Valence band states in Si-based p-type delta-doped field effect transistors

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Abstract. We present tight-binding calculations of the hole level structure of \( \delta \)-doped Field Effect Transistor in a Si matrix within the first neighbors \( sp^3s^* \) semi-empirical tight-binding model including spin. We employ analytical expressions for Schottky barrier potential and the p-type \( \delta \)-doped well based on a Thomas-Fermi approximation, we consider these potentials as external ones, so in the computations they are added to the diagonal terms of the tight-binding Hamiltonian, by this way we have the possibility to study the energy levels behavior as we vary the backbone parameters in the system: the two-dimensional impurity density \( \rho_{2D} \) of the p-type \( \delta \)-doped well and the contact voltage \( V_c \). The aim of this calculation is to demonstrate that the tight-binding approximation is suitable for device characterization that permits us to propose optimal values for the input parameters involved in the device design.

1. Introduction

The field effect transistor with \( \delta \)-doping (\( \delta \)-FET) was proposed firstly by F. Schubert and K. Ploog [1, 2, 3]. They constructed a FET with a Schottky base (metal-semiconductor contact) grown by MBE. The \( \delta \)-doped layer of n-type impurities in this device is located at a fixed distance from the metal-semiconductor contact and spreads the whole region from the source terminal to the drain terminal. The authors compare this transistor with the FET and HEMT (high electron mobility transistor), the latter having an inversion layer channel. The \( \delta \)-FET is a system where a high carrier concentration of the two-dimensional electron gas can be achieved. As a consequence, high transversal conductance \( (g_m) \) results, the latter being inverse proportional to the transversal resistance, then a low dissipation is expected. Additionally, the \( \delta \)-FET has a higher avalanche breaking potential than the other transistors. The reported mobility is higher than 3000 \( cm^2/V \cdot s \) at \( T = 77 K \). The authors interpret the system as a quasi-two-dimensional electron cloud strongly localized in a biased triangular quantum well (V-type) with a constant electrostatic field \( \phi_b/d \) where \( \phi_b \) is the Schottky barrier height and \( d \) is the distance between the well and the barrier.

A \( \delta \)-FET in Si is constructed by Wu et al. [4, 5] with a B \( \delta \)-doped quantum well as conduction channel (\( \delta \)-FET in Si of p-type). Hall measurements observe a hole mobility of 120 \( cm^2/V \cdot s \) at \( T=300 \) K and of 180 \( cm^2/V \cdot s \) at \( T=77 \) K. The authors estimate an impurity density of the carriers in the \( \delta \)-doped layer of \( 1.8 \times 10^{12} cm^{-2} \) approximately and demonstrate this \( \delta \)-FET has an extrinsic transversal conductance \( g_m \) of 640 \( \mu S/mm \) for a gate length of 5 \( \mu m \).
A deep understanding of the physical phenomena in $\delta$-FETs based on different host materials is needed to improve the optimization of the device parameters. The first step in this process has to be a realistic calculation of the electronic structure of these systems. Semi-empirical tight-binding considerations [6] seem to provide additional information to the results obtained by simple effective-mass models. In the present work we have conducted the first tight-binding calculation of the potential barrier influence on the electronic structure of V-shaped quantum well in p-type $\delta$-doped Silicon FET.

2. Model

The main assumption of the model describing the valence band of the semiconductor crystal in p-type Si $\delta$-doped FET is that the potential profile can be constructed within the depletion region approximation in the proximity of the metal-semiconductor contact and by the V-shaped potential profile obtained in the Thomas-Fermi approach [7] that describes correctly the properties of the isolated p-type $\delta$-doped well, this fact is clearly explained in reference [8]. The model has been applied to study the differential capacitance profile of the device [9, 10], the electronic spectra of $\delta$-doped quantum wells of n- and p- types in GaAs [11] and p-type B $\delta$-doped Si quantum wells [12]. The potential model is:

