Table of Contents

Part I
Introduction and Theory .......................................................................................... 1

Part II
Examples: Bulk MOSC’s .......................................................................................... 10
   Example 1: The potential profile and the appropriate charge profile of
   bulk MOSC at zero gate bias ............................................................................. 13
   Example 2: Effect of charge profile on the behavior of sub-100nm
   MOSFETs ........................................................................................................ 19
   Example 3: MOSFET threshold voltage shift, an effect of energy
   quantization .................................................................................................... 26
   Example 4: Triangle well Approximation and Subband population:
   How they vary with Gate voltage .................................................................... 32

Part III
Examples: Single and Double gate SOI-C’s ............................................................ 34
   Example 1: DG-MOSC electrostatics and charge control study;
   classical approach ............................................................................................ 37
   Example 2: Variation of inversion charge with gate voltage in
   DGMOSC ......................................................................................................... 43
   Example 3: Quantum mechanical distribution of inversion
   charge and effect of centroid on DG-MOSC .................................................... 47
   Example 4: Threshold voltage variation with thickness ................................ 54

Appendix
Syntax of Input file ................................................................................................. 59
MATLAB Scripts: part II ....................................................................................... 62
MATLAB Scripts: part III ..................................................................................... 68
Part I

Introduction and Theory
A Brief Tutorial Introduction to
Schred 2.0 and Quantum Confinement in MOS Structures

1.0 Objective of this Tutorial

The main objectives of this tutorial are three fold: 1) to discuss the key quantum mechanical effects in MOS capacitors, 2) to illustrate the fundamentals of SOI structures and 3) in this process provide a quick introduction to Schred 2.0, which is the numerical tool used in this tutorial.

Outline

This tutorial is divided into three parts. Part I reviews the relevant theories that will serve as the background for the rest part of this tutorial. Part II concentrates on the bulk MOSC where a couple of examples are presented to describe some key quantum effects in bulk MOS capacitors. While part III focuses on SOI structures. It gradually develops the basic physics of SOI structures starting from the bulk. Finally an appendix is attached which lists a summary of Schred 2.0 syntax and the Matlab scripts that are used for post processing and generating the figures.

2.0 Theory

It has been well known since the late sixties, that for a better description of the MOS structure, the conventional semi-classical approach is not very adequate. In the semi-classical approach, the density of states above the conduction band is assumed to be continuous, and using this continuous density of states model and the Fermi function, the classical description of the electron concentration can be obtained. This approach works well if the bands are slowly varying.

Fig. 1: Potential well formed at oxide-semiconductor interface.
compared to the electron’s deBroglie wavelength. However, in case of an MOS C, Fig. 1 shows that the band bending near the surface can form a quantum well, which introduces energy quantization. So the semi-classical approach does not work well for these problems, and for a precise description a quantum mechanical approach has to be used.

In the following section, the quantum mechanical approach is described briefly. For an exhaustive review of the quantum mechanical approach and effects on MOS C’s and MOSFETs the reader may read the review article by F. Stern [1]. Also the semiclassical treatment is described in many textbooks like [2].

2.1 The Self-consistent method of solving Schrödinger-Poisson equation

For a quantum mechanical description of MOS structures, we have to solve, the coupled Schrödinger and Poisson’s equation, which can only be done numerically. For an electron, which is confined inside the conduction band potential well $E_c(x)$, its wave function and allowable energies can be found by solving the Effective Mass Schrödinger Equation,

$$\left(-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} + [E_c(x)]\right)\psi_i(x) = E\psi_i(x).$$

This equation gives a set of eigenenergies $\{E_i\}$ and the corresponding set of wavefunctions $\{\psi_i(x)\}$. The available energies above the conduction band are called subbands. As soon as we know the allowable eigenenergies and the spatial distribution of an electron in that eigenstate $(|\psi_i(x)|^2)$, we can calculate the electron density per square cm. in that state according to

$$N_i = F_{2D}(\mu - E_i) = \frac{m^*K_BT}{2\pi \hbar^2} \ln \left(1 + \exp \left(\frac{\mu - E_i}{K_BT}\right)\right).$$

But if there is more than one electron in the system, they will start repealing each other. So, the potential energy that each electron will feel is not only determined by the conduction band edges, but also by the electron-electron interaction, which has to be calculated through Poisson’s equation

$$-\frac{d}{dx} \left(\varepsilon_c(x) \frac{dE_c(x)}{dx}\right) = \frac{q^2}{\varepsilon_0} \left[p(x) - n(x) + N_D(x) - N_A(x)\right].$$
Thus eqs. (1) and (3) are coupled non-linearly and have to be solved self-consistently. The method goes like this:

1. Start with an arbitrary guess for: $E_c(x)$
2. Solve Schrödinger equation with $E_c(x)$ to find eigenstates and wavefunctions.
3. Then using eigenenergies and wavefunctions, calculate $n(x)$ according to Fermi function.
4. Poisson’s Equation

$n(x) \rightarrow \text{Usef}(x)$

This process continues until, both of $n(x)$ and $E_c(x)$ satisfy the Schrödinger equation and the Poisson’s equation simultaneously. In other words, until the difference of $E_c(x)$ between successive iterations become smaller than a predefined small number. This is the essence of quantum mechanical approach to simulating MOS capacitors.

2.2 Silicon Band Structure and Primed and Unprimed Subbands

There is a little modification of the above procedure when applied to the silicon MOSCs. That is due to the band structure of silicon (Fig. 2). As is well known, the effective mass is inversely proportional to the curvature of the constant energy ellipsoids. The two ellipsoids along the x direction have their longitudinal...
effective mass perpendicular to the surface. So they respond to the external field with their longitudinal effective mass, which is 0.916m₀ (where m₀ is the mass of free electron). The other four respond with the transverse effective mass 0.19m₀ because their transverse effective mass is perpendicular to the surface. Thus the Schrödinger equation has to be solved twice, once for the longitudinal effective mass and again for the transverse effective mass. Thus for each effective mass a set of subbands will be obtained. Each set of subbands can be visualized as a ladder. Thus two different ladders will be obtained for each effective mass, as shown in Fig. 3. Subbands from ladder corresponding to the longitudinal effective mass, are called unprimed subbands, and subbands from the other ladder are called primed subbands. It should be noted that, subbands of unprimed ladder have a degeneracy of 2 as there are two ellipsoids in this group, and subbands of primed ladder have a degeneracy of 4.

The unprimed ladder has a larger effective mass, so their energies are relatively smaller than the primed ladder. Normally, the lowest 3 or 4 unprimed subbands and lowest 2-3 primed subbands are occupied at room temperature, other subbands can be safely ignored as they have negligible population.

2.3 Quantum effects in MOS structures

So far we have outlined the mechanics of the quantum mechanical calculation for MOS structures. What we understood is: why we need quantum approach and how we solve the problem quantum mechanically. But, we may want to know how these quantum results differ from the semi-classical result. There are actually two key effects. To see this let us consider Fig. 4 and 5.
Figure 4, shows one of the effects, that is the quantization of the energies above conduction band, which is assumed to be continuous in classical model. The direct effect of this on MOS capacitors or on MOSFETs is an increase of threshold voltage, because the threshold voltage is approximately the gate voltage for which, the conduction band goes below the Fermi level. However, due to the energy quantization, the lowest level that electrons occupy is not the bottom of conduction band, rather it is the first energy level, which is little higher than the conduction band edge. So to bend this band below the Fermi level, a little more gate voltage is needed. This gives rise to a threshold voltage rise in MOSFETs.

