Chapter 1

Introduction

Nowadays high performance CMOS technologies have been investigated with the channel length down to nanometer regime. However, the several unwanted effects seriously degrade the characteristics of nanoscale CMOS device such as gate oxide tunneling, mobility degradation, short-channel effect, and drain induced barrier lowering (DIBL) enhanced leakage. Therefore, some advanced MOSFET structures such as double-gate MOSFETs have been proposed in the past years for these specific devices exhibit the promising ability to alleviate the hurdles described above. The double-gate MOSFETs offer the possibility of channel length scaling down to 10 nm along with the advantages such as high transconductance and near-ideal subthreshold swing. Particularly, the upper and bottom gates can provide good electrostatic integrity which minimizes drain-induced barrier lowering and threshold voltage variations. The physical origin of these nano-scale MOSFETs has been thoroughly examined and there have been a number of mathematical models developed to date. In this thesis, we focus on ultrathin double-gate MOSFETs to establish a new physically based analytic model. The validity of the model is corroborated by sophisticated device simulations such as 1-D Schrödinger – Poisson solving, 2-D ballistic I-V simulations, and 2-D Monte Carlo particle and Green's Function simulations with the scattering in the channel. The developed model can furnish physical insights into double-gate MOSFETs, the potential candidate for the next-generation nanoFETs.

2-D Green's function simulation [1],[2] and 2-D Monte Carlo particle simulation [3],[4] both have recently been conducted on the ultrathin film double-gate MOSFETs. The involved electrical characteristics included ballistic I-V as well as scattering

counterparts. In a 1-D-like treatment [5], a compact model was developed for the width of the k_BT layer, a critical zone according to channel backscattering theory [2]. However, there have been unsolved issues on the modeling of the ultrathin film double-gate MOSFETs: (a) Can a 1-D treatment reflect the above-threshold 2-D behaviors adequately if the *DIBL* is obtained in advance from the subthreshold I-V shift as in bulk case [6]-[8]? (b) Is the relationship, between the ratio of the backward to forward flux at the top of the source-channel barrier and the thermal injection velocity, strong or weak? (c) What is the error if the compact k_BT layer width model does not include the modulation by gate voltage? (d) Can the channel backscattering theory work well in the presence of drain scattering [3],[4]?

In this thesis we present a physically based analytic model established at the peak of the source-channel barrier in a 1.5-nm thick silicon film double-gate MOSFETs with channel lengths down to 10 nm. Through the aid of such transparent model, the above issues of concern can be substantially clarified.

This thesis is organized as follows. In Chapter 2, we will describe 1-D and 2-D Quantum Mechanical simulations. The simulation results are given in Chapter 3. In Chapter 4, a physically based analytic model is established along with comparisons with sophisticated device simulations. Finally, a conclusion of the work is drawn in Chapter 5.

Chapter 2

1-D & 2-D Quantum Mechanical Simulations

2.1 1-D Quantum Mechanical Simulation

As the MOSFET dimension scales down, the quantum effect is more and more important. To study the concerned phenomena due to the quantum effect, the self-consistent Schrödinger - Poisson simulation is needed. In this chapter, we introduce a one-dimensional (1-D) and two-dimensional (2-D) quantum mechanical simulation developed by the group at Purdue university [9].

2.2 The Self-consistent Method of Solving Schrödinger – Poisson Equation

Schred [9], a program of 1-D quantum mechanical simulation, can calculate the envelope wave functions and corresponding bound-state energies in MOS, SOS (Semiconductor - Oxide - Semiconductor), and SOI structure.

For a quantum mechanical description of MOS structures, we have to solve simultaneously Schrödinger and Poisson's equations, which can only be done numerically. When an electron is confined inside the conduction band potential well *Ec(x)*, the effective mass Schrödinger Equation is written as,

$$\left(-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}+\left[E_C(x)\right]\right)\Psi_i(x)=E_i\Psi_i(x) \qquad (2.1)$$

which $\Psi_i(x)$ is wave function and E_i is allowable energies. The available energies above the conduction band are called subbands. As long as we know the allowable eigen-energies and the spatial distribution of an electron through eigen-state ($|\Psi_i(x)|^2$), we can calculate the electron density per unit area in that state according to

$$N_i = \frac{m^* K_B T}{2\pi\hbar^2} \ln\left(1+\exp\left(\frac{E_F - E_i}{K_B T}\right)\right)$$
$$N = \sum_i N_i \tag{2.2}$$

Electrons should be not only determined by the conduction band edges, but also by the electron-electron interaction, so the potential energy has to be calculated through Poisson's equation

$$-\frac{d}{dx}\left(\varepsilon_r(x)\frac{dE_c(x)}{dx}\right) = \frac{q^2}{\varepsilon_0}\left[p(x) - n(x) + N_D(x) - N_A(x)\right] \tag{2.3}$$

Eq. (2.1) and (2.3) are coupled non-linearly and have to be solved self-consistently. The flow chart in Fig. 2-1 shows the solving procedure involving n(x) and E_C(x) to satisfy both Schrödinger equation and Poisson's equation.

