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Tight-binding study of the hole subband structure properties of p-type delta-doped quantum wells in Si by using a Thomas-Fermi-Dirac potential

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Abstract. We present the hole subband structure of p-type delta-doped single, double, multiple and superlattice quantum wells in Si. We use the first neighbors sp^3s^* tight-binding approximation including spin for the hole level structure analysis. The parameters of the tight-binding hamiltonian were taken from Klimeck et al. [Klimeck G, Bowen R C, Boykin T B, Salazar-Lazaro C, Cwik T A and Stoica A 2000 *Superlattice. Microst.* **27** 77], first neighbors parameters that give realiable results for the valence band of Si. The calculations are based on a scheme previously proposed and applied to delta-doped quantum well systems [Vlaev S J and Gaggero-Sager L M 1998 *Phys. Rev. B* **58** 1142]. The scheme relies on the incorporation of the delta-doped quantum well potential in the diagonal terms of the tight-binding hamiltonian. We give a detail description of the delta-doped quantum well structures, this is, we study the hole subband structure behavior as a function of the impurity density, the interwell distance of the doped planes and the superlattice period. We also compare our results with the available theoretical and experimental data, obtaining a reasonable agreement.

1. Introduction

Doping plays a fundamental role in semiconductor physics due to the physical properties of semiconductor systems can be easily modified through the incorporation of impurities. Among the most important doping techniques is the so called delta-doping, which has as key features the amount of charge that can be reached and the precision of the impurity seeding (up to atomic scale). With this technique it is possible to obtain bidimensional doping densities (p_{2D}) above 10^{12} cm^{-2} and doping profile widths of tenth of angstroms, these factors causes a strong electric field that confines the charge carriers in a V-shaped potential or better known as delta-doped quantum well. Studies on p-type B δ-doped Si quantum wells have been reported [1, 2, 3, 4, 5]. Due to the technological importance of Si and the particular properties of the δ-doped systems, they appear to be of interest for application in the electronic device industry and for basic investigation as well. In this particular, the B δ-doped Si QW has been investigated from the theoretical and experimental points of view [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]. It is clear that in the case of p-type systems the simultaneous consideration of the heavy and light hole bands is unavoidable because the electric charge is distributed among them. Some works [5, 6] have shown that, even at $T = 0$ K, the contribution of the split-off(so) band turns out to be important when the value of the impurity density p_{2D} is greater or equal to 2×10^{13} cm^{-2}. The reason for this effect to

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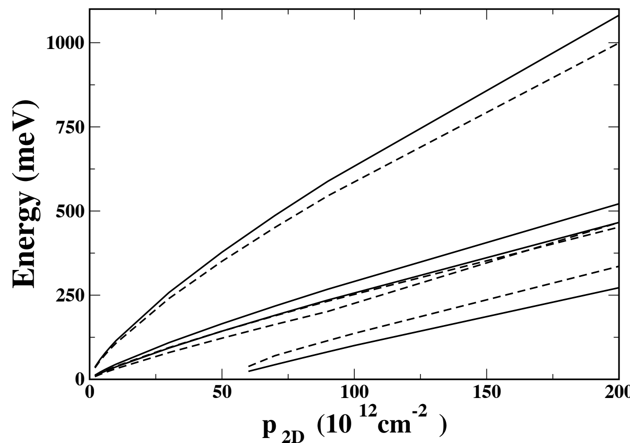

Figure 1. Hole subband structure versus doping density of SDD quantum wells in Si.

occur relies in the relative population of the different bands: for values of p_{2D} above 5×10^{13} cm^{-2}, the relative occupation number of the so_0 level is greater than the corresponding to the lh_0 level, and ranks as the second after the hh_0 population.

In the present work we study the hole subband structure of p-type delta-doped quantum wells in Si. We use a Thomas-Fermi-Dirac scheme and first neighbors sp^{3}s* tight-binding approximation (including spin) for the modeling of the confining potential and the hole subband structure, respectively. We have implemented tight-binding parameters that are suitable for the description of the valence band of Si [11]. We analyze the level structure behavior of single, double and superlattice delta-doped (SDD, DDD and SLDD) quantum wells as a function of the paramount parameters in each of these systems. We find that the split-off band influences the hole subband structure, even for low impurity densities, in a considerable way. We also compare our results with the theoretical and experimental data available obtaining a reasonable agreement.