Another effect comes from the spatial distribution of inversion charge. Both the classical and the quantum distribution of inversion charge along the depth of the device (x direction) are shown in Fig. 5. The classical distribution shows a peak at the oxide semiconductor interface while the quantum mechanical distribution is totally different from that and shows a peak inside. The net effect is that the actual profile (quantum mechanical) has an average distance from the surface that is larger than that predicted by the classical calculations. As we know, the average carrier distance has the effect of increasing the effective oxide thickness. Thus the quantum mechanical calculation predicts a larger effective oxide thickness, which means a lower gate capacitance.

Fig. 4: Potential well formed at the oxide semiconductor interface. Horizontal lines represent the subbands.

Fig. 5: Classical and quantum mechanical charge distribution inside semiconductor.
Thus for a certain gate voltage, the amount of inversion charge will be somewhat smaller than that, predicted by the classical analysis. This is more important as the oxide thickness becomes smaller with each technology generation.

Detailed discussion of quantum effects in MOSFETs can be found in [3] and [4].

3.0 THE SCHRED PROGRAM

Schred 2.0 calculates the envelope wavefunctions and the corresponding bound-state energies in typical MOS, SOS or SOI structures by solving self-consistently the one-dimensional (1D) Poisson equation and the 1D Schrödinger equation. Version 2.0 has the following features:

1. It can simulate both p type and n type silicon bodies for bulk or SOI structures and can assume both n-type and p-type polysilicon or metals with specified workfunction as the gate contact.

2. Both classical and quantum modes of simulation can be done. In a classical simulation either Maxwell-Boltzmann or Fermi-Dirac statistics can be used.

3. For quantum simulation Schred 2.0 assumes the [100] plane to be parallel to the Si/SiO₂ interface.

4. In doing bulk structure quantum mode simulations, version 2.0 can solve both the inversion and accumulation regions quantum mechanically. However in either region only one type of carrier is treated quantum mechanically (electrons in inversion region, for p body) while other type of carriers (holes in inversion region, for p body) are treated classically.

5. In doing SOI quantum mode simulations, both electrons and holes are treated quantum mechanically at the same time.

6. The charge density on the gate is always calculated classically. Version 2.0 allows different gate dielectrics for top and bottom gates.
7. In quantum mode simulations, electrons in the p-body inversion layer are represented by longitudinal and transverse effective masses, which gives rise to unprimed and primed ladder of subbands respectively.

8. For holes, the heavy hole and light hole valence bands are considered, ignoring the split off band.

9. No oxide penetration of wavefunctions are considered, that is wavefunctions are assumed to be zero at the oxide-semiconductor interface.

10. Either full Fermi-Dirac statistics or Boltzman approximation can be used.

11. In quantum mode simulations, it has exchange co-relation correction capability, which can also be turned off.

12. Schred 2.0 produces the following outputs: Conduction-band edge profile, charge density per cm$^3$ and per cm$^2$ in the body, average distance of carriers from the interface, total gate capacitance $C_{tot}$, and oxide capacitance $C_{ox}$. When the quantum mode simulation is chosen, it also provides the subband energies and wavefunctions in the body.

The following output files are useful

<table>
<thead>
<tr>
<th>File name</th>
<th>1$^{\text{st}}$ Column</th>
<th>2$^{\text{nd}}$ Column</th>
<th>3$^{\text{rd}}$ Column</th>
<th>4$^{\text{th}}$ Column</th>
<th>5$^{\text{th}}$ Column</th>
</tr>
</thead>
<tbody>
<tr>
<td>ad_dist.dat</td>
<td>$V_G$</td>
<td>$N_{inv}$</td>
<td>$Z_{avg}$</td>
<td>$\phi_s$ (wrt bulk)</td>
<td></td>
</tr>
<tr>
<td>capacitance.dat</td>
<td>$V_G$</td>
<td>$C_{tot}$ (uF/cm$^2$)</td>
<td>$C_{ox}$ (uF/cm$^2$)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>chrg.dat</td>
<td>$z$ (nm)</td>
<td>$E_c$ (eV)</td>
<td>Elect. Fld.</td>
<td>$n(x)$ (cm$^{-3}$)</td>
<td>$p(x)$ (cm$^{-3}$)</td>
</tr>
</tbody>
</table>

DEBUG

This file contains the information about progress of the current simulation. This file is continuously updated by Schred 2.0 while the simulation is running.

Also valuable information can be found in the output file ( .out ).
REFERENCES


Part II

Examples: Bulk MOSC’s
Simulating the bulk-MOSC, classically and quantum mechanically

As was mentioned in Sec. 2.3, the quantum mechanical calculation primarily has two distinct features that differ from classical results. One is the quantization of available energy (along with different density of states than the classical) and another is the distribution of carriers (electrons as well as holes) inside the semiconductor. Most of the terminal behaviors that are attributed as quantum effects are some sort of manifestation of above two features.

In the examples to follow in this part of tutorial, the main objective will be to address the major quantum effects that are seen in sub 100nm MOSFETs and in the process to learn to use Schred 2.0 to understand some of the physics behind MOSFETs of such small scales.

If we try to put all the main effects all together the story goes like this. The potential well formed near the oxide-semiconductor interface gives rise to energy quantization and a charge distribution that has a peak not right at the surface, rather at some point down the substrate. This is shown in example 1.

The minority carrier distribution inside the semiconductor gives rise to two effects that are seen from terminal behavior. One is due to the finite shifting of the centroid of carrier distribution inside semiconductor, which degrades the total gate capacitance even at strong inversion and also changes the semiconductor surface potential significantly beyond strong inversion; where it is normally assumed to be pinned at some fixed value ($2\varphi_F$ or $2\varphi_F + 6k_BT/q$). And the other effect is due to the oxide-semiconductor interface boundary condition that forces the carrier density to go to zero at the interface giving rise to a small region over which either minority carrier concentration or the majority carrier concentration is significantly smaller (some author call this region as “dark zone”) which give rise to a significant degradation of total gate capacitance even at flat-band condition. These effects are illustrated by example 2.

Quantization of the available electronic states above conduction band and reduced density of states for electrons (assuming nMOS) give rise to threshold voltage shift and degraded transconductance of MOSC than predicted by classical analysis. Example 3 examines these issues.
These are the chief quantum effects seen in sub 100nm MOSFETs. Some of the authors suggested that at low enough electric fields the potential sub-well that form at the oxide-semiconductor interface can be well-described by a triangular well approximation which has analytic solutions. Schred 2.0 is an excellent numerical tool to check this point. So example 4 is an examination of this possibility. These are all the examples of this part. Below the name of the examples are listed:

**Example 1:** The potential profile and the appropriate charge profile of bulk MOSC at zero gate bias.

**Example 2:** The effect of charge profile on the behavior of sub-100nm MOSFETs.

**Example 3:** MOSFET threshold voltage shift, an effect of energy quantization.

**Example 4:** Triangular well approximation.
**Example 1:** The Potential well and the appropriate Charge profile of bulk MOSC at zero gate bias.

**Objective**

1. To show that a potential well is formed by the silicon and oxide conduction bands at the oxide silicon interface.

2. And to compare the classical and quantum mechanical minority carrier charge distribution inside silicon.

As was mentioned earlier, the quantum effect has several consequences. However, why the quantum effect arises anyway. This question was addressed in Sec. 2, part I of this tutorial and there it was stated that this is due to the presence of a potential well, which is formed by the conduction band discontinuity at the oxide-semiconductor interface. This potential well can give rise to significant energy quantization, so that it is no longer accurate to consider the conduction band as a quasi-continuous band as is assumed in semi-classical treatment. So, the first objective of this example is to show this potential well near the interface.

