Analysis of Gate Tunneling Current in MOS Structures using Quantum Mechanical Simulation

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Abstract

We report studies of quantum transport in n^+Si-SiO_2-p Si Metal-Oxide-Semiconductor (MOS) structures based upon a non-equilibrium tight-binding Green's function method. As a result, the quasi-bound states at the SiO_2-p Si interface are found to be lower than those calculated by the conventional Shrödinger-Poisson analysis, since the wavefunctions in this region are coupled with the Bloch functions in the electrodes. It is also found that the leakage current through the oxide consists of not only the intraband tunneling but also the interband tunneling current.

1 Introduction

The recent MOS scaling less than sub-100 nm gate length has changed operating voltage less than 1V and an oxide thickness less than 3 nm, which corresponds to several layers of atom. The progress in the miniaturization has revealed such crucial problems as the gate tunneling, deterioration in device performance i.e. loss of inversion charge and transconductance due to the quantization of carriers in the channel, and polysilicon gate depletion. So far, semi-analytical models [1] and quantum correction models [2] have been applied to analyze such problems. In order to understand these aspects more physically, we have to simulate the transport of carriers quantum-mechanically taking into account the possible tunneling paths as well as quantization in the MOS structure.

In this paper, we present simulations of quantum electron transport in a MOS structure based on a non-equilibrium tight-binding Green's function (NEGF) method.

2 Modeling and Simulation Results

We confine ourselves within an n^+ poly Si-SiO_2-p Si MOS diode as schematically illustrated in Fig. 1. We have employed a tight-binding 2-band model which describes the conduction band (CB) and valence band (VB), and the pure imaginary

band. Figure 2 (a) and (b) show the complex band structures of Si and SiO_2, respectively. The pure imaginary wave number $\mathbf{Im}k_z$ in the band gap implies the decay constant of evanescent electron waves. The evanescent waves should be appropriately matched between Si-SiO_2 interfaces.

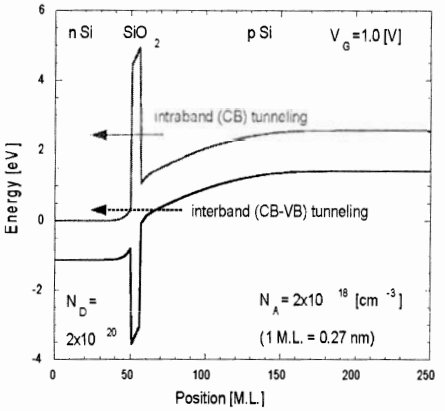

Figure 1: Schematic structure of an n^+ poly Si-SiO_2-p Si MOS diode.

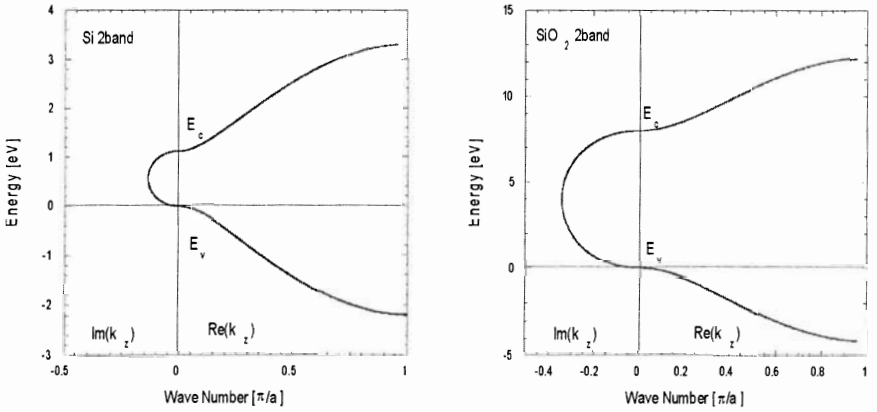

Figure 2: Complex band structures of (a) Si and (b) SiO_2 calculated by the 2B model. The real bands (**Re** k_z) are drawn on the right portion, whereas the imaginary bands (**Im** k_z) are on the left.

Using the band structures, carrier concentrations n and p, current density J, and a spectral function or local density of states (LDOS) A at lattice position L are straightforwardly expressed in terms of the NEGF[3,4]:

$$n_L = -\frac{2i}{S\Delta}\sum_{\boldsymbol{k}_\parallel}\int\frac{dE_z}{2\pi}\mathbf{Tr}\left[G^<_{L,L}(\boldsymbol{k}_\parallel,E_z)\right], \quad (\text{for } p_L, \quad G^< \longrightarrow G^>), \quad (1)$$

$$J_L = \frac{2e}{\hbar S}\sum_{\boldsymbol{k}_\parallel}\int\frac{dE}{2\pi}2\mathbf{Re}\left\{\mathbf{Tr}\left[-t_{L,L+1}\cdot G^<_{L+1,L}(\boldsymbol{k}_\parallel,E_z)\right]\right\}, \quad (2)$$

$$A_{L,L} = 2\mathbf{Im}[G^R_{L,L}(E)] \quad (3)$$

where S is the cross sectional area, Δ monolayer spacing (=0.27 nm), e the electronic charge, $t_{L,L+1}$ is the **hopping matrix** which is related to the matrix elements of the Hamiltonian, and **Tr** denotes trace of the matrix. Poisson's equation is simultaneously solved to include the space charge effect for selfconsistent calculation.