2. Mathematical method

The scheme of calculation starts by modeling the valence band profile, within the local density Thomas-Fermi-Dirac approximation. The outcome of this approach is an analytical expression for the one-dimensional potential energy function describing the band bending in a SDD quantum well considering the exchange effects [12],

$$V^*(z) = \frac{\alpha^2}{(\alpha\,|z| + z_0)^4} - \frac{2\varsigma^2(w)m_a}{\pi^2}\left[1 - \sqrt{1 + \frac{\pi^2}{\varsigma^2(w)m_a}\frac{\alpha^2}{(\alpha\,|z| + z_0)^4}}\right], \quad (1)$$

where α and z_0 are constants that come in terms of the effective masses, dielectric constant and the impurity density, and ς takes account of the coupling between the light and heavy hole bands [12].

The corresponding expression for $V^*(z)$ in DDD and SLDD is constructed with a suitable combination of the potential functions of multiple delta-wells and is incorporated to the diagonal terms of the tight-binding Hamiltonian [13],

$$TB_{ii}(n) = TB_{ii}(0) + V^*(n) \quad (2)$$

where the potential $V^*(n)$ is the potential $V^*(z)$ written in discrete coordinates, in which n numbers the atomic layers.

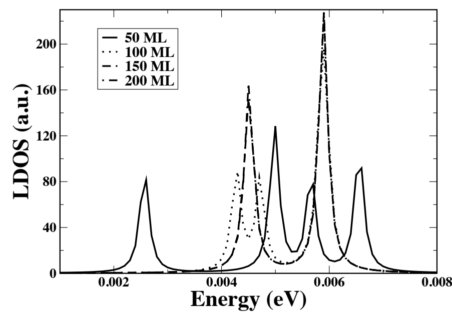

Figure 2. Local denisty of states versus energy of DDD quantum wells in Si. The doping density is fixed at 1×10^{12} cm^{-2}, while the interwell distance takes values of 50, 100, 150 and 200 ML's.

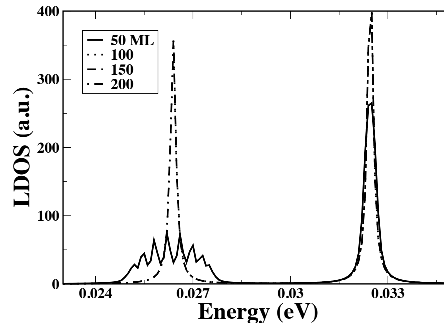

Figure 3. Local density of states versus energy of SLDD quantum wells in Si. The doping density is fixed at 8×10^{12} cm^{-2}, while the interwell distance takes values of 50, 100, 150 and 200 ML's.

3. Results and discussion

We use a set of typical input parameters for the confining potential [14]. At first, we analyze the subband hole level structure of SDD quantum wells taking into account the split-off band contribution and without it by means of the parameter m_a that appears in the kinetic term of the Thomas-Fermi energy functional. In Fig. 1 we can see the behavior of the hole subband level structure as a function of the doping density with (dashed lines) and without the split-off contribution (solid lines). From top to bottom we have the potential depth, ground heavy hole state, ground light hole state and ground split-off state, respectively. As it is possible to see from the mentioned figure the split-off contribution takes relevance in the high density limit in which energy differences from 60 meV to 80 meV are found in the hole subband level structure as compare to the calculations without the abovementioned contribution. The hole level structure behavior is the typical one expected to the delta-doped quantum well systems with a stronger confinement as the doping density is increased.