If quantum mechanical treatment is used, the boundary condition of Schrödinger equation forces the wavefunctions and thus the electron concentration to become negligible at the oxide-semiconductor interface. Thus the charge distribution inside the semiconductor has a peak not at the interface, rather somewhere inside the semiconductor body. This is directly the opposite to our common sense or of classical viewpoint. Our second objective then compares the classical and quantum mechanical charge distribution inside semiconductor.

**Figures and Discussion**

Figure 5 plots the energy band diagram of a MOSC with oxide thickness 4nm, body doping $10^{17}$ cm$^{-3}$ and metal gate of work function 4.05eV. Figure 5a shows the band diagram at zero gate bias and 1b at a gate bias of 3v. It is seen that a potential well is formed inside silicon at the oxide-semiconductor interface, due to the discontinuity of conduction bands between silicon dioxide and silicon, which is shown separately in Fig. 5c. At zero gate bias this potential well is
less stiff and separation between various subbands are relatively small, which means many of the subbands are occupied at the same time. If the gate bias is increased, the potential well becomes stiffer and the separation between subband energies as well as the energy of the lowest subband gets higher as a result only a few lower energy subbands are occupied at this case. Figure 5d compares the potential wells at zero gate bias and at a gate bias of 3.0v and it supports the above argument.

![Graphs showing potential wells at different gate biases](image1)

Fig. 5: Band diagram of MOSC. Complete band diagram (a) at $V_G = 0v$, (b) at $V_G = 3v$. (c) Shows the potential well formed inside the semiconductor and (d) is a magnified plot of (c) near the interface showing that high gate bias causes stiffer potential well.

Intercept from output file `qm.out` containing subband population data is shown in table I, where L1 represents the percentage population of ladder one (unprimed ladder) and L2 represents the percentage population of ladder two (primed ladder). N11, N21, N31 and N41 are
the population of 1st, 2nd, 3rd and 4th subbands of ladder one, while N21 and N22 represents the population of 1st and 2nd subbands of ladder two. It is seen that at $V_g = 0v$, $L1=51\%$ and $L2=49\%$, where as at $V_g = 3.0v$, $L1=78\%$ and $L2=22\%$. This clearly shows that as gate voltage increases (for nMOS), all the electrons tend to occupy the lowest subband.

**Table I**

<table>
<thead>
<tr>
<th>$V_g$ [V]</th>
<th>$N_i$ [1/cm$^2$]</th>
<th>$L1$ [%]</th>
<th>$L2$ [%]</th>
<th>$N_{11}$ [%]</th>
<th>$N_{21}$ [%]</th>
<th>$N_{31}$ [%]</th>
<th>$N_{41}$ [%]</th>
<th>$N_{12}$ [%]</th>
<th>$N_{22}$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.11E+10</td>
<td>51.452</td>
<td>48.548</td>
<td>37.787</td>
<td>9.435</td>
<td>3.076</td>
<td>1.155</td>
<td>44.350</td>
<td>4.198</td>
</tr>
<tr>
<td>3.000</td>
<td>0.13E+14</td>
<td>77.791</td>
<td>22.209</td>
<td>71.746</td>
<td>5.022</td>
<td>0.805</td>
<td>0.217</td>
<td>21.506</td>
<td>0.703</td>
</tr>
</tbody>
</table>

This is because with the increase of gate voltage, potential well becomes stiffer and stiffer (Fig. 5d) as a result, energy of the lowest subband as well as the separation between various subbands increase, so the lowest subband becomes primarily occupied. Table II, which is also an intercept from the *qm.out* file, shows the subband energies for electrons at two gate biases. Note that, at $V_g = 0v$, $E_{11}=48.73$meV, $E_{21}=84.59$meV and so on, while at $V_g = 3v$, $E_{11}=312.18$meV and $E_{21}=357.18$meV. Both the energy of $E_{11}$ as well as the separation between $E_{21}$ and $E_{11}$ increase as $V_g$ increases from 0v to 3v (Table II).

**Table II**

<table>
<thead>
<tr>
<th>$V_g$ [V]</th>
<th>$N_i$ [1/cm$^2$]</th>
<th>$E_f$ [meV]</th>
<th>$E_{11}$ [meV]</th>
<th>$E_{21}$ [meV]</th>
<th>$E_{31}$ [meV]</th>
<th>$E_{41}$ [meV]</th>
<th>$E_{12}$ [meV]</th>
<th>$E_{22}$ [meV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.11E+10</td>
<td>-188.81</td>
<td>48.73</td>
<td>84.59</td>
<td>113.56</td>
<td>138.86</td>
<td>83.70</td>
<td>144.63</td>
</tr>
<tr>
<td>3.000</td>
<td>0.13E+14</td>
<td>312.18</td>
<td>255.26</td>
<td>357.18</td>
<td>406.27</td>
<td>440.34</td>
<td>358.83</td>
<td>449.14</td>
</tr>
</tbody>
</table>

Classical and quantum mechanical electron distribution is shown in Fig. 6. It is seen that, both curves have roughly same pattern for higher values of $x$ (coordinate perpendicular to the surface), but they are completely different at the surface. The classical electron density shows a peak right at the surface and quantum mechanical electron density shows peak at some point inside the silicon body. Whether this difference is negligible or not depends on oxide thickness. If the oxide is thick enough then it doesn’t matter, if we use quantum mechanical or classical
description, but if the oxide itself is very thin then this shift of peak can indeed introduce a significant error, as will be discussed in example 2.

![Graph showing classical and quantum mechanical electron distribution inside semiconductor.]

**Fig. 6:** Classical and quantum mechanical electron distribution inside semiconductor. Here $t_{ox} = 4\text{nm}$, $N_A = 10^{17} \text{ cm}^{-3}$, $V_g = 0.0\text{v}$.

**SCHRED INPUT FILE**

Data for Fig. 5 and Fig. 6 are generated using Schred 2.0. Given the figures, it is now easy to understand what type of simulation needs to be performed. Figure 5, shows band diagram of a MOSC calculated quantum mechanically for two gate voltages, $V_g = 0\text{v}$ and $3\text{v}$, and Fig. 6 shows electron density at zero gate bias but, one is calculated classically and the other is calculated quantum mechanically. Thus we need to perform two simulations for the same MOSC, one in quantum mode and another in classical mode. For quantum mode calculation the following input deck is used.

```
qm.in
*title qm.in: QM STUDY
$-----------------------------------------------------$
device bulk=yes
params temp[K]=300, tox[nm]=4, kox=3.9
body uniform=true, Nb[cm-3]=1.e17
gate metal=true, phi[eV]=4.05
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage Vmin[V]=0.0, Vmax[V]=3.0, Vstep[V]=3.0
charge quantum=yes, Fermi=yes, exchange=no, e_nsub1=4, e_nsub2=2
calc CV_curve=no, file_cv=cv.dat
save charges=yes, file_ch=chrg.dat,
+ wavefunc=yes, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
```

16
The statement,

```
charge    quantum=yes, Fermi=yes, exchange=no, e_nsub1=4, e_nsub2=2
```

Specifies that a quantum mechanical simulation has to be performed. Note that, four subbands from unprimed ladder \((e_{nsub1}=4)\) and two from primed ladder \((e_{nsub2}=2)\) are to be considered in this simulation. Whether these numbers are adequate or not, cannot be told in advance, but we can guess them and then look at the subband population section of `.out` file to verify this. As is seen from table I, at \(V_g = 3v\), \(N41=0.2\%\) and \(N22=0.7\%\), which are below \(1\%\). Thus occupation of higher subbands can be safely neglected. However, for \(V_g = 0v\), it is seen that \(N41=1.15\%\) and \(N22=4.2\%\), none of them are below \(1\%\), which means more subbands need to be included for a better accuracy at zero gate bias simulation for this MOSC. As a rule of thumb, for simulations near flatband or subthreshold regions it is safe to start with a higher value for \(e_{nsub1}\) and \(e_{nsub2}\), then by checking the subband populations, then can be adjusted accordingly for the final simulation. However when doing a simulation at several gate voltages, it is necessary to adjust the numbers carefully to avoid lengthy simulation time.

