Self–Consistent Solution of the Schrödinger and Poisson Equations for Accumulated MOS Capacitors with Ultra–thin Layers

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Abstract

We present a full quantum–mechanical method for the study of quantum effects in a MOS capacitor with ultra–thin oxide which may contain several layers in the accumulation mode, thereby extending the earlier work that is restricted to the inversion regime. The method is based on a self–consistent solution of Schrödinger and Poisson equations for the entire device composed of the metallic gate, the oxide layers, the conduction channel and the substrate region. The energy levels as well as the corresponding quantum states are calculated for both bound and mobile holes of an accumulated p–type semiconductor. These levels are then used to calculate the leakage gate tunneling current and the carrier charge distribution as a function of the bulk acceptor concentration, the temperature and the hole concentration.

1. Introduction

During the last decades, the development of the electronic devices has reached a size limit where quantum effects become important. These phenomena might change drastically the behavior of the devices, and the consequences of such changes have attracted much attention both theoretically and experimentally [1, 2]. More recently there has been considerable work on quantum effects that arise when the oxide thickness scales down such that the leakage current flowing through the insulator becomes significant. This current is due to direct tunneling through the ultra thin–oxide (around 20 Å). The study of such structures has shown that this effect must be included in the modeling and simulation of deep–submicron CMOS in order to have an accurate electronic device description.

In a previous paper[3], it has been demonstrated that in order to predict the carrier charge distribution in the channel and the tunneling leakage current flowing between the gate and the channel it is required to give a full quantum–mechanical treatment, in which the metal gate, the oxide layers and the semiconductor are considered on the same footing. Such an approach was used for a p–type inversion layer in a MOS capacitor.

The main purpose of this paper is to extend this method to the case of a p–type semiconductor in accumulation under general external conditions of the temperature and doping concentration. In this regime, the situation is more complicated. In fact, in addition to the holes which are spatially bound in the discrete energy levels reflecting the quantized motion perpendicular to the interface, there exist carriers of which the motion is not quantized and for which the wave functions are traveling waves extending into the bulk. These carriers are holes that form the positive charge which compensates the negative charge of ionized acceptors in the bulk region and also contribute to the self–consistent potential near the interface. In the following, we give a brief description of the model and discuss some of the results.

2. Description of the method

We solve Schrödinger and Poisson equations self–consistently using a full quantum mechanical description in which the whole MOS structure is treated as a single system. Using the effective–mass approximation and assuming translation invariance in the lateral directions, the normalized hole-wave function and the corresponding eigenvalue $E_{\alpha k}$ can, respectively, be written as:

$$\psi_{\alpha k}(x, y, z) = \frac{1}{\sqrt{L_x L_y}} \exp[i(k_x x + k_y y)] \phi_{\alpha}(z)$$

$$E_{\alpha k} = W + \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_{ax}} + \frac{k_y^2}{m_{ay}} \right),$$

where the $z$ direction is chosen to be perpendicular to the silicon/oxide interface. The lengths $L_x$ and $L_y$ are the device dimensions in the $x$ and $y$ directions, respectively. The quantities $k_x$ and $k_y$ are the components of the wave vector, $\mathbf{k}$, for the lateral motion, $\alpha$ stands for light and heavy holes and $\phi(z)$ is the envelope wave function solution to the following one–dimensional Schrödinger equation with eigenvalue $W$

$$-\frac{\hbar^2}{2m_{az}} \frac{d^2}{dz^2} \phi_{\alpha}(z) + [U(z) - W] \phi_{\alpha}(z) = 0.$$
appearing in Eq. (3), relates to the top of the valence-band energy according to $U(z) = -E_V(z)$. The profile of the latter characterizing the device in accumulation, $E_V(z)$ is represented schematically in Fig. 1. $U(z)$ is determined by solving self-consistently the above-mentioned Schrödinger equation and the following Poisson equation

$$\frac{d^2 U(z)}{dz^2} = -\frac{e^2}{\epsilon_s} [p(z) - n(z) - N_A(z)] ,$$

where $p(z)$, $n(z)$ and $N_A(z)$ denote hole, electron and ionized acceptor concentrations, respectively, and $\epsilon_s$ is the silicon dielectric constant. In our calculations, all energies are measured with respect to the top of the valence band, $E_V$, far enough from the silicon/oxide interface. With this choice, the bound states are associated with negative values of $W$, whereas the extended states correspond to positive values of $W$. The boundary conditions imposed on the potential are

$$U(z = \infty) = 0 ,$$
$$U(z = 0) = -U_s .$$

Consequently, all the allowed eigenvalues for the hole, $W$, are exceeding $-U_s (W \geq -U_s)$ and $-U_s$ is the value of the potential energy at the interface.