Figure 3 shows the LDOS around the oxide region. Darker portions have higher density of states. Several quasi-bound states are observed without assuming infinite wall boundaries at the electrodes. For comparison, Fig. 4 shows the result calculated by the Schrödinger-Poisson analysis (SPA) with infinite wall boundaries. Note that in the present NEGF analysis, each quasi-bound state lies below corresponding one calculated by the SPA, since the NEGF correctly takes into account the open boundary conditions at electrodes through self-energies which include couplings between the electrodes and the device region. The shift of the quasi-bound states may change the threshold voltage of the MOS predicted by the conventional SPA.

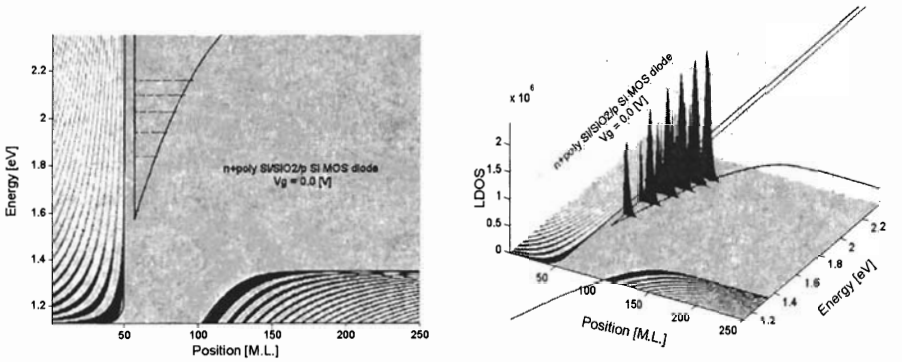

Figure 3: Local density of states (LDOS) in the MOS diode at gate bias $V_g = 0$ V. Six quasi-bound states are drawn in the triangular quantum well from which electrons are injected into the gate electrode when intraband tunneling occurs. The contribution of states from the transverse energies have been ignored for clarity.

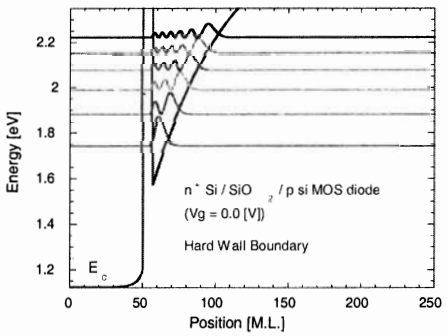

Figure 4: Bound-states calculated by the Schrödinger-Poisson analysis with infinite-wall boundaries at the ends of the electrodes. Probability densities are also shown.

Figure 5 (a) shows the I-V characteristics of the MOS diode with $t_{ox} = 1.6$ and 2.5 nm, which is qualitatively in agreement with the experimental data[5]. The current density under the inversion condition is fairly large due to the tunneling current. The tunneling current is found to be made up of both the injection from the quasi-bound states and the VB-CB interband tunneling as shown in the LDOS in Fig 5(b). The interband tunneling can be understood from the overlap of the local density of state between the CB and VB.

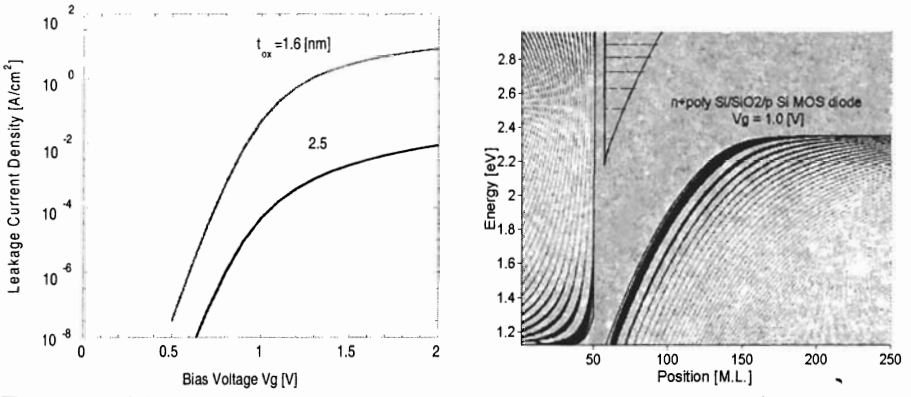

Figure 5: (a) Oxide thickness dependence of the tunneling current ($t_{ox} = 1.6$ and 2.5 nm). (b) Local density of states at $V_g = 1.0$ V. Overlapping of the states can be observed arount $E = 1.2$ eV.

3 Conclusion

We have applied the non-equilibrium tight-binding Green's function (NEGF) formalism to analyze tunneling in the MOS structure. As a result, the NEGF method is found to include correctly the open boundary conditions. The quasi-bound states in the MOS triangular well are found to become lower due to the boundary condition, which may change the threshold voltage predicted by the conventional method. The amount of the tunneling current under the inversion biased condition is so large that we have to be careful in comparing the simulated C-V characteristics with experimental data.

References

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