Following statement

```
voltage    Vmin[V]=0.0, Vmax[V]=3.0, Vstep[V]=3.0
```

causes the simulation to be performed for two bias points; first for \(0v\) and next for \(3v\). In order to generate Fig. 5, we need conduction band data and to generate Fig. 6 we need electron density data. All these data are found in a single file named `chrg.dat`. An intercept of the `chrg.dat` file is shown below.

```
chrg.dat :
%-----------------------------------------------------------------------------------
% POTENTIAL, E_FIELD, CHARGES, DOPING for Vg =  0.000  [V]
% Ec  ==> conduction band edge
% FD  ==> electrical field
% n   ==> electron density
% p   ==> hole density
% ro  ==> p - n - Na + Nd
% dop ==> Na - Nd (ionized)
%-----------------------------------------------------------------------------------
-0.6995E+01  0.190734863437E-06  0.000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.4200E+01  0.190734863437E-06  0.000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.4000E+01  0.315000019073E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.3800E+01  0.315944074431E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.3587E+01  0.316947482292E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.3361E+01  0.318013974246E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.3121E+01  0.319147516378E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.2871E+01  0.320352058510E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.2611E+01  0.321636590642E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.2341E+01  0.322901122774E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.2061E+01  0.324145654905E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.1771E+01  0.325370187036E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.1471E+01  0.326584719167E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.1161E+01  0.327779251299E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.0841E+01  0.328953783430E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.0521E+01  0.330108315561E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
-0.0191E+01  0.331242847692E+01  0.472028E+06  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00  0.000000000000E+00
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .
  .     .     .     .     .     .     .     .

```
%--------------------------------------------------------------------------------
% POTENTIAL, E_FIELD, CHARGES, DOPING for Vg = 3.000 [V]
% Ec  ==> conduction band edge
% FD  ==> electrical field
% n   ==> electron density
% p   ==> hole density
% ro  ==> p - n - Na + Nd
% dop ==> Na - Nd (ionized)
%--------------------------------------------------------------------------------

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>-.6995E+01</td>
<td>-.299999980927E+01</td>
<td>0.000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.4854E+01</td>
<td>-.299999980927E+01</td>
<td>0.000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.4200E+01</td>
<td>-.299999980927E+01</td>
<td>0.000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.4000E+01</td>
<td>0.150000190735E+00</td>
<td>0.671954E+07</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.3800E+01</td>
<td>0.284390991585E+00</td>
<td>0.671954E+07</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.3587E+01</td>
<td>0.427230920635E+00</td>
<td>0.671954E+07</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.3361E+01</td>
<td>0.579051173235E+00</td>
<td>0.671954E+07</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
<tr>
<td>-.3121E+01</td>
<td>0.740416340885E+00</td>
<td>0.671954E+07</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
<td>0.000000000000E+00</td>
</tr>
</tbody>
</table>

Note that, results for V_g = 0v and V_g = 3v are appended in the same file in the appropriate order.

Classical simulation is needed only at zero gate bias. Following file does a classical mode simulation.

**cl.in**

*title cl.in: CLASSICAL STUDY*

```bash
$-----------------------------------------------------$
device bulk=yes
params temp[K]=300, tox[nm]=4, kox=3.9
body uniform=true, Nb[cm-3]=1.e17
gate metal=true, phi[eV]=4.05
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage Vmin[V]=0.0, Vmax[V]=0.0, Vstep[V]=0.1
charge quantum=no, Fermi=yes
calc CV_curve=no, file_cv=cv.dat
save charges=yes, file_ch=chrg.dat,
+ wavefunc=yes, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
```

Here the statement

```
charge quantum=no, Fermi=yes
```

specifies classical mode simulation. Note that, in order to generate the char.dat file, charges=yes have to be set (line 11 of the above file).

After executing the *qm.in* file chrg.dat file is saved as *ex1qms.dat* and after executing *cl.in* file, chrg.dat is saved as *ex1cl.dat* file, then Matlab script *ex1.m* is executed to generate Fig.5 and Fig. 6.
**Example 2: Effect of charge profile on the behavior of sub-100nm MOSFETs.**

**Objective**

1. To show the effect of inversion charge distribution on band bending inside semiconductor.
2. And to discuss the degradation of gate capacitance, originating from voltage drop due to inversion charge inside semiconductor.

In the most simplified description of MOSC, it is assumed that the inversion charge builds up right at the oxide-semiconductor interface like a sheet of charge. This means, the potential drop inside semiconductor is only due to the ionized acceptors and inversion charge will not introduce any potential drop at all. It is also assumed in this simplified model that, if after strong inversion the gate voltage is increased, there is always sufficient inversion charge at the interface to screen out the extra gate charge so that no further penetration of flux lines into semiconductor is possible, and thus the depletion width becomes fixed at its maximum value.

Thus two points come out from the above model, 1) semiconductor band bending only depends on depletion charge that is the effect of inversion charge profile on semiconductor voltage drop is negligible and 2) depletion layer width becomes constant after strong inversion, in other words there is always total screening of gate charge after strong inversion, where by strong inversion it normally means the condition for which semiconductor potential drop at the interface becomes $2\phi_F$ [1]. The question is; is the effect of inversion charge profile on semiconductor band bending really negligible? Also to what extent is the idea of perfect screening valid? If perfect screening at all exits then at what surface potential does it happen? Is it the normally used value $2\phi_F$, or the value $(2\phi_F + 6k_BT/q)$ that is suggested by Tsividis[2]? The first objective of this example is to explore these questions.

If semiconductor voltage drop due to inversion charge is not negligible, then it is equivalent to a capacitor in series with the oxide. Thus the total gate capacitance will be smaller than oxide capacitance, this is known as degradation of gate capacitance. If this degradation is significant, then it suggests a non-negligible voltage drop compared to the drop across oxide. To what extent
does this inversion drop degrade the gate capacitance also depend on oxide thickness. Our second objective is to study this capacitance degradation.

**Figures and Discussion**

To answer the above questions the straightforward method is to plot the semiconductor band bending with respect to gate voltage using Schred 2.0, as is shown in Fig. 7 and use it to explain the above. However, before discussing Schred 2.0 results, let us briefly see what electrostatic predicts. According to Gauss’s law

\[
\varepsilon \xi(x) = q \int_{-\infty}^{\infty} N_A(x) dx + q \int_{-\infty}^{\infty} n(x) dx.
\]

\[
-\frac{\varepsilon}{q} \frac{d\phi}{dx} = \int_{-\infty}^{\infty} N_A(x) dx + \int_{-\infty}^{\infty} n(x) dx.
\]

\[
-\frac{\varepsilon}{q} \Delta \phi = \int_{-\infty}^{\infty} N_A(x) dx + \int_{-\infty}^{\infty} n(x) dx.
\]

\[
-\frac{\varepsilon}{q} \Delta \phi = \left[ \int_{-\infty}^{\infty} N_A(x) dx \right]_{0}^{\infty} - \int_{0}^{\infty} x N_A(x) dx + \left[ \int_{0}^{\infty} n(x) dx \right]_{0}^{\infty} - \int_{0}^{\infty} x n(x) dx.
\]

\[
\Delta \phi = \left( \int_{0}^{\infty} x N_A(x) dx \right) \frac{q}{\varepsilon} \int_{0}^{\infty} N_A(x) dx + \left( \int_{0}^{\infty} x n(x) dx \right) \frac{q}{\varepsilon} \int_{0}^{\infty} n(x) dx.
\]  

\[
\Delta \phi = \left( z_d \right) \frac{Q_d}{\varepsilon} + \left( z_i \right) \frac{Q_i}{\varepsilon}.
\]  

\[
\phi_s = \phi_{dep} + \phi_{inv}.
\]

