Electronic structure of \(pn\) delta-doped quantum wells in GaAs

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We present the electron and hole subband structure in a coupled \(p\)- and \(n\)-type delta-doped quantum well in GaAs. The study is performed in the framework of the envelope function approximation via analytical expressions for the Hartree potential previously obtained through the lines of the Thomas-Fermi approximation. The calculations are focused on the electronic structure and specially on the determination of the one-dimensional \(p\)- and \(n\)-type Bohr radius as a function of the two dimensional acceptor and donor concentrations, respectively, in order to obtain the minimum distance between the delta-doped layers that avoids or generates a reduction in the potential barriers, which is essential in the design of devices based on the coupling of \(p\)- and \(n\)-type delta-doped structures.

Keywords: Electronic structure; \(pn\) \(\delta\)-doped quantum wells; Thomas-Fermi approximation.

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1. Introduction

The everyday improvement in doping and growth techniques allows the realization of semiconductor structures with delta-function doping profiles. In particular \(p\)- and \(n\)-type delta-doped structures present electron and hole confinement due to the bending of the conduction and valence band caused by the ionized impurities. Systems in which \(p\)- and \(n\)-type delta-doped (\(pnDD\)) layers are used as conductive channel and punchthrough stopper (ALD-FET), respectively, are of special interest due to the high transconductance observed \([1,2]\).

\(pnDD\) quantum wells are also important because they form the basic elements in delta-doped \(nipi\) superlattices (also called sawtooth superlattices), which have the following features: tunable band gaps at energies below that of the bulk, long carrier recombination life times, strong nonlinearity and improved optical properties over homogeneously doped \(nipi\) superlattices \([3]\). All these properties make the sawtooth superlattices attractive for technological applications in light emitting diodes and lasers \([4]\), infrared detectors and modulators, \([5]\) and optical computing \([6]\). The \(nipi\) delta-doping structures are also ideal systems to investigate interesting phenomena like the disorder effects caused by the random distribution of impurities \([7,8]\), the band edge relaxation effects \([9,10]\), high field electron transport \([11]\) and the metal-insulator transition \([12]\).

In the present paper we study the electron and hole level structure in \(pnDD\) quantum wells in GaAs within the effective mass envelope function approximation. The Thomas-Fermi approximation has been applied to obtain analytical expressions for the bending of the conduction and valence band. The electronic structure for electrons and holes is analyzed as a function of the distance between the acceptor and donor layers. We paid special attention to the one-dimensional Bohr radius (1DBR) of the electron and hole ground levels and its variation with the acceptor and donor concentration. With the data presented here, it is possible to find the minimum distance between the donor and acceptor layers to avoid a reduction in the potential barrier whether for electrons or holes, which is essential in parallel and vertical transport devices based on these structures.

2. Theoretical framework

The scheme of calculation starts by modeling the conduction and valence band profile, within the local density Thomas-Fermi approximation. The outcome of this approach is an analytical expression for the one-dimensional potential energy function describing the band bending in a single delta-doped quantum well (SDDQW) \([13,14]\).

For a single \(n\)-type delta-doped quantum well centered in \(z = a\), the confining potential can be written as \([13]\),
\[ V_{Hn}^*(z) - \mu_n^* = -\frac{\beta^2}{(\beta |z - a| + z_{0n})^4}, \quad (1) \]

with
\[ \beta = \frac{2}{15\pi} \quad \text{and} \quad z_{0n} = \left( \frac{\beta^3}{\pi m_n^* a} \right)^{1/5}. \]

\[ V_{Hn} = V_{Hn}/R_{yn}^* \quad \text{and} \quad \mu_n^* = \mu/R_{yn}^* \quad \text{are given in units of the effective Bohr radius and effective Rydberg,} \]
\[ a_{0n}^* = \frac{\epsilon_r \hbar}{m^* e^2} \quad \text{and} \quad R_{yn}^* = \frac{\epsilon^2}{2 \epsilon_r a_{0n}^*}. \]

In the case of a single p-type delta-doped quantum well centered in \( z = b \), the confining potential can be written as [14],
\[ V_{Hp}^*(z) - \mu_p^* = \frac{\alpha^2}{(\alpha |z - b| + z_{0p})^4}, \quad (2) \]

with
\[ \alpha = \frac{2 m_p^{3/2}}{15\pi} \quad \text{and} \quad z_{0p} = \left( \frac{\alpha^3}{\pi m_{p}^{*} a} \right)^{1/5}. \]

\[ V_{Hp} = V_{Hp}/R_{yp}^* \quad \text{and} \quad \mu_p^* = \mu/R_{yp}^* \quad \text{are given in units of the effective Bohr radius and effective Rydberg,} \]
\[ a_{0p}^* = \frac{\epsilon_r \hbar}{m_{p}^* e^2} \quad \text{and} \quad R_{yp}^* = \frac{\epsilon^2}{2 \epsilon_r a_{0p}^*}. \]

