Schrödinger-Poisson solver for half-open MOS structures

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1. Introduction

Since the dimensions of Metal- Oxide-Semiconductor (MOS) transistors are shrunken, quantum mechanical effects play a growing role in device operations and performance. The thickness of the gate insulator layers reaches up to 2 nm in modern state of the art devices. The size scaling of oxide layer leads to a dramatically rise of the gate leakage current, which produces a large amount of heat in the devices. Therefore, deeper theoretical investigation of the leakage current, to suggest preventive measures how to reduce it, become very important.

Suggestion of quantum corrections to the classical characteristics in the framework of classical models is one of the widely used method. The effective potential (EP) approach [1-3] and the density gradient (DG) [4-5] approach which are based on the Bohmian interpretation of quantum mechanic are the most important models in this category. Although the quantum corrections improve the classical data, these approaches are not able to model and to predict all quantum mechanical effects. Modern studies of the leakage current in ultrathin oxides are focused on pure quantum mechanical modelling of field- effect devices.

In a fully quantum mechanical continous material model the Schrödinger and Poisson equations are solved self consistently. The Schrödinger equation is solved within the effective mass approximation. The boundary condition of the Schrödinger and Poisson equations are also an important issue. In many activities the Schrödinger equation has been solved in a quantum box with closed boundaries, containing only the semiconductor substrate [6-8], or the semiconductor substrate and the gate insulator [9-12], or even the whole device [13].

In this work we present results of our self-consistent computation of quantum- particle distribution in a MOS with closed boundaries in the inversion regime. Using closed boundary condition one obtains quantum mechanical bound-states in the inversion layer.

By improving this model, we have solved the Schrödinger equation with one open boundary condition to understand the effect of open boundarys and the mechanism of crossover from bound states into a quasi bound states.

2. Self-consistent solution with closed boundary condition

In the effective mass approximation, the one- electron wave function is given by the product of Bloch functions in x, y directions parallel to the $Si-SiO_2$ interface with an envelope function in z-direction perpendicular to the interface, which is the solution of the following one dimensional Schrödinger equation:

$$-\frac{\hbar^2}{2m_j^*}\Delta\Psi_j(z)+V(z)\Psi_j(z)=E_j\Psi_j(z), \quad (1)$$

where $\Psi_j(z)$ and E_j are the envelope function and the energy eigenvalue of the jth sub-band; m_j^* is the effective mass in z-direction and $V(z)$ is the potential energy. The above equation is solved in a closed quantum box under the following boundary conditions:

$$\Psi_j(0)=0 \text{ and } \Psi_j(L)=0. \quad (2)$$

Using the Fermi- Dirac statistic and summing up over all x, y direction quantum states, the electron distribution can be expressed by the following equation:

$$n_s(z)=\sum_j \frac{n_{vj}m_{dj}^*k_BT}{\pi\hbar^2}\left|\Psi_j(z)\right|^2 \ln\left[1+\exp\left(\frac{E_F-E_j}{k_BT}\right)\right] \quad (3)$$

where E_F is the Fermi energy, n_{vj} is the valley degeneracy and m_{dj}^* is the density of states effective mass per valley. The potential $V(z)$ is obtained as a solution of the Poisson equation

$$\frac{d^2V(z)}{dz^2}=\frac{e\rho(z)}{\varepsilon_0\varepsilon_s} \quad (4)$$

under the following boundary conditions:

$$V(0) = 0\,,\ \frac{dV}{dz}\Big|_{z=L} = 0$$

To find the eigenfunctions and eigenenergies of a particle, the Schrödinger equation (1) has to be solved self-consistently with Eq.(4).