Where \( \phi_s = \Delta \phi_s \) : \( \phi_{dep} = \left( z_d \right) \frac{Q_d}{\varepsilon} = \left( \phi_s - \left( z_i \right) \frac{Q_i}{\varepsilon} \right). \)

Thus it is seen that semiconductor voltage drop depends on total depletion charge and its centroid as well as on total inversion charge and its centroid. So, the inversion charge can indeed be thought of as a sheet of charge of charge density \( Q_i \) (coul/cm\(^2\)), but not at the interface, rather located at its centroid \( \langle z_i \rangle \). And location of this centroid depends on the distribution of inversion
charge. Had it happened that the inversion charge located right at the interface then there were no potential drop in semiconductor due to inversion charge, no matter what the charge density is. That’s why this is called the effect of inversion charge “distribution”. Thus the distribution of inversion charge really introduces drop inside semiconductor. However, the concept of perfect screening can only be justified by numerical calculations.

Let us now consider Fig. 7. In Fig. 7a, semiconductor voltage drop is plotted with respect to gate voltage. Blue curve represents semiconductor drop ($\phi_s$) and red curve is the depletion drop term of eq. (3), which is obtained by subtracting the inversion drop term (calculated from second term of eq. (2)) from surface potential. It is seen that up to a certain gate voltage red curve and blue curve coincides, which means inversion drop term is negligible in that region. This is because there is...
so little inversion charge \((Q_i)\) that, the inversion drop is negligible compared to the depletion drop term. As the gate voltage increases, the red curve becomes constant. This shows that the screening effect really takes place, however, the surface potential at which this happens is neither \(2\Phi_F\), nor \((2\Phi_F + 6k_BT/q)\). The \(2\Phi_F\) value is too small as shown by the lower horizontal line and the value \((2\Phi_F + 6k_BT/q)\), which is represented by the upper horizontal line, is closer to the saturated value. It is not easy to come up with a fixed criterion for strong inversion, but obviously \((2\Phi_F + 6k_BT/q)\) is a better approximation for this. Also the inversion drop part becomes increasingly important after strong inversion and it is not very good approximation to treat the inversion charge at the interface. However how good or how bad this approximation is, depends on oxide thickness also, as will be discussed with connection to gate capacitance degradation. Fig. 7b is the same plot as 1a, except the body doping is 1.E17 cm\(^3\). Figure 7c is a of depletion charge calculated using \(\phi_{dep}\) and depletion approximation.

![Fig. 8: Average distance of inversion charge from the interface. The top most curve represents the average distance for a doping level of 10\(^{17}\) cm\(^{-3}\), while lower two shows for a doping of 10\(^{18}\) cm\(^{-3}\). The bottom dotted curve is the average distance calculated from classical charge distribution, while the middle one is calculated quantum mechanically for the same MOSC. It shows that the quantum mechanical inversion charge centroid is always higher than classical value.](image)

Figure 7d compares the semiconductor voltage drop calculated classically and quantum mechanically. As, inversion charge density is almost zero at the interface, its centroid is more
shifted from the interface than classical analysis predicts. This is also shown in Fig. 8, where the dotted curve represents the average inversion charge distance from interface calculated classically and the next higher curve represents the average distance calculated from quantum mechanical charge distribution. It is seen that, classically the inversion charge is more shifted towards the interface.

This means, classically total gate capacitance will be slightly higher than given by quantum mechanical calculation. Also the percentage degradation of total gate capacitance depends on oxide thickness, because, if the oxide is thicker, most of the voltage will be dropped across the oxide then the voltage drop due to inversion charge is not important, so capacitance degradation (degradation from oxide capacitance value) is less important. This is also seen in Fig. 9 and Fig. 10. Figure 9, shows cv curve for an MOSC with 10nm oxide thickness and Fig. 10 is for 2nm oxide thickness. Effect of inversion charge centroid is more pronounce in latter case than in the former. The percentage degradation for 10nm oxide thickness is about 3% and for 2nm oxide thickness is about 9.5%.
In order to generate Fig. 7 and Fig. 8, we need to know the semiconductor surface potential, total inversion charge and average penetration of inversion carrier at various gate voltages. For this following two Schred files can be used. Qm.in is for quantum mode calculation and cl.in is for classical calculation.

**Qm.in**

*title qm.in: (QM) VARIATION OF US WITH VG

device bulk=yes

params temp[K]=300, tox[nm]=10, kox=3.9

body uniform=true, Nb[cm-3]=1.e17

gate metal=true, phi[eV]=4.05

ionize ionize=no, Ea[meV]=45, Ed[meV]=45

voltage Vmin[V]=0.0, Vmax[V]=8.0, Vstep[V]=0.2

charge quantum=yes, Fermi=yes, exchange=no, e_nsub1=9, e_nsub2=5

calc CV_curve=yes, file_cv=cv.dat

save charges=no, file_ch=chrg.dat,

+ wavefunc=no, file_wf=wfun.dat

converge toleranc=5.e-6, max_iter=2000

The above file is executed once with doping $10^{17}$ cm$^{-3}$ and then with $10^{18}$ cm$^{-3}$. Outputs are extracted from qm.out file. A portion of the intercept from the output file, which is saved as a different file for post processing is shown below.

%--------------------------------------------------------------------------------
%AVERAGE DISTANCE OF THE INVERSION LAYER CARRIERS FROM THE Si/SiO2 INTERFACE:
%Vg ==> Gate bias voltage
%Vs ==> Si/SiO2 interface voltage measured with respect to the body voltage
%Nt ==> 2D total charge density divided by q
%Ni ==> 2D inversion layer carrier density
%Ne ==> 2D electron density
%z_av ==> average distance of the inversion layer
%--------------------------------------------------------------------------------
% Vg[V]  Vs[V]  Nt[1/cm^2]  Ni[1/cm^2]  z_av[nm]  Ne[1/cm^2]
0.000  0.135  -0.546E+13  0.000E+00  0.000  0.000E+00
0.200  0.174  -0.581E+13  0.000E+00  0.000  0.000E+00
0.400  0.218  -0.615E+13  0.000E+00  0.000  0.000E+00
0.600  0.266  -0.648E+13  0.917E-03  1.565  0.917E-03
0.800  0.319  -0.679E+13  0.124E-01  2.013  0.124E-01
1.000  0.374  -0.710E+13  0.666E-01  1.716  0.666E-01

Data files are saved as ex2qm1.dat for $N_A=10^{17}$ cm$^{-3}$ and ex2qm2.dat for $N_A=10^{18}$ cm$^{-3}$. For classical simulation following Schred file is used. And intercept of the above mention section from cl.out file is saved as ex2cl2.dat.
To generate Fig. 9 and Fig. 10, above two files can be used by changing the oxide thickness to 2nm and then to 10nm; also the voltage sweep range have to be changed into -5v to 5v with a step size of 0.2v. In this case, output are obtained from cv.dat file, which registers the capacitances directly. The cv.dat file is saved according to following convention

<table>
<thead>
<tr>
<th>Name</th>
<th>Mode</th>
<th>Oxide Thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>qmcv10.dat</td>
<td>Quantum</td>
<td>10nm</td>
</tr>
<tr>
<td>qmcv2.dat</td>
<td>Quantum</td>
<td>2nm</td>
</tr>
<tr>
<td>qlcv10.dat</td>
<td>Classical</td>
<td>10nm</td>
</tr>
<tr>
<td>qlcv2.dat</td>
<td>Classical</td>
<td>2nm</td>
</tr>
</tbody>
</table>
Example 3: MOSFET threshold voltage shift, an effect of energy quantization.

