Introduction

As MOS field-effect transistors are scaled down to a nanometer regime, quantum effects in both transverse and transport directions start playing a major role in determining device characteristics. In order to address a new challenge, SILVACO has started a deployment of new quantum mechanical models based on Non Equilibrium Green’s Function (NEGF) approach. This is a fully quantum mechanical approach which treats such effects as source-to-drain tunneling, ballistic transport, and quantum confinement on equal footing. The new NEGF solver is suitable to model ballistic quantum transport in such devices as Double Gate or Surround Gate MOSFET, using rectangular or cylindrical geometries in ATLAS. The method used is based on references [1] and [2].

Simulations

This article considers a silicon Double Gate transistor, schematically depicted in Figure 1. The gate length is 10 nm, channel length in 15 nm, channel thickness is 3 nm, gate oxide thickness is 1 nm. The device has flared-up source and drain regions taken to be 9 nm thick and doped to 1e20 1/cm$^3$. The channel is kept undoped. We used metal gates with a workfunction of 4.7 eV. In this simulation a single valley with an isotropic effective mass of 0.3 was considered in Si for simplicity. The non uniform cross-section of such a device immediately suggests that the confinement in both channel and source has to be taken into account. Moreover, the interface between wide source and drain regions and narrow channel may cause additional reflection of electrons and a decrease of current. That is the quantum mechanical coupling between electron modes in the source and channel is important.

![Figure 1. A layout of a double gate transistor.](image1)

![Figure 2. Converged eigen functions found by a 1D Schrodinger equation in the source (a) and channel (b). Only two lowest states are shown.](image2)
The modeling starts with a solution of 1D Schrödinger equation in the transverse slices of the device in order to find eigen functions and eigen energies, shown in Figure 2 and 3 respectively. Note that the penetration of electrons into oxide is accurately taken into account. ATLAS will automatically decide on the number of required eigen states in each slice, as this number changes from source to drain and is different for different biases. If desired, the number of eigen states may be set manually.

After finding eigen states, NEGF quantum transport equations are solved in the mode space. Due to an abrupt wide-narrow interface, ATLAS will use a Coupled Mode Space (CMS) approach, to account for mode mixing. In a simpler case of constant cross-section, an Uncoupled Mode Space (UMS) is used which is essentially a number of 1D transport equations for each subband. By estimating the geometry of the device, ATLAS automatically chooses the appropriate method. A particular method (CMS or UMS) can also be enforced by a user.

The NEGF equations are solved for each electron energy on an internally constructed non uniform energy grid. A user can change the size of the energy grid to optimize a trade-off between precision and computation time. After solving NEGF equations, quantum electron concentration is computed and plugged into Poisson equation for self-consistent solution. The convergence

Figure 3. Eigen energies in the source (a) and channel (b). Note that the minimum number of eigen states required in the source (and drain) is usually higher than that in the channel.

Figure 4. Contour plot of electron concentration at low (a) and high (b) gate voltage.
is typically achieved within several iterations, which utilize a predictor-corrector scheme. A user has a control over the number of predictor iterations and convergence criteria. The converged electron concentration is shown in linear scale in Figure 4 (a) and (b) for low and high gate bias. A wave nature of electron is clearly manifested near the Si-SiO2 interface, where the concentration's value oscillates away from the interface. At high gate voltage electron concentration increases in the channel. The quantum OFF (low Vg) and ON (high Vg) current density is shown in Figure 5 (a) and (b). While the current flow is uniform in the channel, it shows spatial oscillation in the wide source and drain regions, suggesting a possible access geometry optimization to increase ON-current and improve device performance.

In Figure 6, electron concentration (a) and conduction band energy (b) as functions of coordinate in transport direction are shown for Vd=0.6 V and Vg=0, 0.2, 0.4, 0.6, 0.8 and 1V. Since here we consider only a ballistic transport, there is no voltage drop in the source and drain regions. Von Neumann boundary conditions are used for potential in the source and drain and consequently the potential may float. The contact Fermi levels are, however, kept fixed at the boundaries. In Figure 7, electron concentration (a) and conduction band energy (b) as functions of coordinate in transport direction are shown for Vg=0.6 V and Vd=0, 0.2, 0.4, 0.6, 0.8 and 1V. Note that there is a significant drain induced barrier lowering (DIBL) in the channel.

Figure 5. Contour plot of current density at low (a) and high (b) gate voltage.

Figure 6. Electron concentration (a) and conduction band edge at Y=0 as a function of X at different gate voltages.
Current-voltage characteristics are shown in Figure 8. In Figure 8 (a), the Id-Vg shows a nearly ideal 68 mv/decade subthreshold slope and threshold voltage Vt=0.6V. The DIBL effect results in a poor saturation of Id-Vd characteristics at Vg=0.6, 0.7 and 0.8 V in Figure 8 (b). This behavior is also related to a source-to-drain tunneling, which was taken into account by the NEGF method.

A user can probe various energy dependent quantities to gain an insight into the device characteristics. The quantities that can be probed and stored in a separate log file for each bias point are transmission coefficient, local density of states, local electron concentration per energy, local current density per energy. These quantities can be stored for a particular effective mass band (valley) and subband.
or summed over these indices. Figure 9 (a) shows the total transmission coefficient, where the two steps correspond to the contribution due to two subbands in the channel. The energy of the steps roughly correspond to the maximum value of eigen energy in the channel.

Figure 9 (b) shows that the lowest subband gives the major contribution to current, as the population of the second subband is much lower. Finally, Figure 9 (c) shows a contribution of various subbands to a total density of states in the source.

**Conclusion**

This article has presented a modeling of nanoscale Double Gate MOSFET using an NEGF approach. The model predicts the eigen energies and eigen functions, quantum electron concentration and current density, current-voltage characteristics and also gives insight into the interplay of various quantum effects in the nanoscale transistors.

**References**
