Extended Abstracts of the 2001 International Conference on Solid State Devices and Materials, Tokyo, 2001, pp. 382–383

F-5-1

70 nm MOSFET Device Simulation Considering Two Dimensional Channel Quantization and Self-Consistent Non-Equilibrium Carrier Transport

Tatsuya Ezaki, Philipp Werner* and Masami Hane

Silicon Systems Research Laboratories, NEC Corporation,
1120 Shimokuzawa, Sagamihara, 229-1198, Japan
Phone: +81-42-771-0797, Fax: +81-42-771-0886, E-mail: t-ezaki@ap.jp.nec.com

1. Introduction

In small MOS transistors with thin gate oxide and high substrate doping concentrations, a strong transverse electric field near the Si/SiO_2 interface leads to significant quantization effects in the direction perpendicular to the interface. There have been several papers related to the quantum mechanical (QM) device modeling. In these previous works, however, only the QM charge distribution has been taken into account, and drain currents have been simulated based on the classical drift-diffusion (DD) model [1, 2]. In this work, we have developed the self-consistent two dimensional (2D) QM Monte Carlo (MC) device simulator in order to evaluate QM effects on the drain current. There are three major improvements in our simulation: 1) QM calculation is extended over the whole device region, 2) the quantum transport is taken into account considering the electron transition between quantized states, 3) the charge density, the potential profile and the non-equilibrium distribution function are calculated self-consistently. In order to identify the impact of the full 2D QM calculation, drain currents of 70nm n-MOSFET are simulated and are compared to those obtained from the DD device simulator [3].

2. Model

Assuming that the variation of the potential along the channel is small over an electron wavelength, the electron wave function can be written as the product of a plane wave traveling parallel to the interface and an envelope function in the direction perpendicular to the interface [1]. Therefore, 2D eigenstates can be constructed from solutions of the one dimensional (1D) Schrödinger equation at many different positions along the channel direction (Fig. 1 and Fig. 2). The non-parabolicity of the Si energy band near the X-points is introduced into our simulator in the analytical form of $\varepsilon(1+\alpha\varepsilon) = \hbar^2 k_y^2/2m_y^* + \hbar^2 k_z^2/2m_z^*$ with non-parabolicty parameter being $\alpha = 0.5\mathrm{eV}^{-1}$. Note that 1D eigenstates (Fig. 2) are calculated by the effective mass Schrödinger equation under the non-parabolic band structure [4]. As shown in Fig. 2 (b), we extend the QM calculation to the entire simulated domain. This approach does not require any prescription for the transition of electrons between two- and three-dimensional states near the channel edges. The electron distribution in the MOSFET is calculated by using the one particle MC method. By using this method, the current continuity along the channel can be satisfied automatically. Especially the quasi-ballistic transport near the source junction [5] is also properly simulated. For the self-consistent potential calculation, the inversion charge within the channel is replaced by the latest QM charge distribution obtained from the MC simulation (Fig. 3). The QM charge distribution (Fig. 3) is rescaled to satisfy the charge neutrality in the source and the drain region. Since the non-equilibrium nature is included in the charge distribution of itself, the consistency between the potential and the non-equilibrium distribution function can be guaranteed. Scattering mechanisms included in our simulation are the intra-valley acoustic- and the inter-valley optical-phonon scattering [6].

3. Results and Discussion

Drain current calculations successfully converged within 25 iterations as shown in Fig. 4. For the first iteration, the potential obtained from the DD device simulator was used (Fig. 5). Since the subband energy profile after the self-consistent QM calculation is much lower than the initial profile (Fig. 6), QM effects cannot be captured by the classical potential (Fig. 6) and charge distribution (Fig. 7), and only the self-consistent QM calculation is capable of producing meaningful results. There is an increase of nearly 0.1V in the threshold-voltage predicted by the quantum mechanical device simulator compared to the DD simulation incorporating the van Dort QM correction [7] (Fig. 8). This shift can easily be understood by plotting the bottom of the conduction band and the energy of the lowest subband as shown in Fig. 9. The classical threshold-voltage coincides with the gate voltage, for which the bottom of the conduction bands crosses the Fermi level. For the quantum mechanical case, the lowest subband has to be considered. The importance of the self-consistent calculation is also obvious from the figure. The transconductance obtained from the QM simulation is 1.5 times lower than the classical result (Fig. 8), because the quantum dark space depleted of the free carriers near the interface (Fig. 7) acts as an effective gate dielectric for device operations. The lower total current predicted by the QM simulation (Fig. 8) is the consequence of a lower charge density in the channel (Fig. 10), since the mean carrier velocities are almost the same near the source edge in both cases (Fig. 11). There is no saturation velocity incorporated in the QM simulator, as is the case for the DD simulator. The reasonable mean carrier velocity is the result of phonon scattering. Some velocity overshooting ($v > v_{\mathrm{sat}} \approx 10^7$ cm/s) occurs near the drain edge (Fig. 11), resulting from the non-equilibrium carrier transport near the drain.