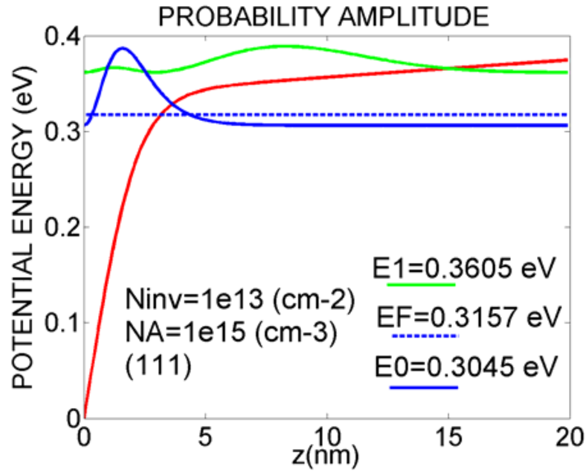

Fig.1. *The probability amplitude for the first two sub-bands at the inversion layer of a p-type semiconductor.*

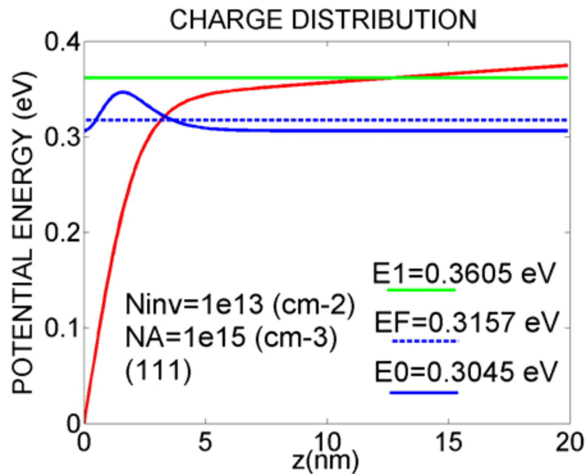

Fig. 2. *Charge distribution and the contribution of two first sub-bands to the electron density at the inversion layer.*

Figs. 1 and 2 show the bound-states, wave functions and charge distribution of the first two sub-bands at the inversion layer for a p-type semiconductor.

As it is shown in Fig. 2 the main contribution of the electron density comes from the first sub-band and the contribution of the higher sub-bands are nearly zero. Fig. 3 shows the total electron distribution at inversion layer. The average distance of the charge distribution is shifted about 2 nm from the interface. The quantum charge- distribution strongly differs from the classical distribution, where the maximum of charge distribution is placed at the Si/SiO_2 interface.

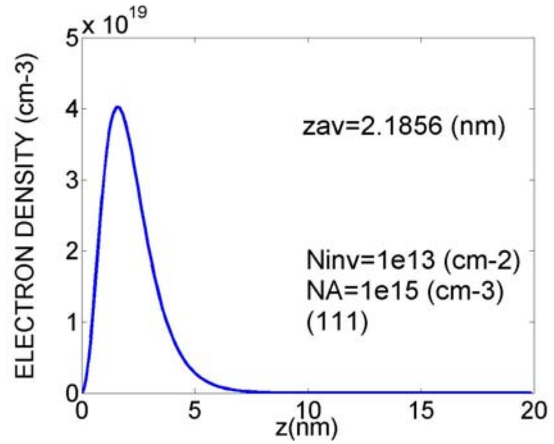

Fig. 3. *Total electron distribution at the inversion layer for a p-type semiconductor.*

3. Open boundary and the quasi bound-states

Bound character of electronic states near the Si/SiO_2 interface, formed due to the band bending, means that there is no leakage from such states and, therefore there is no tunnelling current from inversion layer into the gate. This is an acceptable assumption, if the oxide layer is thick enough ($t_{ox} > 4\,nm$). Unfortunately this assumption is not reasonable for MOSFETs with ultra-thin oxide layers.

Simulation of devices with extremely thin oxide layers require to solve the Schrödinger equation using open boundary condition. As soon as the boundary is opened the bound-states change into quasi bound-states. An electron can never leave a bound state. In other words, the life time of electron in a bound-state is infinite. But electrons in quasi bound-states can leave the state by tunnelling through the barrier; therefore they have a finite life time. In order to characterize quasi bound-states we need to define the eigenenergy and the wave function of a quasi- bound state, like for a bound-state, but also the life time for this state.