**Objective**

1. To see how energy quantization leads to threshold voltage shift.

The threshold voltage is an important parameter of MOSFET. Accurate prediction of threshold voltage for a technology generation is very important. If the channel length is small enough, then in order to keep the short channel effects under control substrate doping have to be increased and oxide thickness have to be decreased. In this case, threshold voltage predicted by classical analysis is significantly lower than what is obtained experimentally [1]. This change in threshold voltage that originates from quantum mechanical effects, are no more negligible for these heavily doped MOSFETs. This example is a study on threshold voltage, calculated both classically and quantum mechanically.

**Definition of Threshold Voltage**

Classically the threshold voltage of MOSFET is defined as the gate voltage, for which the minority carrier concentration at oxide-semiconductor interface equals to the doping concentration there (and this condition is known as on-set of strong inversion). Classical theory predicts maximum concentration to be at the surface, hence the definition of threshold voltage in terms of surface concentration makes sense. And this happens, when the semiconductor surface potential \( \phi_s \) equals to twice of \( \phi_b \), where \( \phi_b \) is the position of the equilibrium Fermi level with respect to intrinsic Fermi level (in electron volt).

However, problem with this definition is that it is not applicable to quantum mechanical calculations. Defining in terms of surface concentration does not make sense, because carrier concentration is negligible there anyway. The alternative could be to define the on-set of strong inversion not at the surface but at the point inside the semiconductor body where minority carrier concentration is maximum, but the position of the peak is not fixed and is unknown a-priori. Thus it is more appropriate to define the threshold voltage in terms total number of inversion
charge, instead of concentration. A modified definition of threshold voltage, which reduces to the familiar definition in classical limit, while also applicable to the quantum regime is [2]

\[ \frac{dQ_{inv}}{d\phi} \bigg|_{\phi_{ST}} = \frac{dQ_{depl}}{d\phi} \bigg|_{\phi_{ST}}, \]  

(1)

which is equivalent to

\[ \frac{dQ_{inv}}{dV_G} \bigg|_{V_T} = \frac{dQ_{depl}}{dV_G} \bigg|_{V_T}. \]  

(2)

In this example, the above definition will be used for threshold voltage, in order to study how and why threshold voltage changes by quantum effects.

**DISCUSSION**

According to eq. (1), at threshold voltage, both inversion capacitance and depletion capacitance become equal. Figure 11a shows the variation of inversion charge with surface potential for both classical (red curve) and quantum mechanical (black curve) cases in a logarithmic scale. Both vary linearly in a log scale, which means the dependence is exponential with surface potential. However, classical curve is always higher than quantum, which means the classical approach over estimates the co-efficient of the exponent. The depletion charge varies as square root of surface potential.

Thus the depletion capacitance, which is the derivative of depletion charge with respect to (w.r.t.) \( \phi \), has an inverse square root variation with \( \phi \), and the inversion capacitance, which is the derivative of inversion charge (w.r.t.) \( \phi \), has an exponential variation. When plotted in the same logarithmic scale, with inversion capacitance, as shown in Fig. 11b, the depletion capacitance is more or less constant (with a small negative slope). The point where these two capacitance curves intersect represents the threshold condition. As the classical analysis shows a stronger dependence on surface potential, the classical threshold voltage is always smaller than the actual value.
Fig. 11: Showing the variation of inversion carrier and depletion carrier and with gate voltage surface potential. Red curve represents classical calculation and black curve represents quantum calculation. Parameters are, \( t_{ox} = 10 \text{nm}, \ N_A = 10^{18} \text{ cm}^{-3}, \) metal work function = 4.05 eV. (a) Inversion carrier with surface potential, (b) depletion and inversion capacitances with gate voltage. Flat curve represents depletion capacitance and the other represent inversion capacitance. (c) And (d) show total inversion carrier density with gate voltage in linear scale and logarithmic scale respectively. Note that (c) shows a threshold voltage shift of 1.0v, which is due to choosing very large oxide thickness of 10nm, which is not practical for a doping level of \( 10^{18} \text{ cm}^{-3}. \) Higher value is used for illustration purpose only.

Physically it can be explained this way. In classical approach, the conduction band is assumed to be quasi-continuous, which means the discrete eigenstates are so finely separated that, they can be assumed continuous for practical calculations with the conduction band edge representing the lowest energy level. Thus for a certain increase of gate voltage (nMOS is assumed throughout the discussion), the Fermi level shifts towards the conduction band and a lot of subbands contribute to the total number of electron population according to the three dimensional Fermi function. In quantum mechanical approach, neither the lowest subband is the conduction band, nor the separations between successive subbands are negligible. Thus, for a given position of Fermi level, the quantum mechanical calculation always gives smaller amount of inversion charge than classical analysis predicts.
In short, due to the quantization of energy (energy for motion perpendicular to the surface), conduction band edge no more represents the lowest energy level and the total number of eigenstates that contribute to the electron concentration is also reduced. Thus same gate voltage produces smaller amount of inversion charge than is predicted by the classical calculation. That is to generate a certain amount of inversion charge (other way of saying the threshold condition), a larger gate voltage is necessary than is given by classical calculations. This is known as threshold voltage shift.

![Graph](image)

**Fig. 12:** Variation of threshold voltage with doping concentration, calculated classically and quantum mechanically

![Graph](image)

**Fig. 13:** Threshold voltage shift for 10nm oxide thickness and 2.5nm oxide thickness.

Figure 12 shows, variation of threshold voltage with doping concentrations, calculated both classically and quantum mechanically. Figure 13, shows the shift of threshold voltage with doping for two oxide thickness. It is seen that, higher doping concentration causes greater threshold voltage shift, this is because at higher doping concentrations, potential well become stiffer making the quantization effect more pronounce. On the other hand, for thinner oxide threshold voltage shift is smaller (Fig. 13). As we know, with the shrinkage of gate length, doping level increases and at the same time oxide thickness decreases, these two having opposite effect on threshold voltage shift reduces the threshold voltage somewhat. Still, the threshold voltage shift in today’s MOSFETs is of the order of 0.2v, which is not negligible any more, especially due to the reduction of operating voltage.
Schred Input File

Figure 11 is plotted from the data files generated from example 2. To avoid repetition, the Schred input files are not shown here, which can be found in example 2. For this figure, `ex2cl2.dat` and `ex2qm2.dat` files were used. The procedure for calculating depletion capacitance is discussed in the following paragraph.