4. Conclusion

We have developed the quantum mechanical MC simulator for n-MOS transistors in which the QM calculation is extended to the whole device region. A simple and effective self-consistent iterative method to obtain meaningful results with good convergence is also proposed. Our "parameter fitting free" simulator can provide the microscopic insight into the deep sub-100nm CMOS device operation.

References

[1] A. S. Spinelli *et al.*, IEEE Trans. Electron Devices, **45**, 1342 (1998).
[2] T. Janik*et al.*, IEEE Trans. Electron Devices, **ED-45**, 1263 (1998).
[3] I. Yokota *et al.*, Proc. 1998 Electronics Society Conference of IEICE, 77 (1998).
[4] C. Jungemann *et al.*, Solid State Electronics, **36**, 1529 (1993).
[5] M. Lundstrom *et al.*, 2000 International Conference on Semiconductor Processes and Devices, 1 (2000).
[6] S. Yamakawa *et al.*, J. Appl. Phys. **79**, 911 (1996).
[7] M. J. van Dort *et al.*, IEEE Trans. Electron Devices **ED-39**, 932 (1992).

*Present address: Department of Biochemistry University of Zurich, Winterthurerstrasse 190 8057 Zurich, Switzerland.

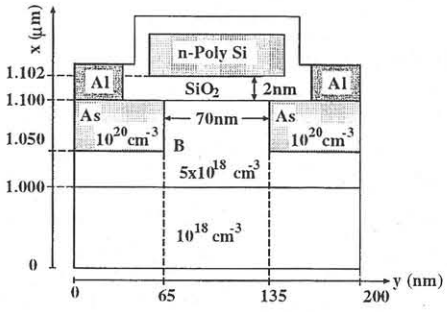

Figure 1: Cross-section of the n-MOS transistor under investigation.

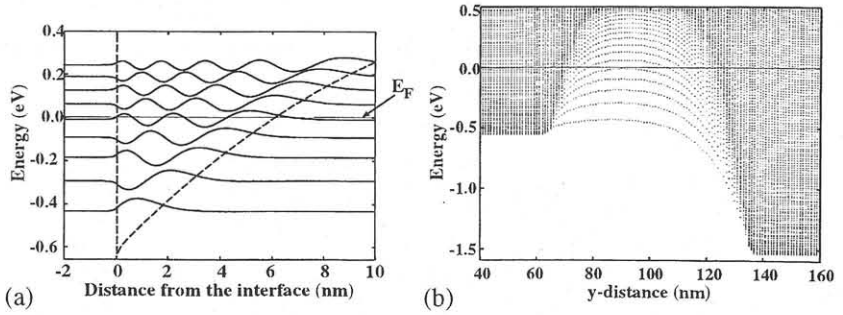

Figure 2: (a) The lowest nine eigenfunctions at $y = 90$nm and (b) the profile of eigenenergies along the channel ($V_S = 0$V, $V_D = 1$V and $V_G = 1.4$V).

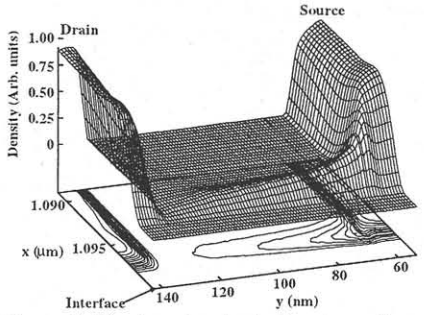

Figure 3: Electron density in the channel region for $V_G = 1.4$V. The repulsion from the interface can clearly be seen.

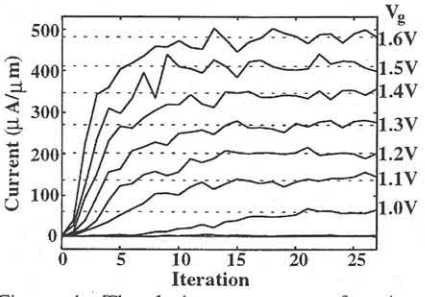

Figure 4: The drain current as a function of iterations for gate voltages ranging from $V_G = 0.8$V to $V_G = 1.6$V. The initial currents were calculated by using the potential obtained from the DD device simulator.

