk upper valence band edge at $\Gamma$. According to the system of units adopted we have that:

$$
\begin{align*}
  a_\Gamma &= \frac{2}{15\pi} \\
  a_X &= \frac{2}{15\pi} \left( \frac{m_\Gamma}{m_X} \right)^{3/2} \\
  z_0\Gamma &= \frac{2}{15\pi} \left( \frac{225\pi}{4N_2D} \right)^{1/5} \\
  z_0X &= \frac{2}{15\pi} \left( \frac{225\pi}{4N_2D} \right)^{1/5} \left( \frac{m_\Gamma}{m_X} \right)^{1/2},
\end{align*}
$$

where $N_2$ is the 2D electron density.
whereas $N_{2D}$ is the two-dimensional density of ionized impurities in the delta doping spike.

The calculation of the ground state of the mixing Hamiltonian in equation (1) is performed variationally. The off-diagonal elements are set to be $V_{\Gamma X} = V_{X\Gamma} = \mathcal{V}$, which will be one of the variational parameters in the energy functional $\int \Psi^\dagger H \Psi dz$. The second variational parameter, $\alpha$, appears in the choice of the two components of the trial vector wavefunction $\Psi$ [21]:

$$
\begin{align*}
\psi_{\Gamma}(z) &= \alpha \phi_{\Gamma}(z) + \sqrt{1 - \alpha^2} \phi_X(z) \\
\psi_X(z) &= -\sqrt{1 - \alpha^2} \phi_{\Gamma}(z) + \alpha \phi_X(z).
\end{align*}
$$

The functions $\phi_j(z)$ are proposed to have the following form:

$$
\phi_j(z) = A e^{-b_j |z|}, \quad \text{with} \quad b_j = \sqrt{\mathcal{E}_{0j} - \left( \mathcal{E}_{Gj} - \frac{\alpha_j^2}{\mathcal{E}_{0j}} + \beta_j \mathcal{V} \right)},
$$

where $\beta_j = \alpha^2$ if $j = \Gamma$ and $\beta_j = 1 - \alpha^2$ if $j = X$. $\mathcal{E}_{0j}$ represents the values of the ground level calculated exactly with the single-minimum Hamiltonian of equation (2).

The inclusion of the hydrostatic pressure effects is made via the dependence upon $P$ of the main input parameters. That is, effective masses, energy gaps, and the dielectric constant. We are using the input data previously dealt with in ref. [15].

3. Results

Now, we go back to the use of traditional units. Figure 1 show the results of the variational calculation for the ground state of the mixed system with variational Hamiltonian (1). The value chose for the two-dimensional ionized impurity density is $N_{2D} = 5 \times 10^{12} \text{cm}^{-2}$. The cases of pure GaAs (left figure) and $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ (right figure) are considered. Reported pressure intervals were chosen in such a way that the point of crossing between the ground levels of the unmixed DDQW at both minima is included within.

![Figure 1](image_url)

**Figure 1.** The ground state (in black) of the mixed $\Gamma - X$ n-type delta doped quantum well with $N_{2D} = 5 \times 10^{12} \text{cm}^{-2}$ as a function of the hydrostatic pressure. For comparison, the corresponding independent energy ground levels at the $\Gamma$ (in red) and $X$ (in blue) points are plotted as well. Left figure corresponds to the case of GaAs. Right figure shows the results for a n-delta-doped $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ quantum well.

The off-diagonal variational parameter is found to depend linearly with pressure: $\mathcal{V} = \sigma P$. The values obtained for the slope, in each range of $P$ considered are $\sigma(\text{GaAs}) = 2.83 \text{meV kbar}^{-1}$, and $\sigma(\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}) = 2.68 \text{meV kbar}^{-1}$. As the calculation was performed using effective
atomic units, the values resulting for the variational parameter $\alpha$ after minimization are constant and independent of $P$ because the effective Rydberg is defined for each value of pressure, thus leaving the differential diagonal operators in $H$ unaltered. That is, in effective units, both variational parameters have a fixed value, which is independent of $P$. When going back to "normal" units, it is necessary to multiply by $Ry^*(P)$ if the quantities involved do have units of energy. That is the case of $V$. We have obtained $\alpha = 0.305$ for both cases.

It is seen that the effect of mixing is to bring down the ground state of the coupled system, when it is compared with the values $E_{0j}$ calculated without the presence of hydrostatic pressure. Furthermore, the correct behaviour of $E_0$ as a function of pressure is detected. That is, the ground state must reproduce the a very close to $E_{0\Gamma}$ when $P = 0$. In fact, there might be some kind of interaction between $\Gamma$ and $X$ minima even for null pressure; but it is always neglected. $E_0$ must also tend to $E_{0X}$ for sufficiently high hydrostatic pressure.

However, it can be observed in the case of Al$_{0.3}$Ga$_{0.7}$As that there will be a small difference between $E_0$ and $E_{0\Gamma}$. We explain this by indicating that the choice made for the trial wavefunctions $\phi_j(z)$ is not the more accurate. They are, perhaps, the simplest option. Although they qualitatively reproduce the decaying of the electronic probability density with the distance away from the origin, these functions do not have a continuous first derivative at $z = 0$. Therefore, they can not be taken as any expansion of the eigenfunctions of the Hilbert space associated with the Hamiltonian $H$.

4. Conclusions
The mixing effect between $\Gamma$ and $X$ conduction band states due to the hydrostatic pressure in Al$_x$Ga$_{1-x}$As-DDQW appears to be not negligible. Several tens of meV are the amount of the difference between the ground state of $H$ and the eigenstates of the single-conduction-band-minimum Hamiltonians of equation (2) for the n-type DDQW. This indicates that further consideration should be taken of this phenomenon when studying the properties of delta-doped systems under pressure in such materials. A more convenient selection of the single-minimum variational trial wavefunctions is required for that purpose. It would be interesting, for instance, the inclusion of finite temperature effects. In this case, the self-consistent solution for the single minimum eigenstates would be the correct starting point for the application of the variational scheme here proposed.

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