For Fig. 12 and 13, two Schred 2.0 files were used, one is for quantum mode and another is for classical mode. For each doping level both classical and quantum mode simulations were done. To get the threshold voltage, the depletion and inversion capacitances have to be calculated. Calculation of inversion capacitance is easy because total number of inversion carrier is given by Schred (or even the inversion capacitance itself is registered). However, for calculating depletion capacitance, first the inversion drop is subtracted from surface potential to obtain the depletion drop and then using depletion approximation depletion charge can be calculated from this drop. Once inversion and depletion charges are known, capacitances can be calculated at once, and the threshold voltage is where the two capacitances intersect. Matlab script `ex3f2.m` and `ex3f3.m` do the calculations on the data files to generate Fig. 12 and Fig. 13. For output data intercept from the `.out` (cl.out or qm.out) file was copied and saved as a data file. A sample intercept from `.out` file is shown below.

```
%--------------------------------------------------------------------------------
%AVERAGE DISTANCE OF THE INVERSION LAYER CARRIERS FROM THE Si/SiO2 INTERFACE:
%Vg ==> Gate bias voltage
%Vs ==> Si/SiO2 interface voltage measured with respect to the body voltage
%Nt ==> 2D total charge density divided by q
%Ni ==> 2D inversion layer carrier density
%Ne ==> 2D electron density
%z_av ==> average distance of the inversion layer
%--------------------------------------------------------------------------------
%  Vg[V]  Vs[V]  Nt[1/cm^2]  Ni[1/cm^2]  z_av[nm]  Ne[1/cm^2]
-0.400  0.473 -0.201E+15  0.870E+07   23.706  0.870E+07
-0.390  0.482 -0.201E+15  0.126E+08   23.408  0.126E+08
-0.380  0.492 -0.201E+15  0.183E+08   23.120  0.183E+08
-0.370  0.502 -0.201E+15  0.265E+08   22.843  0.265E+08
-0.360  0.512 -0.201E+15  0.385E+08   22.576  0.385E+08
-0.350  0.522 -0.201E+15  0.559E+08   22.317  0.559E+08
-0.340  0.532 -0.201E+15  0.811E+08   22.067  0.811E+08
```

30
**cl.in**

*title cl.in: CLASSICAL MODE

$-----------------------------------------------------$

device  bulk=yes
params  temp[K]=300, tox[nm]=4, kox=3.9
body    uniform=true, Nb[cm-3]=1.e17
gate    metal=true, phi[eV]=4.05
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage Vmin[V]=0.0, Vmax[V]=0.0, Vstep[V]=0.1
charge quantum=no, Fermi=yes
calc    CV_curve=no, file_cv=cv.dat
save    charges=yes, file_ch=chrg.dat,
+       wavefunc=yes, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000

$-----------------------------------------------------$

**qm.in**

*title qm.in: QM STUDY

$-----------------------------------------------------$

device  bulk=yes
params  temp[K]=300, tox[nm]=2.5, kox=3.9
body    uniform=true, Nb[cm-3]=1.e15
gate    metal=true, phi[eV]=4.05
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage Vmin[V]=-0.3, Vmax[V]=0.0, Vstep[V]=0.01
charge quantum=yes, Fermi=yes, exchange=no, e_nsub1=9, e_nsub2=5
calc    CV_curve=yes, file_cv=cv.dat
save    charges=no, file_ch=chrg.dat,
+       wavefunc=no, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000

$-----------------------------------------------------$

**REFERENCES**


Example 4: Triangle well Approximation and Subband population: How they vary with Gate voltage.

**Objective**

1. To see how well the triangular well approximation is for various low and high gate voltages.

As Taur and Ning discuss in section 4.3.4.1 (page 195), in the text [1], under subthreshold condition the triangular well approximation is good. And the eigenenergies are given by

\[
E_j = \left[ \frac{3\hbar q^2_s}{4\sqrt{2m_s}} \left( j + \frac{3}{4} \right) \right]^{2/3} \tag{1}
\]

\[
E'_j = \left[ \frac{3\hbar q^2_s}{4\sqrt{2m'_s}} \left( j + \frac{3}{4} \right) \right]^{2/3} \tag{2}
\]

\( j = 0, 1, 2, ..., \) \( m_s \) and \( m'_s \) are the effective mass of unprimed and primed subbands respectively. We take \( m_s = 0.916m_0 \) and \( m'_s = 0.19m_0 \)

We will see how good these approximations are at low and high gate voltages. Further discussion on triangular well approximation can be found in [2].

**Schred Input file**

```plaintext```
*title Example 4:
$-----------------------------------------------------$
device bulk=yes
params temp[K]=300, tox[nm]=4, kox=3.9
body uniform=true, Nb[cm^-3]=1.e17
gate metal=true, phi[eV]=4.05
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage Vmin[V]=0.1, Vmax[V]=3.0, Vstep[V]=2.9
charge quantum=yes, Fermi=yes, exchange=no, e_nsub1=4, e_nsub2=2
calc CV_curve=no, file_cv=cv.dat
save charges=yes, file_ch=chrg.dat,
+ wavefunc=no, file_wf=wfun.dat
```
```
**RESULT AND DISCUSSION**

From `qm.out` file we get the following subband energies:

<table>
<thead>
<tr>
<th>Vg [V]</th>
<th>ni [1/cm^2]</th>
<th>Ef [meV]</th>
<th>E11 [meV]</th>
<th>E21 [meV]</th>
<th>E31 [meV]</th>
<th>E41 [meV]</th>
<th>E12 [meV]</th>
<th>E22 [meV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.100</td>
<td>0.264E+11</td>
<td>-103.36</td>
<td>51.12</td>
<td>88.52</td>
<td>118.65</td>
<td>144.96</td>
<td>87.61</td>
<td>150.97</td>
</tr>
<tr>
<td>3.000</td>
<td>0.134E+14</td>
<td>312.18</td>
<td>255.26</td>
<td>357.18</td>
<td>406.26</td>
<td>440.34</td>
<td>358.83</td>
<td>449.14</td>
</tr>
</tbody>
</table>

Here, E11, E21, E31, E41, E12 and E22 are subband energies. E11 to E41 represents subband energies from unprimed ladder and E12 and E22 represents subband energies from primed ladder. In general, the second index represents the ladder, if it is 1 then it represents unprimed ladder and if it is 2, then it refers to primed ladder. The first index represents subband numbers in that particular ladder.

Using the above expressions for triangular potential well we get the following results:

<table>
<thead>
<tr>
<th>Vg [V]</th>
<th>E11 [meV]</th>
<th>E21 [meV]</th>
<th>E31 [meV]</th>
<th>E41 [meV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.100</td>
<td>52.47</td>
<td>92.30</td>
<td>124.76</td>
<td>153.42</td>
</tr>
<tr>
<td>3.000</td>
<td>284.06</td>
<td>499.71</td>
<td>675.43</td>
<td>830.58</td>
</tr>
</tbody>
</table>

From the above results it is clear that, the triangular well approximation is quite good, at least for back of the envelope calculations in the sub-threshold regime, but cannot be used at all in the inversion region.

**REFERENCE**


Part III

Examples: Single and Double gate SOI-C’s
Simulating the SOI/DG-MOSC, using Schred 2.0

The first example examines the essential electrostatics and charge control of DG-SOI structures. However for a better understanding and for the comparison with the bulk, it is better to start with a bulk MOSC then add a second gate to it (thus making it SOI) while keeping the body thickness relatively larger. Then the body thickness is gradually shrunk down to 10nm to observe how the electrostatics and inversion charge change compared to the bulk MOSC. Three important issues, such as what surface potential should one use in classical modeling of the DG-MOSC, the unpredictability of the surface potential (with gate voltage) at the middle of the silicon body and finally the concept of volume inversion are addressed in this example. Thus showing how the program Schred 2.0 can be used in understanding the essential physics.

As discussed in example 1, mid-width surface potential changes with gate voltage in a manner that cannot be modeled easily, but it remains essentially constant in the sub-threshold region. Example 2 shows this point, and uses it for a qualitative understanding of how the inversion charge builds inside the silicon body as gate voltage increases.

Example 3 focuses on how to calculate the inversion layer centroid in case of symmetric double gate structures. Also some interesting C~V curves are presented in this example.

Example 4 is about the threshold voltage of DG-SOI. Common sense says that, decreasing the body thickness will lower the threshold voltage, it indeed does, but only up-to a certain thickness, after that the threshold voltage starts to increase. This quantum mechanical effect on threshold voltage and also comparison of threshold voltage between bulk and DG-MOSC are discussed in example 4. Finally, example 5 is devoted to a study of subthreshold slope of DGMOSFETs from electrostatic point of view.

All these examples have been chosen to demonstrate the very basics of SOI physics through some concrete numerical simulations. The specific examples to be considered are:

**Example 1:** DG-MOSC electrostatics and charge control study; classical approach.

**Example 2:** Variation of inversion charge with gate voltage in DG-MOSC.
Example 3: Effect of inversion layer centroid on DG-MOSC.

Example 4: Threshold voltage variation with thickness in DG-MOSC.

Example 5: Subthreshold slope of Double gate MOSFET.
**Example 1: DGMOSC electrostatics and charge control study; classical approach.**

**OBJECTIVE**

1. To understand the essential electrostatic changes in DGMOS capacitor due to the close proximity of back gate.

2. To study the charge control mechanism of the DGMOSC.

It is obvious that if the silicon body thickness of a DGMOSC is thick enough (in this example, > 220nm), then the electrostatics will be essentially that of bulk MOSC. However, if body thickness is enough small then the electrostatics will be significantly different and as a result, the inversion charge distribution inside and its total amount will differ. This example is a study of the electrostatics and inversion charge distribution with different body thickness. A classical description, although unable to capture important features of DGMOSCs, is an excellent way to decipher the essential physics.

Three figures will be generated using Schred and using these figures the physics will be discussed.

**Schred input files**

`scl.in`

