Miniband structure analysis of n-type delta-doped GaAs superlattices

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The miniband structure of n-type delta-doped GaAs superlattices is studied using the nearest neighbors $sp^3s^*$ tight-binding model including spin. The confining potential caused by the ionized impurities is obtained analytically within the lines of the Thomas-Fermi approximation. This potential is considered as an external perturbation in the tight-binding methodology and it is added to the diagonal terms of the tight-binding Hamiltonian. Special attention is paid to the miniband energy-width variation caused by the change in the impurity density and the interwell distance. The results are compared with the available experimental and theoretical data and a good agreement is found.

**Keywords:** Delta-doped superlattices; miniband structure; tight-binding model.

Se estudia la estructura de minibandas en superredes delta dopadas tipo n en GaAs dentro del modelo tight-binding a primeros vecinos y la base $sp^3s^*$ incluyendo el espín. El potencial de confinamiento causado por las impurezas ionizadas se obtiene analíticamente con el uso de la aproximación de Thomas-Fermi. Este potencial es considerado como una perturbación externa en la metodología tight-binding y es sumado a los términos diagonales del Hamiltoniano tight-binding. Se presta especial atención a la variación en el ancho energético de las minibandas causado por el cambio en la densidad de impurezas y la distancia entre los planos dopados. Los resultados obtenidos también son comparados con los datos teóricos y experimentales disponibles obteniendo un buen acuerdo.

**Descriptors:** Superredes delta dopadas, estructura de minibandas, modelo tight-binding.

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1. Introduction

The delta-doped semiconductor superlattices are important structures for the optoelectronic devices due to their particular properties -high carrier density and miniband formation- that can be exploited in devices based on parallel or vertical transport [1]. Besides, these structures are ideal systems to test the resolution of image techniques [2], to study self-compensation [3] and intermixing effects [4], as well as to analyse the disorder effects [5].

In particular, Si delta-doped GaAs superlattices have been studied both theoretically and experimentally by several authors [6-14]. Photoluminescence [8, 10, 14], photoreflectance [13], Raman scattering [12-14] and magnetotransport measurements [7] have been used to investigate the miniband structure formation in various Si delta-doped GaAs superlattices.

In the present paper we analyse the miniband structure formation of Si delta-doped GaAs superlattices within the nearest neighbors $sp^3s^*$ tight-binding model including spin. The confining potential induced by the ionized impurities and the electronic charge is obtained analytically in the Thomas-Fermi theory. This potential is considered as an external perturbation in the tight-binding methodology, and it is added to the diagonal terms of the tight-binding Hamiltonian. Detailed information of the miniband structure formation as a function of the impurity density and the interwell distance is given, and a comparison with the available theoretical and experimental data is discussed.

2. Theoretical framework

The scheme of calculation starts by modelling the conduction 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) [15],

$$V_H^*(z) = -\frac{\alpha^2}{(\alpha |z| + z_0)^4}$$

The corresponding expression for $V_H^*(z)$ in superlattices (SL’s) is constructed with a suitable combination of the potential functions of multiple delta-wells and it is incorporated to the diagonal terms of the tight-binding Hamiltonian [16],

$$TB_{ii}(n) = TB_{ii}(0) + V_H^*(n)$$

where the potential $V_H^*(n)$ is the potential $V_H^*(z)$ written in discrete coordinates $n$ numbering the atomic layers.

3. Results and Discussion

The tight-binding calculations in the present paper are performed in the spin-dependent $sp^3s^*$ basis (nearest neighbors) at the center of the two-dimensional Brillouin zone for the (001) direction of the delta-doped GaAs. The size of the inhomogeneous doped region (the width of the SL) is varied as the interwell distance and the number of periods vary. The finite inhomogeneous slab is matched with two homogeneous semi-infinite GaAs barriers within the frame work of the surface Green function matching method [17, 18]. The Green function of the inhomogeneous part is obtained through an algorithm previously presented and applied to this kind of systems [18], while the Green functions of the barrier are calculated within the usual transfer matrix approach [19].
The tight-binding parameters are taken from [16]. These parameters give good band structure values at \( \Gamma \) point for zero temperature (0 K) taking into account the spin as well as the commonly accepted effective mass values \( m^*_e = 0.068m_0 \), \( m^*_h = 0.62m_0 \) and \( m^*_\text{hh} = 0.081m_0 \) according to the formulas of Boykin et al. [20]. The values of the diagonal tight-binding parameters and the parameters \( V_{xx}, V_{ss} \) are the same as in the work of Priester et al. [21].

The following values of the system parameters were used in the calculations: \( n_{2D} = 0.068m_0c^2, \) \( \varepsilon_r = 12.5, \) and the impurity density ranging from \( 1 \times 10^{12} \text{ cm}^{-2} \) to \( 10 \times 10^{12} \text{ cm}^{-2} \).

In Fig. 1 we present our results for the potential well profiles in a SDDQW and a SL. Both ionized impurity density and interwell separation length were chosen, in order to give an overall idea of the formation of the energy minibands due to the interaction between the multiple delta-doped wells.