The next step is the construction of the pnDD potential well, so the potential can be written as
\[ V_{H}^*(z) = -\frac{\beta^2}{(\beta |z| + z_{0n})^4} + \frac{\alpha^2}{(\alpha |z| - |l| + z_{0p})^4}, \quad (3) \]

where \( a \) and \( b \) have been taken as 0 and \( l \).

The latter equation summarized the model for the conduction and valence band bending profile. Instead of carrying out numerically troublesome self-consistent calculations, we simply solve the Schrödinger-like effective mass equations at the zone center \( k = 0 \), thus obtaining the corresponding subband electron and hole levels.

### 3. Results and Discussion

The input parameters for the delta-doped quantum wells are:
\[ m^*_e = 0.067m_0, \quad m^*_h = 0.52m_0, \quad m^*_l = 0.087m_0, \quad \epsilon_r = 12.5 \quad \text{and} \quad 10^{12} \leq p_{2D} \leq 10^{14} \text{ cm}^{-2}. \]

In Fig. 1 the potential profiles of the pnDD quantum wells are depicted for various interwell distances for fixed impurity density in the delta-doped layers, \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( p_{2D} = 1 \times 10^{13} \text{ cm}^{-2} \). We can see that the width of the confining region increases as the potential barrier is moved away from the n-type delta-doped layer. This is reflected in the number of electron and hole states and their effective confinement, see Fig. 2.

![Figure 1. Potential profile of pnDD quantum wells in GaAs for various distances between the donor and acceptor layers. The donor and acceptor densities are: \( n_{2D} = 1 \times 10^{12} \text{ cm}^{-2} \) and \( p_{2D} = 1 \times 10^{13} \text{ cm}^{-2} \).](image1)

![Figure 2. Electron and hole levels versus the interlayer distance of pnDD quantum wells in GaAs. The impurity density in the donor and acceptor layers is the same as that in Fig. 1.](image2)

![Figure 3. Electron 1DBR versus the donor density (n-type) in a delta-doped quantum well.](image3)
The electronic structure of $P/N$ delta-doped quantum wells in GaAs is studied. In Fig. 4, we present the 1DBR ($\sigma_1^{1D}$) for the electron ground level as a function of the donor density. The impurity concentrations managed are in the experimental range of interest. The 1DBR changes from 47 to 22 Å for the lower and the higher donor densities considered, which constitute a reduction of 50%. In general, the 1DBR depends on the effective mass, the relative dielectric constant, the confinement of the carriers and the impurity density. In the case of delta-doped wells, 1DBR is inversely proportional to the density as it is seen in Figs. 3 and 4. At first sight, we can expect that the dependency of 1DBR on the impurity density to be proportional to some power law of the latter, and inversely proportional to the confinement as in the 3D case. However, in delta-doped wells, the confinement of the carriers is proportional to the impurity density ($E \approx n_2^{2/3}$); as a consequence, the 1DBR inversely depends on the impurity density. This behavior resembles what happened in atoms in which the atomic number takes the role of the impurity density. In Fig. 4 we depict the same as in Fig. 3 but for the ground level of heavy holes, $p$-type delta-doped wells. The range of acceptor densities considered is larger compared to electrons due to the experimental interest. The main difference between Figs. 3 and 4 comes from the heavy hole effective mass that is approximately six times greater than that of the electron, which affects primarily the hole confinement and reflects on a reduction of the 1DBR. This reduction is nearly of 50% as compared to electrons for the same impurity range.

Figures 3 and 4 also permit us to discern the distance between the donor and acceptor layers to avoid or generate a shrink in the potential barrier whether for electrons or holes, which is essential in devices based on $pnDD$ quantum wells, ALD-FET and sawtooth superlattices.

4. Conclusions

In summary, we have presented the electronic structure in $pnDD$ quantum wells within the envelope function approximation. The Thomas-Fermi approach has been used to model the bending of the conduction and valence band for electrons and holes, respectively. The electronic structure is analyzed as a function of the distance between the donor and acceptor layers. Special attention is paid to the 1DBR, where we find the optimum interwell distances to avoid a reduction in the potential barriers of the $pnDD$ quantum wells, which is essential in electronic devices based on these structures.

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