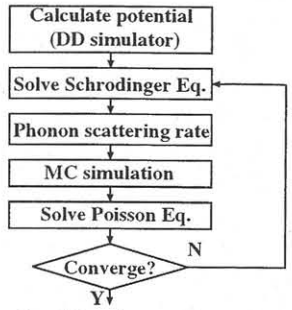

Figure 5: The flow chart of the self-consistent QM simulator. The initial potential is calculated by the DD device simulator.

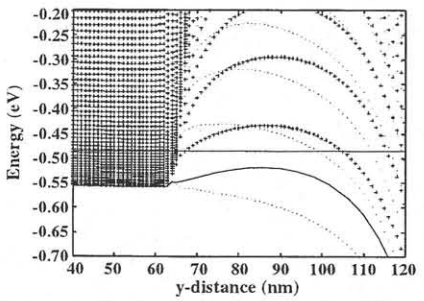

Figure 6: Subband energy levels for $V_S = 0$V, $V_D = 1$V, $V_G = 1.4$V. The horizontal line and the solid curve show the Fermi level and the bottom of the conduction band, respectively. Dots indicate subband energy levels after the self-consistent calculation.

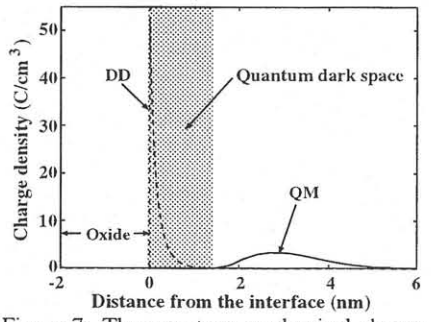

Figure 7: The quantum mechanical charge density after self-consistent calculation. Broken line shows the result obtained from the DD device simulator.

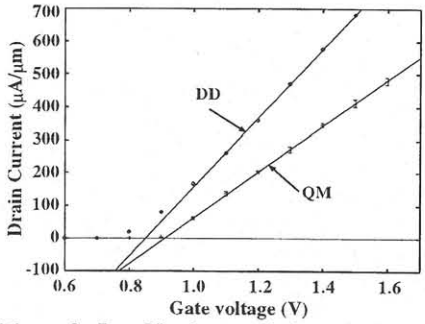

Figure 8: $I_D - V_G$ characteristics calculated by the self-consistent QM simulator and by the DD device simulator.

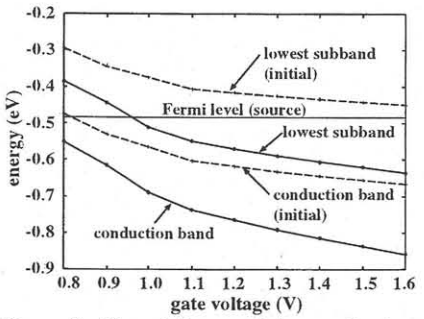

Figure 9: The minimum of the conduction band and the lowest subband energy at $y = 90$nm where the maximum of the potential barrier is approximately located (Fig. 6). Solid lines show the results after the self-consistent calculation.

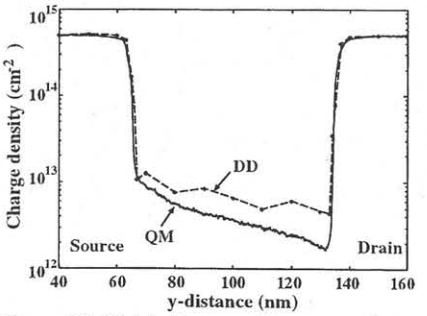

Figure 10: Total electron charge as a function of position ($V_G = 1.4$V). The broken line shows the result obtained from the DD device simulator.

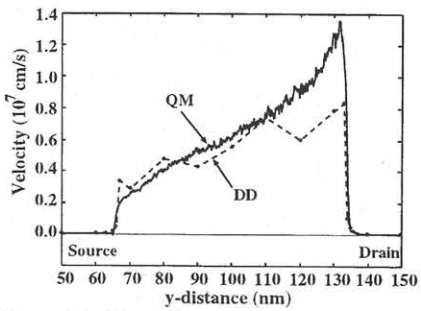

Figure 11: Mean electron velocity as a function of position ($V_G = 1.4$V). The broken line shows the result obtained from the DD device simulator.