In Table I the miniband width is presented as a function of the impurity density and the interwell distance. The number of periods in each case is 10. As it is clearly seen from the table, an increase in the interwell distance makes the miniband narrower. If the interwell distance is large enough, the delta wells don’t interact and the electronic structure of an isolate delta-doped well is recovered. For example, the miniband energy-width of the basic miniband changes from 23.5 meV for 40 ML’s to 3.6 meV for 60 ML’s and 0 for 80 ML’s at a fixed concentration of \( 5 \times 10^{12} \text{ cm}^{-2} \). The minibands are wider for the excited states due to the deeper penetration of these states into the barriers, which results in a stronger overlap between their wave functions. At a concentration of \( 5 \times 10^{12} \text{ cm}^{-2} \), the energy-width of the first excited miniband is 35.3, 31.5 and 12.4 meV for interwell distance 40, 60 and 80 ML’s, respectively. A similar behavior is observed when the impurity density at a fixed distance increases; however, in this case the confinement of the miniband levels is stronger because the wells are deeper.

Ke and collaborators [8] have reported the photoluminescence spectra of Si delta-doped GaAs superlattices. The observed peaks in the PL spectra have been assigned to the direct transition between the photogenerated holes localized in the barriers and the conduction minibands. (The doping creates wells in the valence band.) The samples consist of ten periods with an impurity density per delta doping spike of \( 5 \times 10^{12} \text{ cm}^{-2} \) and period widths of 350 and 100 Å. They obtained a peak at 1.493 eV in the case of 100 Å assigned to the recombination of electrons in the basic conduction miniband (\( \Delta_0 \)) and the photogenerated holes in the valence band, while in the case of 350 Å the peak is located at 1.510 eV and is assigned to the recombination with the first miniband (\( \Delta_1 \)). The basic levels don’t form a miniband and are completely degenerated and independent. According to our calculations we obtain an energy of 1.5196 eV in the first case (100 Å), while in the second case (350 Å) the energy is 1.5229 eV, which represents an error less than five percents with respect to the PL data.

A selfconsistent study of the electronic properties of n-type delta-doped GaAs superlattices is presented in Ref. 9. In particular, for a superlattice with a period of (1) 500 Å \( (1 \times 10^{12} \text{ cm}^{-2}) \) and (2) 300 Å \( (5 \times 10^{12} \text{ cm}^{-2}) \) the calculated mean energy distances between the occupied minibands are 20 and 8 meV, and 70, 25 and 10 meV, respectively, in fair agreement with the spectral data cited in [9] (see the references therein). Our calculations give mean energy distances of 19.5 and 7 meV for (1) and 65, 26 and 15 meV for (2).

The diamagnetic effects in delta-doped structures are analysed in Ref. 11. It is found that the diamagnetic depopulation characteristics dominate when an in-plane magnetic field is applied to single or two couple delta layers, while in

<table>
<thead>
<tr>
<th>( n_{2D} )</th>
<th>( \Delta E_{c1} )</th>
<th>( \Delta E_{c2} )</th>
<th>( \Delta E_{e1} )</th>
<th>( \Delta E_{e2} )</th>
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<td>1</td>
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<td>4.8</td>
<td></td>
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<tr>
<td>5</td>
<td>23.5</td>
<td>35.3</td>
<td>3.6</td>
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<td>14.7</td>
<td>73.2</td>
<td>0.6</td>
<td>24.8</td>
</tr>
</tbody>
</table>

Table I. Energy-width (meV) of the basic and the first excited minibands for 40 ML's, 60 ML's and 80 ML's for impurity densities 1, 5 and 10 in units of \( 10^{12} \text{ cm}^{-2} \).
the case of multiple delta layers the edge effects become less important. An energy-width of 20 meV for the basic miniband in ten couple delta layers with an impurity density of $3 \times 10^{12} \text{cm}^{-2}$, a period width of 135 Å and a zero magnetic field is also reported. We obtain for the same delta-doped structure an energy-width of 17 meV.

De Sousa and colleagues [13] have measured the photoreflectance spectrum of n-type GaAs delta-doped superlattices. They discuss three different contributions: (1) The intrinsic GaAs; (2) The Frans-Keldysh (FKO) oscillations due to the surface electric field; and (3) The FKO attributed to the buffer/superlattice interface. In the case of a twenty five period superlattice with a period width of 200 Å and an impurity density per period of $1.2 \times 10^{12} \text{cm}^{-2}$ the main peak attributed to (3) is located at 1.5158 eV. We find for the same system parameters an energy difference between the $\Delta_0$ miniband and the basic heavy hole level of 1.5324 eV.

4. Conclusions

The miniband structure formation of n-type delta-doped GaAs superlattices is analysed within the framework of the nearest neighbors $sp^3s$ tight-binding model including spin. The miniband structure computation relies on an analytical expression for the SL confining potential obtained in the Thomas-Fermi approximation. The doping concentration and the interwell distance act as useful tuning parameters for the miniband position, the miniband energy-width and the number of minibands. These results can be used in the design of the optoelectronic devices based on vertical transport. The tight-binding model combined with the Thomas-Fermi approximation seems to be an efficient tool in the studies of electronic properties in inhomogeneous semiconductor structures, such as delta-doped superlattices.

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