$$V(z) = -\frac{2\pi e^2}{\varepsilon_r} P_d(z - l)^2 \delta(l - z) + \frac{\alpha^2}{(\alpha |z - d| + z_0)^4} \delta(p - z), \quad (1)$$

where $\alpha = \frac{2m_a^{3/2}}{(15\pi^2)}$ and $z_0 = \left(\frac{\alpha^3}{\pi^3 P_d}\right)^{1/5}$, with $m_a = \left[1 + (m_{lh}/m_{hh})^{3/2} + (m_{so}/m_{hh})^{3/2}\right]^{2/3}$. $P_d$ being the background impurities density, $\varepsilon_r$ is the electric permittivity constant of Silicon, $d$ is the distance at which the p-type $\delta$-doped well is positioned, $p_{2D}$ is the two-dimensional impurities density of the well. And finally $l$ is the screening distance for the electrical field given by:

$$l = \sqrt{\frac{\varepsilon_r V_c}{4\pi e^2 P_d}} \quad (2)$$

where $V_c$ is the contact voltage, that is an input parameter in our calculations.

To take into account an external constant electric field applied to a planar heterostructure in the growth direction in the tight–binding formalism, the value of the external potential is introduced to all diagonal elements of the Hamiltonian matrix in each atomic layer [13]:

$$TB_{ii}(n) = TB_{ii}(0) + neF \quad (3)$$

In the equation 3 the discrete variable $n$ is used, instead of the continuous variable $z$, to label the atomic layers in the growth direction. The zero of the external potential is in the atomic layer $n=0$, $e$ is the electron charge, $F$ is the magnitude of the constant electric field applied along to the growth direction, and $TB_{ii}$ are the diagonal tight-binding parameters ($i$ being the atomic orbitals index). This approximation is considered a reasonable one, at least as a first step, and will not change the nondiagonal tight-binding parameters. This equation shows a shift in the energetic positions of all atomic orbitals in a given atomic layer $n$ with the potential drop $neF$ of the field potential.

In the present work we consider the potential $V(z)$ from Eq. 1 as an external potential applied to a finite region of the projected bulk in the growth direction. Similarly to Eq. 3, we have

$$TB_{ii}(n) = TB_{ii}(0) + V(n) \quad (4)$$
The potential $V(n)$ is the potential $V(z)$ from equation 1, written in discrete notation. The tight-binding (TB) calculations in the present paper are made in spin-dependent $sp^3s^*$ basis (nearest neighbors) at the center of the two-dimensional Brillouin zone for the (001) growth direction of $\delta$-doped Silicon. The Silicon tight-binding parameters were taken from the work [14].

We applied this parameterization to calculate the Stark shifts in quantum wells with different potential profiles [15, 16] and obtained very good results. A next step could be the incorporation of the charge neutrality in a self-consistent way, as in [17], to obtain quantitative dependence of the electronic properties on the contact potential.

The semi-empirical tight-binding model complements the EFA approximation giving information about the dependence of the delta-FET electronic structure on the crystal and band structure of the host material and on the orbital components. Our model can provide also a more detailed study of the total density of states taking into account the electron plane motion considering explicitly all three dimensions of the system. This fact could be a serious advantage in the calculations of many macroscopical properties of the $\delta$-FET.

**Results and discussion**

We present the electronic spectrum description of the $\delta$-FET in a Silicon host material with p-type $\delta$-doping. The following values of the system parameters are used: the background impurities density $P_d = 1.0 \times 10^{18}$ cm$^{-3}$, the contact potential $V_c$ was varied between -100 meV and -1200 meV, the two-dimensional impurities density is $p_{2D} = 3.5 \times 10^{12}$ cm$^{-2}$, the Silicon electric permittivity $\varepsilon_r=11.7$, the heavy hole effective mass $m_{hh}=0.52$, the light hole effective mass $m_{lh}=0.16$ and the split-off one is $m_{so}=0.23$. The distance between the Schottky barrier and the p-type $\delta$-doped well was fixed to 300 Å.