2.3 Silicon Band Structure

In silicon the conduction band edges are six valleys along the equivalent ＜100＞ directions in the Brillouin zone shown in Fig. 2-2, and each valley has an elliptically equi-energy surface. The effective mass is inversely proportional to the curvature of the constant energy ellipsoids. In our simulation, the thickness of the silicon body is

only a few nanometers (1.5 nm), so the charge inside the channel can be modeled as 2-D electron gas in a quantum well [13]. Then, there are two different ladders of energy levels from two different effective masses. The first ladder has higher longitudinal effective mass m_l and has two-fold valley degeneracy with $m_l = 0.916m_0$ (where m_0 is the free electron mass). The second ladder has transverse effective mass m_t and has four-fold valley degeneracy with $m_t = 0.19m_0$. Thus the Schrödinger equation should be solved twice, one for the longitudinal effective mass and the other for the transverse effective mass.

2.4 2-D Quantum Mechanical Simulation

NanoMOS [9], a program of 2-D quantum mechanical simulation, is a self-consistent (Poisson with a transport model) 2-D simulator for the ultrathin body (less than 5 nm), fully depleted, double-gate n-MOSFETs. NanoMOS accounts for quantum effects in the confinement direction (threshold voltage shift) exactly by solving Schrödinger equation, and uses five different models to treat transport along the channel. The five transport models are classical ballistic, quantum ballistic, drift-diffusion, energy transport and quantum dissipative. With given "x" (transmission direction) point, the quantum effects in the confinement direction (y direction) are treated exactly by solving a 1-D Schrödinger equation, then yielding a set of subband profiles (ESUB(x)) shown in Fig. 2-3. Besides, NanoMOS also utilizes the 1-D program Schred to solve 1-D Schrödinger equation.

2.5 The Transport Models of NanoMOS

2.5-1 Classical Ballistic Transport Model (clbte)

With given “x” (transmission direction) point, the quantum effects in the confinement direction (y direction) are treated exactly by solving a 1-D Schrödinger equation, then yielding a set of subband profiles (ESUB(x)). Carrier transport in each subband only accounts for the thermionic emission, and quantum tunneling through the source-channel barrier is assumed to be zero.

2.5-2 Quantum Ballistic Transport Model (qbte)

With given “x” point, the quantum effects in the confinement direction are treated exactly by solving a 1-D Schrödinger equation, then yielding a set of subband profiles (ESUB(x)), as in the case of model clbte. Carrier transport in each subband uses the non-equilibrium Green’s function method, and is treated by solving a 1-D Schrödinger equation in the transmission direction. Therefore, it accounts for quantum tunneling through the source-channel barrier, which is different from Classical Ballistic Transport Model.

2.5-3 Drift Diffusion (dd)

This model is a quantum corrected drift diffusion model, where quantum effects in the confinement direction are accounted for exactly. With given “x” point, the quantum effects in the confinement direction are treated exactly by solving a 1-D Schrödinger equation, as in the case of model clbet, to yield a set of subband profiles (ESUB(x)). Carrier transport in each subband is then treated by solving a 1-D drift-diffusion equation in the transmission direction.

2.5-4 Energy transport model (et)

The 1-D energy transport model implemented in nanoMOS is identical to that of Medici simulator except that the degree of freedom of thermal random motion of the 2-D electron gas in the energy balance equation becomes 2 instead of 3. NanoMOS uses the same parameter names in the input deck as those of Medici.

2.5-5 Quantum Dissipative Transport model (qdte)

With given “x” point, the quantum effects in the confinement direction are treated exactly by solving a 1-D Schrödinger equation, as in the case of model clbet, to yield a set of subband profiles (ESUB(x)). Dissipative transport in MOSFETs is treated through the Green’s function formalism using a simple Büttiker-probe model. Scattering centers are treated as reservoirs similar to the source and drain except that they only change the energy of the carriers and not the total number of carriers in the system. Each scattering center is modeled through a perturbation strength characterized by a position dependent self-energy.