In the case of DDD we can figure out the hole level structure behavior with respect to the interwell distance through the evolution of the local density of states (LDOS). In Fig. 2 we present the LDOS of DDD quantum wells with a doping density of 1×10^{12} cm^{-2} and four interwell distances (50, 100, 150 and 200 ML). As it is clearly seen the DDD systems is practically degenerate for 150 and 200 ML meanwhile for 100 ML the ground light hole state splits in two levels with energy difference of about a 1 meV. In the case of 50 ML both the ground light hole state and the heavy hole state splits in two levels with energy differences of 2.5 meV and 1 meV, respectively. In a similar fashion the SLDD quantum well system presents a energy level splitting, however is only evident for the ground hole light state for a period width of 50 ML. The impurity density considered in Fig. 3 is 8×10^{12} cm^{-2}. In order to discern the evolution of the hole level structure, of both DDD and SLDD quantum well systems, as a function of the impurity density we have considered DDD and SLDD quantum wells with a fixed interwell distance (50 ML) and doping densities of 3, 7, 20, 60, 100 and 200 in units of 10^{12} cm^{-2} that corresponds to the top left, top middle, top right, bottom left, bottom middle and bottom right of Figs. 4 and 5, respectively. The hole level structures of the bottom part of both figures belong practically to the level structure of SDD quantum wells which means that the delta-doped quantum wells do not interact at all as a consequence of the stronger confinement experience by the carriers as the doping density is increased. On the contrary, the top part of both figures shows a clear level splitting for low doping densities due to the better sloping of the

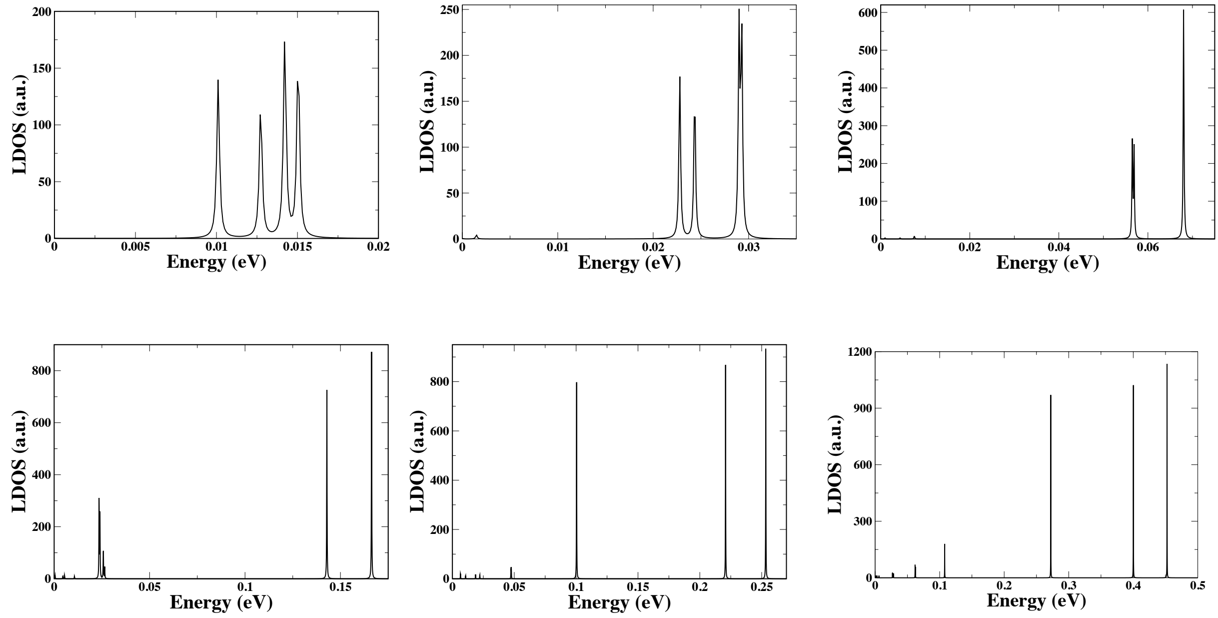

Figure 4. Local density of states versus energy of DDD quantum wells in Si with interwell distance of 50 ML and doping densities of: (Top) 3 left, 7 middle and 20 right; (Bottom) 60 left, 100 middle and 200 right. The doping density is in units of 10^{12} cm^{-2}.

hole subband levels.