We have considered a slab of 600 monolayers containing the whole system. This size is sufficiently large to avoid the truncation effect for the confined states. The small imaginary part added to the energy as well as the energy step in the Green function numerical calculations were chosen to be 1 meV. We have calculated the density of states to obtain the energies of the confined states and then for each energy we have calculated also the spatial distribution of the state over the slab to determine the symmetry and the type of the confined hole states. The finite slab models our semi-infinite system. One of the surfaces matches the vacuum and here we have a free surface without reconstruction. The second surface is artificial, this is because we consider a large slab. By this way we avoid the influence of the second free surface to the discrete energy spectrum. We have applied this model in [18] obtaining very good results.

In figure 1 we show the density of states (DOS) of p-type $\delta$-doped Silicon FET for different contact potential values. The energy zero coincides with the flat band region of the valence band. The confining potential and the spatial distributions of the ground heavy and light hole states are presented in figure 2 when $V_c=-500$ meV. We can understand the electronic spectrum of our system in terms of the confining potential and interpret qualitatively the features of all spectra in terms of this potential, but only the realistic calculation based on the resolution of the Schrödinger equation in the framework of the model presented in the previous section permit us to obtain semi-quantitative results. Finally in figure 3 we show influence of the contact potential on the energies of the confined hole states for this system, the ground states are mainly affected for contact potentials higher than -800 meV and we obtain that the first heavy hole excited state escapes at contact potential value of -900 meV.

Tight-binding calculations of the electronic spectrum in p-type $\delta$-doped quantum wells in Si are presented in [19]. The confining potential is treated as an external one and the diagonal
The elements of the tight-binding Hamiltonian are modified adding the corresponding terms as in the present work. The authors have used the TB parameters from [14], the same set of parameters we have used in our calculations. The comparison of the results obtained within the EFA and TB approximations given in [19] demonstrates that such kind of approach is suitable for this type of calculations. The agreement between the calculations and the experimental data reported in [19] is quite well.

![Figure 1. DOS for a p-type \( \delta \)-doped Silicon FET when \( p_{2D} = 3.5 \times 10^{12} \) cm\(^{-2}\), and \( V_c = -700 \) meV (pointed line), \( V_c = -800 \) meV (dashed line) and \( V_c = -900 \) meV (solid line).](image)

3. Conclusions
In summary, we present the first tight-binding calculation of the electronic structure of a p-type \( \delta \)-doped silicon FET. The computation relies on analytical expressions for the Schottky barrier and \( \delta \)-doped potentials obtained previously [10] within the depletion and Thomas-Fermi approximation, respectively. These potentials are considered as external ones in the tight-binding formalism and added to the diagonal terms of the tight-binding Hamiltonian. It is shown that the tight-binding formalisms is suitable for the device characterization because the computed energy level behavior reflects the presence of the Schottky barrier potential. The presented scheme permits also to consider the dependence of the electron properties of the \( \delta \)-doped FET on the band structure, growth direction and orbital components.

Acknowledgments
J.C.M.O and S.J.V acknowledge to the National Science and Technology Council (CONACyT) from México, through the retention program, J.C.M.O also acknowledges to the Universidad Autónoma de Zacatecas (UAZ) and to the Consejo Zacatecano de Ciencia y Tecnología (COZCyT) for the financial support.
Figure 2. Potential profile and hole wave function for a p-type δ-doped Silicon FET with \( p_{2D} = 3.5 \times 10^{12} \text{ cm}^{-2} \) and \( V_c = -500 \text{ meV} \).

Figure 3. Energy levels versus the contact voltage for a p-type δ-doped silicon FET with \( p_{2D} = 3.5 \times 10^{12} \text{ cm}^{-2} \) and \( d = 300 \text{ Å} \).

4. References

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