![Figure 1](image_url)

Figure 1. Typical potential energy profile of the electron in the valence band in a MOS structure of a p-type semiconductor in accumulation

The hole density $p(z)$, which appears in Eq. (4), is composed of two parts:

$$p(z) = p_b(z) + p_m(z) .$$

Here $p_b(z)$ and $p_m(z)$ respectively represent the hole concentration of the bound and mobile states, that are given by the expressions

$$p_b(z) = 2 \sum_{\alpha k} \int_{-U_s}^0 dW |\phi_\alpha(W, z)|^2 F(E_{\alpha k}, E_F) ,$$
$$p_m(z) = 2 \sum_{\alpha k} \int_0^\infty dW |\phi_\alpha(W, z)|^2 F(E_{\alpha k}, E_F) ,$$

where the factor 2 arises from spin degeneracy and the function $F(E_{\alpha k}, E_F)$ is the Fermi–Dirac distribution function. For the electron density in the conduction band we used the local density approximation in which $n(z)$ is expressed in the form

$$n(z) = N_C \exp (\beta (E_C - U(z) - E_F)) ,$$

where $\beta = 1/k_B T$, $N_C$ is the effective conduction band density, $E_C$ and $E_F$ are respectively the conduction band edge and the Fermi energy in the substrate.

Setting up a computational grid and assuming a piecewise constant profile in each grid cell for the energy potential $U(z)$, and moreover, using the transfer matrix approach described in [3], we determine both the quasi-bound and the extended states which are normalized according to

$$\int_{-\infty}^{+\infty} dW \phi_\alpha^*(W', z) \phi_\alpha(W, z) = \delta(W' - W).$$

In addition, the quasi–bound states are required to vanish asymptotically deep inside the substrate ($z \to \infty$) as

$$\phi_\alpha(W, z) = A_s(W) \exp (-k_{as} z) z \geq a ,$$

where the coefficient of the wave function, $A_s(W)$, is a function of energy and $a$ is the width of the well. The quantity $k_{as}$ describes the exponential decay of the motion along the $z$ direction and is given by

$$k_{as} = \sqrt{-\frac{2m_{as} W}{R^2}} .$$

The minus sign in Eq. (13) is due to the fact that bound states are associated to negative values of energy $W_\alpha$. On the other hand, the mobile states are plane waves propagating along the $z$ direction and of the form

$$\phi_\alpha(W, z) = A_s(W) \exp(\pm ik_{as} z) z \geq a ,$$

with $k_{as}$ given by

$$k_{as} = \sqrt{\frac{2m_{as} W}{R^2}} .$$

To proceed further, we find it convenient to use the technique developed in [3] to identify the bound states or the resonances and their corresponding spectral widths which will be, in turn, used in the calculation of their contribution to the leakage current density. This technique is based on tracing the peaks of the presence probability of holes in the well near the silicon/interface as a function of energy. A typical plot of this probability, $P_\alpha(W)$, is shown.
in Fig. 2. In this figure, the position and the width of the peaks determine the resonance energies, $W_{\alpha r}$, and their lifetimes, $\tau_{\alpha r}$, respectively. These peaks are well defined even for oxide thicknesses as low as 1 nm. Finally using Eqs. (8,9,11) and solving Eqs. (3,4), self–consistently, we determine the hole density profile, $p(z)$, and the leakage current density, of both bound and mobile holes. These results will be the subject of the next section.

3. Results and discussion

The main result of this paper is the determination of the leakage current density due to direct tunneling of charge carriers though the barrier. This current is composed of two parts. One is due to quasi–bound states living in the well near the silicon/oxide interface while the other part is associated to mobile states, extended over the whole device.

In contrast to the mobile states, the direct calculation of the current carried by a quasi–bound state, $\psi_{\alpha k}$, based on the equation

$$J_{\alpha k}(z) = \frac{e^2}{2m_{\alpha r}}[\psi_{\alpha k}^* \frac{\partial \psi_{\alpha k}}{\partial z} - c.c.], \quad (16)$$

would lead to zero contribution to the total current. However, on physical grounds, we know that the finite lifetime, $\tau_{\alpha r}$, of these states, due to their decay into the oxide region, leads to a non zero current. To circumvent this problem, at least two different approaches have been proposed [3, 4]. In our calculation we focused on the method based on Gamow’s picture of nuclear decay [5] which is described in [3]. This method leads to the following expression for the resonance contribution, $J^{\text{res}}$, to the total current:

$$J^{\text{res}} = \frac{e^2}{\pi \hbar^2} \sum_{\alpha r} \frac{\sqrt{m_{\alpha r} m_{\alpha y}}}{\tau_{\alpha r}} \times \log \frac{1 + \exp \left( - \beta (W_{\alpha r} - E_F - eV_G) \right)}{1 + \exp \left( - \beta (W_{\alpha r} - E_F) \right)}, \quad (17)$$

where $V_G$ is the electrostatic potential at the gate. Finally, we evaluate the extended quantum states and use Eq. (16) together with Eq. (17) for the bound states, we obtain the total current density. The result is represented in Fig. 3.

4. Conclusion

We have developed a full quantum mechanical approach for the MOS capacitor with ultra–thin oxide which may be composed of many stacks for a p-type semiconductor in accumulation. This approach is an extension of a previous model for MOS inversion layers[3] to account for the presence of mobile states in addition to bound ones. It is based on a self–consistent solution of Schrödinger and Poisson equations for the holes in the presence of electrons and ionized acceptors. Using the effective mass–approximation and lateral translational invariance assumption, we give an alternative method for a straightforward calculation of the leakage current density, the local hole density as well as the energy potential profiles under various external conditions of temperature, doping concentration and stack materials.