Finally, in table 1 we present a comparison of our results with respect to the experimental data based on absorption and conductance measurements [3, 4, 2] as well as the theoretical data based on the $\mathbf{k} \cdot \mathbf{p}$-Envelope Function Approximation (EFA) [6, 14]. Our results agree within a 15 % for doping densities of 35 and 90 (in units of 10^{12} cm^{-2}) meanwhile for a doping density of 24 (in units of 10^{12} cm^{-2}) our approximation is frankly far from the experimental value within an error of 30 %.

Table 1. SDD hole subband energy comparison with respect to the experimental [3, 4, 2] and theoretical data [6, 14]. The doping density is in units of 10^{12} cm^{-2} and the energies in units of meV.

p_{2D}	TB	EFA	Exp.
24	79	99	110 ± 20
35	107	129	125
90	232	274	270

4. Conclusions

In summary, we have presented the hole subband level structure of quantum well systems in Si. We adopted a Thomas-Fermi-Dirac scheme for the confining potential as well as the nearest neighbors sp^{3}s* Tight-Binding approximation including spin for the hole subband level structure. We have analyzed the single, double and superlattice delta-doped quantum wells as a function of

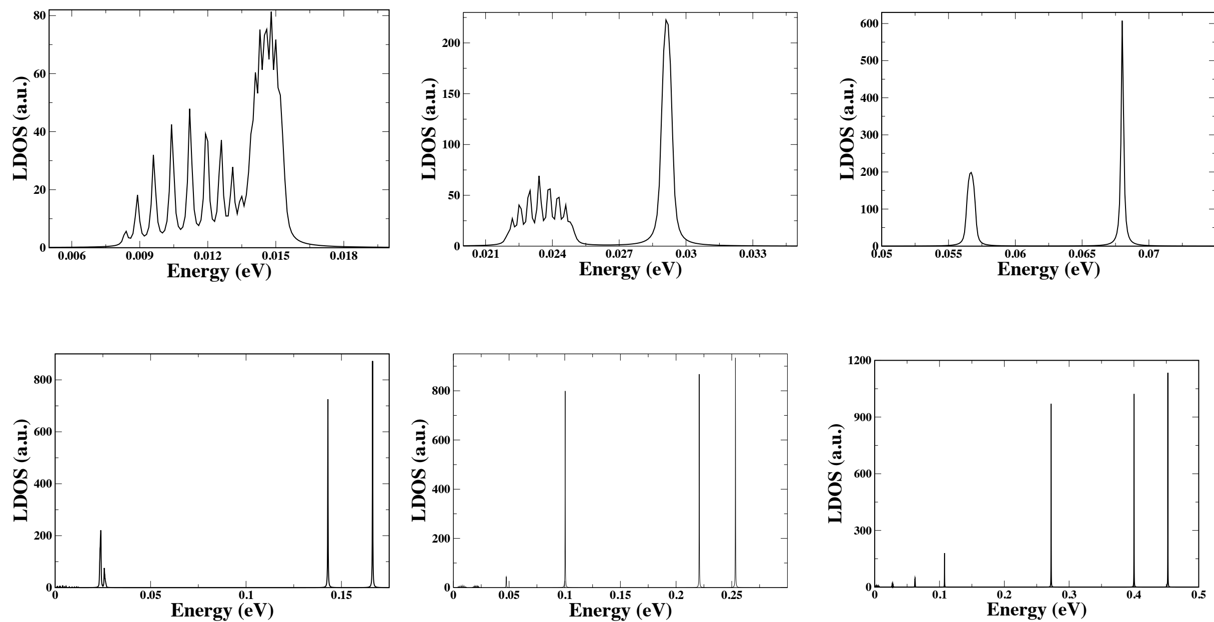

Figure 5. Local density of states versus energy of SLDD quantum wells in Si with a period of 50 ML and doping densities of: (Top) 3 left, 7 middle and 20 right; (Bottom) 60 left, 100 middle and 200 right. The doping density is in units of 10^{12} cm^{-2}.

the main parameter in each case. We also compare our results with the available experimental data obtaining a good agreement.

Acknowledgments

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