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ELECTRON SUBBAND STRUCTURE AND MOBILITY TRENDS IN *P*-*N* DELTA-DOPED QUANTUM WELLS IN *SI*

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Abstract—We present the electronic spectrum of a n-type delta-doped quantum well in Si coupled to a p-type delta-doped barrier within the envelope function effective mass approximation. We applied the Thomas-Fermi approximation to derive an analytical expression for the confining potential, and thus, we obtain the electronic structure in a simple manner. We analyzed the electron subband structure varying the distance between the doping planes (l) as well as the impurity density in them (n_{2D}, p_{2D}). We also study the mobility trends through an empirical formula that is based on the electron levels, the electron wave functions and the Fermi level. We find a monotonic decrease in the mobility as the p-type barrier moves away from the n-type well, and optimum parameters, $l = 70\,\text{Å}$ and $n_{2D} = 5 \times 10^{12}\,\text{cm}^{-2}$ and $p_{2D} = 5 \times 10^{13}\,\text{cm}^{-2}$, for maximum mobility.

1. INTRODUCTION

Recently, the delta-doping has been used as a backbone technique to improve important characteristics, such as the linearity, in field effect transistor devices for application in millimeter-wave integrated circuits

(MMIC) and wireless components [1–7]. The better performance of the mentioned devices relies on an improvement in the transport properties via optimization of the coupling between the delta layers and the heterostructure region.

In particular, high carrier densities, two-three orders of magnitude greater than in $GaAs$ systems, can be achieved in Silicon systems by means of delta-doping [8]. Delta-doped quantum wells in Si are ideal structures to study the transport properties of ultra dense two dimensional electron gases (2DEG) [9, 10] Important parameters are the mobility, mean free path and phase coherent length due to their implications in ballistic and coherent nanodevices. Meanwhile the carrier concentration in this kind of systems is ultra high, the mobility is very low, which is opposite to what happen in $GaAs/AlGaAs$ systems [11]. An improvement in the conductivity, not properly the mobility, could be reach via the coupling of delta-doped layers [12]. The main proposal relies in finding the interwell distance at which the mobility is maximum in conjunction with the high carrier density coming from the two doped planes, such that the conductivity -the product of the mobility and the carrier density-enhances [13].

The aim of the present study is to analyze the implications that represent a p-type delta-doped barrier near a n-type delta-doped quantum well in Si. The electronic structure and the mobility trends as a function of the interlayer distance and the impurity concentration are obtained. The Thomas-Fermi approximation and the effective mass theory are combined to obtain the confining potential and the electron subband levels. The mobility calculations are performed via an empirical formula previously proposed and applied to n, p, and p-n delta-doped systems [12, 14, 15]. We find that the electron confinement plays an important role to improve the mobility. We obtain an optimization in the mobility at interwell distance of 70 Å and donor and acceptor concentrations of 5 and 50 in units of $10^{12}\,\mathrm{cm}^{-2}$.

2. MATHEMATICAL METHOD

For a single n-type δ-doped quantum well in Si centered at $z = a$ the confining potential can be written as [12],

$$V_{Hn}^{*}(z) - \mu_n^{*} = -\frac{\beta^2}{(\beta\,|z-a| + z_{0n})^4}, \tag{1}$$

with $\beta = \frac{2}{15\pi}$ and $z_{0n} = \left(\frac{\beta^3}{\pi n_{2D}^{au}}\right)^{1/5}$. $V_{Hn}^{*} = V_{Hn}/R_{yn}^{*}$ and $\mu^{*} = \mu/R_{yn}^{*}$ are given in units of the effective Bohr radius and effective Rydberg, $a_{0n}^{*} = \frac{\epsilon_r \hbar}{m^{*} e^2}$ and $R_{yn}^{*} = \frac{e^2}{2\epsilon_r a_{0n}^{*}}$.

In the case of a single p-type δ-doped quantum well in Si centered at $z = b$ the confining potential can be written as [16],

$$V_{Hp}^{*}(z) - \mu_p^{*} = \frac{\alpha^2}{(\alpha\,|z-b| + z_0)^4}, \tag{2}$$

with $\alpha = \frac{2m_a^{3/2}}{15\pi}$ and $z_{0p} = \left(\frac{\alpha^3}{\pi p_{2D}^{au}}\right)^{1/5}$. $V_{Hp}^{*} = V_{Hp}/R_{yp}^{*}$ and $\mu_p^{*} = \mu/R_{yp}^{*}$ are given in units of the effective Bohr radius and effective Rydberg, $a_{0p}^{*} = \frac{\epsilon_r \hbar}{m_{hh}^{*} e^2}$ and $R_{yp}^{*} = \frac{e^2}{2\epsilon_r a_{0p}^{*}}$.

The next step is the construction of the p-n delta-doped ($pnDD$) potential well through a proper combination of the potentials for electrons and holes

$$V_H^{*}(z) = -\frac{\beta^2}{(\beta\,|z| + z_{0n})^4} + \frac{\alpha^2}{(\alpha\,|z+l| + z_0)^4} \tag{3}$$

where a and b have been taken as 0 and l.

The latter equation summarizes the model for the conduction band bending profile. Instead of carrying out numerically troublesome self-consistent calculations, we simply solve Schrödinger-like effective mass equations at the zone center $\mathbf{k} = \mathbf{0}$, thus obtaining the corresponding subband longitudinal and transverse electron levels.