Big effort has been done to indirectly calculate the life time of a quasi bound-state in inversion and accumulation layer of MOS structure, using the transfer Hamiltonian approach [10], transverse resonant method [11] and Breit-Wigner theory of nuclear decay [12].

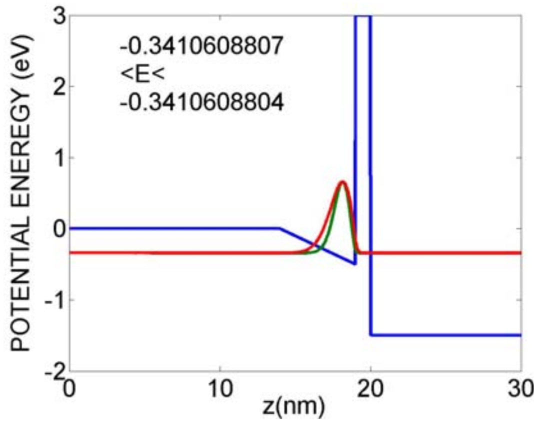

Fig. 4. *The first quasi bound state in a potential well with a 3 eV high and 1 nm thick barrier.* $\Delta E = 3\times10^{-10}(eV)$. *Red and green colour curves correspond to the wave function and the probability amplitude, respectively.*

We calculate the life time directly from the solution of Schrödinger equation with open boundary. We integrate the Schrödinger equation, providing a zero boundary condition in the deep bulk of the Si substrate, and letting the other boundary to be open. Instead of the closed boundary at the oxide side we force the wave function to satisfy the following conditions:

(i)Absolute value of the wave function at the $Si-SiO_2$ interface has to be larger than that in the interface of SiO_2/polysilicon gate;

(ii) the wave function can not change sign in the oxide layer, and the derivative of the probability amplitude can not be positive in the oxide.

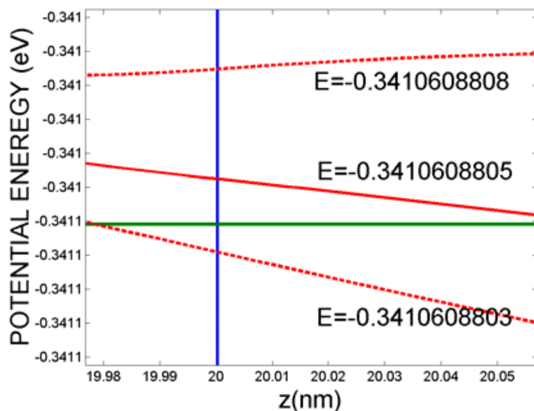

Fig. 5. *a closer shot of the figure 4 at the oxide-gate interface. The dotted wave functions fail to satisfy the conditions of an acceptable wave function.*

Under these conditions we find, that the possible energy states are placed in a close vicinity ΔE of the bound state, obtained under closed boundaries. This ΔE depends on the barrier height and thickness. Figs. 4 and 5 show the first eigenvalue with $\Delta E = 3\times10^{-10}\,eV$. Changing the barrier height from 3 eV to 2 eV, ΔE changes from $3\times10^{-10}\,eV$ to $1\times10^{-8}\,eV$. Shift in the thickness of the barrier from 1 nm to 0.7 nm, changes ΔE from $1\times10^{-8}\,eV$ to $1\times10^{-7}\,eV$.

The life time of an electron in the quasi- bound state can be calculated by using the Heisenberg uncertainty relation $\Delta t\times\Delta E = \hbar/2$. ΔE increases with decreasing the barrier height or thickness, which consequently decreases Δt leading to high leakage current.

4. Conclusion

As the oxide layers in MOS transistors becomes ultrathin the bound-state approximation is not a reasonable approximation. The states should be characterized as quasi bound-states by solving the Schrödinger equation with open boundaries.

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