2.6 Conclusions

The program Schred shows several physically based techniques to describe the nano-scale double-gate MOSFETs. The quantum confinement effect is difficult to analyze using closed-form formula due to complex mathematical and nonlinearity. This explains why we use numerical analysis program such as Schred. In this work, we apply the 1-D quantum mechanical simulator to provide 1-D datails. Then we establish a physically based analytic model while accounting the 2-D effects. The validity of the model will be justified by sophisticated device simulations.

Chapter 3

Simulation Specifications and Results

3.1 Device Parameters and Bias Conditions

Fig. 3-1 depicts schematically cross section of the device under study: a 1.5-nm thick silicon film double-gate MOSFETs with channel lengths down to 10 nm. The oxide thickness is 1.5 nm. The gate length L is equal to the channel length. The top and bottom gate oxide thickness are t_{ox}=1.5 nm, and the Si body thickness t_{Si} is also 1.5 nm. The n^+ source and drain are degenerately doped at a level of $10^{20}/cm^3$, and the whole channel region is undoped. The low-field mobility is assumed to be 120 cm^2/ V-sec, and the work function of the top and bottom gate is 4.25 eV. All the simulations are conducted at room temperature (T=300 K). To obtain the steady-state behavior of the device, the same voltage is applied to both the top gate and bottom gate, and resulting in the same work function with the symmetric property. The top and bottom gate voltage are swept from 0.4 V to 0.55 V, while the drain voltage is swept from 0.1 V to 0.5 V. Table 3-1 shows the details.

3.2 Simulation Results

With the specified conditions, we can obtain the results by running 2-D simulation program. The I_{DS}-V_{DS} curve of ballistic double-gate MOSFET with L=20nm is shown in Fig.3-2. The drain voltage is swept from 0 V to 0.5 V while the gate voltage changes from 0.4 V to 0.55 V with a 0.05 V step. Fig. 3-3 and Fig. 3-4 show the I_{DS}-V_{DS} curve of ballistic double-gate MOSFETs with the same specifications for

L=15 nm and L=10 nm, respectively. In Fig. 3-3 and Fig. 3-4, we can observe that in the conventional saturation region the drain current increases with increasing drain voltage. This phenomenon can be attributed to drain induced barrier lowering as described in Chapter 4. Fig. 3-5 shows the first subband energy profile along the channel for different V_{GS}. As V_{GS} increases, the subband energy barrier will drop down while the top of the barrier approaches close to the source side. In a response, the electron density increases with increasing gate voltage applied. Similarly, the subband energy profile for different V_{DS} is shown in Fig. 3-6. 2-D electron densities along the channel for different V_{GS} and V_{DS} are shown in Fig. 3-7 and Fig. 3-8. From Fig. 3-5 to Fig. 3-8, we can see that the described trend of the simulated device is consistent each other and thus we can confirm the validity of the simulator. Fig. 3-9 and Fig. 3-10 show the subband energy profiles along the channel and 2-D electron densities of the subbands along the channel. In Fig. 3-9, we can observe the subband energy of two-fold is lower than four-fold, indicating that the 2-D electron density of two-fold is higher than four-fold. In other words, electrons preferably occupy the lower energy subband. In Fig. 3-11, we can observe the conduction band edge potential. Obviously, conduction band edge is almost constant for each given x point, and this phenomenon is evident in Fig.3-12, where the cross section of the same conduction band edge is located at the top gate (Y=0 nm) and the bottom gate (Y=1.5 nm). Indeed, the symmetrical property supports the self consistency of the simulation. The relative difference between Y=0.75 nm and Y=0 nm is less than 1%, thus guaranteeing that we can approximate the conduction band edge by assuming that the conduction band edge is almost independent of Y-axis. Besides, a maximum electron density appears in the middle of the channel as shown from electron density profile in Fig. 3-13.

Chapter 4

Physically Based Analytic Model

4.1 Model Establishment

Fig. 3-1 describes the double-gate MOSFET structure discussed in Section 3.1. With the concepts above, we establish a new model for the double gate system. First of all, a self-consistent Schrödinger-Poisson simulation [9] was performed on a 1-D upper metal-gate oxide-silicon film-gate oxide-bottom metal system, yielding channel subband levels and Fermi level as shown in Fig. 4-1 versus gate voltage. This figure clearly reveals that the lowest subbands associated with the two-fold valleys are the primary factors, rendering the establishment, while taking into account the MOS electrostatic at the top of the source-channel barrier [10], of a physically based analytic model possible. Fig. 4-2 sketches the conduction-band profile from source to drain along with electron energy versus wave vector plot at the peak of the barrier showing the ratio of backward to forward flux, r_{BF}. The forward flux from the source side brings a carrier density $n_s(+)$ and the backward flux is $n_s(-)$. Then the ratio r_{BF} can be defined as