For the mobility calculations we implement an empirical formula previously proposed and applied to n, p and p-n delta-doped systems [12, 14, 15],

$$\mu_{rel}^{\delta} = \frac{\mu_{pnDD}}{\mu_{SDD}} = \frac{\displaystyle\iint \rho_e^{\delta}(z')\rho_{imp}^{\delta}(z)\,|z-z'|\,dzdz'}{\displaystyle\iint \rho_e^{pn\delta}(z')\rho_{imp}^{pn\delta}(z)\,|z-z'|\,dzdz'}, \tag{4}$$

where ρ_e^{δ} and ρ_{imp}^{δ} ($\rho_e^{pn\delta}$ and $\rho_{imp}^{pn\delta}$) represent the density of electrons and impurities of SDD (of $pnDD$), respectively. Substituting the density of electrons and impurities and integrating over z we obtain,

$$\mu_{rel}^{\delta} = \frac{\displaystyle\sum_{ij} m_j \int \left|F_{ij}^{\delta}(z')\right|^2 (k_F^{\delta} - E_{ij}^{\delta})\,|z'|\,dz'}{\displaystyle\sum_{ij} m_j \int \left|F_{ij}^{pn\delta}(z')\right|^2 (k_F^{pn\delta} - E_{ij}^{pn\delta})\,|z'|\,dz'}, \tag{5}$$

where $F_{ij}^{\delta}(z')$, k_F^{δ} and E_{ij}^{δ} ($F_{ij}^{pn\delta}(z')$, $k_F^{pn\delta}$ and $E_{ij}^{pn\delta}$) are the envelope function, the Fermi level and the ith level respectively of the SDD (of $pnDD$).

3. RESULTS AND DISCUSSION

We have found the potential and electronic mobility of a p-n delta-doped quantum wells in Si. The donor and acceptor concentrations goes from $5 \times 10^{12}\,\text{cm}^{-2}$ to $5 \times 10^{13}\,\text{cm}^{-2}$.

In Fig. 1, we present the p-n potential profile for various interwell distances, from 500 to 50 Å. We can see that there is a small decrement in the altitude of the p-type well for 100 and 50 Å and a reduced wide in n-type well, because of the recombination. But in these distances still persist a good confinement of electrons and holes densities. Fig. 2

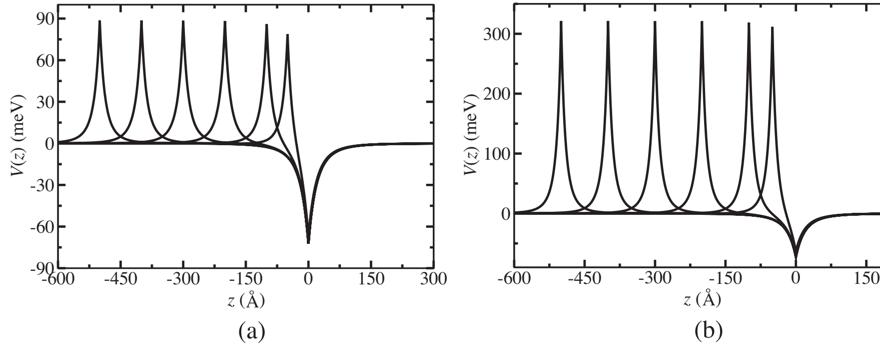

Figure 1. Potential profile of p-n delta-doped quantum wells for different interwell distances with: (a) $n_{2D} = 5 \times 10^{12}$ and $p_{2D} = 1 \times 10^{13}\,\text{cm}^{-2}$, (b) $n_{2D} = 5 \times 10^{12}$ and $p_{2D} = 5 \times 10^{13}\,\text{cm}^{-2}$.

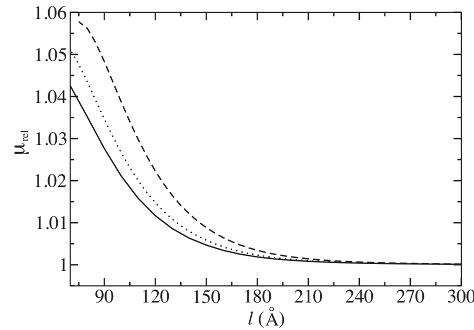

Figure 2. Relative mobility versus the distance between the n-type well and the p-type barrier. The donor density remains fix at $5 \times 10^{12}\,\text{cm}^{-2}$, meanwhile the acceptor concentration takes three values 5 (solid), 10 (dot) and 50 (dash) in units of $10^{12}\,\text{cm}^{-2}$.

sketches the mobility, for three concentrations in the p-type delta-doped barrier remaining fix the donor concentration, as function of the p-n separation. We found a monotonic growth in the mobility as the p-n distance decrease. The best improvement in mobility was found in 70 Å interwell distance with donor and acceptor concentrations of 5×10^{12} and $5 \times 10^{13}\,\mathrm{cm}^{-2}$. The improvement in mobility is attributed to a good confinement of electron densities, so this is a way to enhance the transport properties in p-n delta-doped quantum wells in Si.

4. CONCLUSION

In summary, we study the effects that produces a p-type barrier near a n-type delta-doped quantum well in Si. The Thomas-Fermi theory combined to the effective mass approximation are used for the electron level calculations. An empirical formula is implemented for the mobility-trend analysis. The electronic structure and mobility trends are analysed as a function of the backbone parameters in the system, interlayer distance and impurity density. We find that the electronic confinement plays an important role to optimize the mobility. We obtain an optimization in the mobility at interwell distance of 70 Å and donor and acceptor concentrations of 5 and 50 in units of $10^{12}\,\mathrm{cm}^{-2}$.

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