$$r_{BF} = \frac{n_S(-)}{n_S(+)} \tag{4.1}$$

At the top of the source-channel junction barrier, the total carrier density n_S is

$$n_S^i = n_S(+) + n_S(-) \tag{4.2}$$

and according to MOS electrostatics [10], we have

$$qn_s = 2C_{eff}[V_G - (V_{tho} - DIBL \times V_D)] \tag{4.3}$$

For one-subband approximation, $n_S = n_S^i$, where

$$n_S^i = (1 + r_{BF})\left[\frac{m_d^i}{\pi\hbar^2}\right]\frac{n_v^i}{2}k_B T \ln\left(1 + e^{\frac{E_F - E_i}{k_B T}}\right) \tag{4.4}$$

Here n_s^i is the carrier density with subband i, n_v^i is the valley degeneracy, m_d^i is the density-of-states effective mass for subband i. According to the 1-D simulation results in Fig. 4-3, nearly all of the electrons occupy the first subband, so we can reasonally calculate the charge density on the first subband (i.e. i=1). The effective gate capacitance C_{eff} and quasi-equilibrium threshold voltage V_{tho}, which can be assessed via the Schrödinger-Poisson solver under *DIBL* = 0 and in turn produce the value of the Fermi level minus the lowest subband level. With the same subband and Fermi-level, the effective thermal injection velocity at the top of source-junction barrier is

$$v_{inj}^i = \sqrt{\frac{2k_B T m_C^i}{\pi m^{2i}_d}}\left(\frac{\Im_{1/2}(\eta_F)}{\ln(1 + e^{\eta_F})}\right) \tag{4.5}$$

$$\Im_{1/2}(\eta_F) = \frac{1}{\Gamma\left(\frac{3}{2}\right)}\int_0^\infty \frac{\eta^{1/2}d\eta}{1 + e^{\eta - \eta_F}} = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{\eta^{1/2}d\eta}{1 + e^{\eta - \eta_F}}$$

$$\eta_F = \frac{E_F - E_i}{k_B T}$$

where m_C^i is the conductivity effective mass for subband i, E_i is the energy level of subband i, E_F is the Fermi-level, $\Im_{1/2}$ is the Fermi-Dirac integral of order one-half. For two-fold valley, $m_C^i = m_d^i = m_t$, and for four-fold valley, $m_C^i = \frac{2m_l m_t}{m_l + m_t}$ and $m_d^i = \sqrt{m_l m_t}$, where the longitudinal mass $m_l = 0.916m_0$ and the transverse mass $m_t = 0.19m_0$. When the device scales down, the mean-free-path can be compared with the length of the critical length. Under this situation, quasi-ballistic transport occurs. If the ratio of backward to forward flux r_{BF} is equal to the channel backscattering coefficient r_C, then the drain current and the mean-free-path for backscattering λ can be expressed as

$$I_{DS} = qn_s \upsilon_{inj} \frac{1 - r_C}{1 + r_C} \tag{4.6}$$

$$r_C = \frac{1}{1 + \frac{\lambda}{l}} \tag{4.7}$$

$$\lambda = 2\frac{k_B T}{q}\frac{\mu}{\upsilon_{inj}}\frac{\left(1 + e^{\eta}\right)\ln\left(1 + e^{\eta}\right)}{e^{\eta}} \tag{4.8}$$

where μ is the quasi-equilibrium mobility, and l is the k_BT layer width. The calculated inversion-layer charge density and thermal injection velocity are respectively given in Fig. 4-4 and 4-5 versus gate voltage with r_{BF} as a parameter. It can be seen that the ratio of backward to forward flux can significantly affect the thermal injection velocity while producing little change in total inversion-layer charge as expected from the MOS electrostatics [10]. The calculated results are confirmed by

self-consistent Schrödinger-Poisson simulation, as depicted in Fig. 4-4 and 4-5.

4.2 *DIBL* Extraction

From the total inversion-layer charge and thermal injection velocity by self-consistent Schrödinger-Poisson simulation [9], the linear relationship can be obtained in Fig. 4-6 ：

$$\upsilon_{inj} = 2.9035 \times 10^{12} (Q_{inv} + 4.2474 \times 10^{-6}) = aQ_{inv} + b \tag{4.9}$$

where a and b are numerical constants. (4.10) establishes the relationship between the thermal injection velocity and drain current. Through substituting (4.9) into (4.10), followed by differentiation with respect to V_{DS}, we can obtain an analytic model expressing I-V slope as function of DIBL. The detailed analysis process is shown below

$$I_D = Q_S v_{inj} = Q_S (aQ_S + b) = aQ_S^2 + bQ_S \tag{4.10}$$

$$\begin{aligned} \frac{\partial I_D}{\partial V_D} &= 2aQ_S \frac{\partial Q_S}{\partial V_D} + b\frac{\partial Q_S}{\partial V_D} \\ &= (2aQ_S + b)\frac{\partial Q_S}{\partial V_D} = (2aQ_S + b)2C_{eff} \times DIBL \end{aligned} \tag{4.11}$$

$$Q_S = 2C_{eff}(V_G - V_{tho} + DIBL \times V_D) \tag{4.12}$$

$$\begin{aligned}\frac{\partial I_D}{\partial V_D} &= (2aQ_S + b)2C_{eff} \times DIBL \\ &= 8a(C_{eff})^2 (V_G - V_{tho} + DIBL \times V_D) DIBL + 2bC_{eff} \times DIBL \\ &= 8a(C_{eff})^2 (V_G - V_{tho}) \times DIBL + 8a(C_{eff})^2 V_D \times DIBL^2 + 2bC_{eff} \times DIBL \\ &= 8a(C_{eff})^2 V_D \times DIBL^2 + \left[2bC_{eff} + 8a(C_{eff})^2 (V_G - V_{tho})\right] \times DIBL\end{aligned} \tag{4.13}$$

From the Green's function simulation results in Fig. 3-2 to 3-4, we can obtain different I-V slopes for different channel lengths, which create different DIBL values through (4.13).

4.3 Effect of *DIBL* on Ballistic I-V

2-D Green's function simulation [9] was applied to furnish ballistic I-V characteristics for three channel lengths as shown in Fig. 4-7 to 4-9. With *DIBL* as the only adjusting parameter, the proposed model was found to be able to handle the 2-D behaviors as clearly seen in these figures. Moreover, by comparing the extracted *DIBL* with that from the shift of the subthreshold I-V curves as created by the 2-D Green's function simulation, we found that they are comparable each other as shown in Fig. 4-10.

4.4 On the Validity of the Channel Backscattering Theory

To examine the validity of the channel backscattering theory, we replaced the r_{BF} in the model with the channel backscattering coefficient r_C [2] and compared the calculated results with those from 2-D Monte Carlo particle simulation [4]. First of all, the k_BT layer widths were cited from the simulated potential profiles for different

scattering areas (see Fig. 6 of [4]) as shown in Fig. 4-11. Then the drain current was calculated and strikingly, the calculation values are quite consistent with those from Monte Carlo simulation as revealed in Fig. 4-12. Further corroborating evidence in terms of the change in the peak of the barrier as the scattering area changes is given in Fig. 4-13. Therefore, the channel backscattering theory remains valid. However, as the mobility or scattering time is increased by a factor of 5, implying that the channel length is effectively reduced from 25 nm down to 5 nm, the calculated drain currents appear to lie above the Monte Carlo ones as shown in Fig. 4-14, suggesting the increasing importance of the drain scattering [3],[4]. The existing channel backscattering formula might be improved (see [8] for the bilk case) to meet this issue.

4.5 Improved Compact Expression for the k_BT Layer Width

We have established a new compact expression for the bulk case [11]: (a) the k_BT layer width l is a weak function of gate voltage in the linear region; (ii) in the saturation region l follows the amount of injected carriers (through gate voltage minus effective threshold voltage) while the drain voltage tends to shift the l versus gate voltage curve; and (iii) $l \propto (k_BT/q)^{0.5}$. This model can readily apply to a specific double-gate device [12] with the results in Fig. 4-15 and 4-16. Evidently, excellent agreements are achieved as long as the modulation by gate voltage is taken into account.

Chapter 5

Conclusion

A physically based analytic model of the ultrathin film double-gate MOSFETs has been established. The validity of the model has been confirmed using sophisticated device simulations such as 1-D Schrödinger – Poisson solving, 2-D ballistic I-V simulations, and existing 2-D Monte Carlo particle and Green's Function simulations with the scattering in the channel. The issues of concern have been clarified the effect of backward to forward flux ratio on the thermal injection velocity at the top of the barrier, the comparison of DIBL extracted from the model with that from subthreshold I-V shift, the validity of the channel backscattering theory once the backward to forward flux ratio is replaced by the channel backscattering coefficient, and the potential applications of an improved expression for the width of the k_BT layer (a critical zone, part of the barrier).

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