```plaintext
*title EXAMPLE 1: (Fig. 1): CLASSICAL DGMOSC SIMULATION
$-----------------------------------------------------$
$ VARY t_b[nm]: 250.0, 150, 50 $  
$-----------------------------------------------------$
device  bulk=no
params  temp[K]=300, tox1[nm]=10.0, tox2[nm]=10.0,  
       +  kox1=3.9, kox2=3.9,
body    uniform=true, t_b[nm]=250.0, Nb[cm-3]=1.e17
gate    metall=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,  
       +  N1[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize  ionize=no, Ea[meV]=45, Ed[meV]=45
voltage dual=yes, Vmin[V]=1.5, Vmax[V]=1.5, Vstep[V]=0.01,  
       +  V2min[V]=1.5
charge  quantum=no, Fermi=yes
calc    CV_curve=no, file_cv=cv.dat
save    charges=yes, file_ch=chrg.dat,  
       +  wavefunc=no, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
```

37
This \texttt{sl.in} file is executed three times, with body thickness 250nm, 150nm and 50nm. The corresponding \texttt{chrg.dat} files are saved as \texttt{scl250.dat}, \texttt{scl150.dat} and \texttt{scl50.dat} respectively in a separate folder. These three data files contain the conduction band and charge density data for DG-SOIC’s (classical mode).

\texttt{bcl.in}

\begin{verbatim}
\*title EXAMPLE 1: (Fig. 1) CLASSICAL BULK SIMULATION
$---------------------------------------------------$
device    bulk=yes
params    temp[K]=300, tox[nm]=10, kox=3.9
body      uniform=true, Nb[cm-3]=1.e17
gate      metal=true, phi[eV]=4.05
ionize    ionize=no, Ea[meV]=45, Ed[meV]=45
voltage   Vmin[V]=1.5, Vmax[V]=1.5, Vstep[V]=0.01
charge    quantum=no, Fermi=yes
calc      CV_curve=no, file_cv=cv.dat
save      charges=yes, file_ch=chrg.dat,
          + wavefunc=no, file_wf=wfun.dat
converge  toleranc=5.e-6, max_iter=2000
$---------------------------------------------------$
\end{verbatim}

To compare the results to a bulk MOSC, the \texttt{bcl.in} file is then simulated, and the corresponding \texttt{chrg.dat} file is saved as \texttt{bcl.dat} in the same folder where the previous data files were saved for example 1. Next the Matlab script \texttt{ex1_f1.m} is executed within this folder to produce Fig. 14 and Fig. 15. In this example all the files concerning Fig. 14 are kept in a folder named \texttt{ex1_f1}. This folder then contains the following files:

\begin{verbatim}
/ex1_f1/
scl250.dat scl.in ex1_f1.m
scl150.dat bcl.in
scl50.dat bcl.dat
\end{verbatim}

\texttt{sl.in}

\begin{verbatim}
\*title EXAMPLE 1: (Fig. 2) CLASSICAL MODE DG-SOI
$----------------------------------------------------------------$
$ VARY t_b[nm]: 10, 25, 50, 100, 150, 170, 190, 210, 230, 250  $
$----------------------------------------------------------------$
device      bulk=no
params      temp[K]=300, tox1[nm]=10.0, tox2[nm]=10.0,
            + kox1=3.9, kox2=3.9,
body        uniform=true, t_b[nm]=250.0, Nb[cm-3]=1.e17
gate        metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
            + NL[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize      ionize=no, Ea[meV]=45, Ed[meV]=45
voltage     dual=yes, Vmin[V]=1.5, Vmax[V]=1.5, Vstep[V]=0.01,
\end{verbatim}

38
This file is simulated for each value of body thickness $t_b\,[\text{nm}]$, varying from 250nm to 10nm. Following values of thickness are used: 250, 230, 210, 190, 170, 150, 100, 50, 25 and 10nm. And after each simulation value of $N_i$ is read from $\text{av\_dist.dat}$ file and are saved in a separate file $\text{nil.dat}$. Then the Matlab script $\text{ex1\_f2.m}$ is executed to generate Fig. 16. Files are saved in folder $\text{ex1\_f2}$ for this figure. The following files should appear in this folder:

$\text{/ex1\_f2/}$

$\text{ni\_l.dat}$    $\text{sl.in}$    $\text{ex1\_f2.m}$

**FIGURES AND DISCUSSION**

![Band-diagram of DGMOS capacitors of different body thickness at same $V_G$. Also shown the band diagram of bulk MOSC (red-dashed line). $t_{ox} = 10$nm, $N_A = 1.1E17$ cm$^{-3}$, $V_G = 1.5v$. Classical mode calculation.](image-url)
Fig. 15. Classical charge distribution inside the DGMOSC of different body thickness at same $V_G$. The Dashed line is for bulk MOSC. $V_G = 1.5v$

Fig. 16. Influence of thickness on the amount of total Inversion charge inside of DGMOSC. $V_G = 1.5v$, $N_A = 1.1E17cm^{-3}$, $t_{ox} = 10nm$. 
In all the figures above, the gate voltage is fixed at 1.5v. For a body thickness much greater than twice the maximum depletion width, there is no difference in electrostatics between bulk and DGMOSC, as shown by the dashed (red) and the blue lines of Fig. 14 and Fig. 15. Decreasing the body thickness has no effect as long as \( 2t_{si} > w_{dm} \). This is clear from the right most flat portion of Fig. 16 where, both the inversion and depletion charges are fixed irrespective of body thickness. However, as soon as \( 2t_{si} \) becomes less than \( w_{dm} \), amount of depletion charge starts to decrease linearly with \( t_{si} \) because \( Q_b = -qN_{a}t_{si} \). This is seen in Fig. 16 (\(-Q_b/q \) term). But the total gate charge is held fixed (fixed \( V_G \)) and also

\[
Q_G = -Q_s = Q_b + Q_i
\]

\[
Q_G = |Q_b| + q|N_s|.
\]

So, if \( Q_b \) reduces, electrostatic requires that, \( qN_i \) will increase by the same amount to restore the total charge. The purpose of Fig. 16 is to confirm this point numerically. Thus the flux lines that were left uncompensated due to reduced \( Q_b \) are now paired with extra inversion charges. However, how these extra inversion charges come can be explained using Fig. 14 and Fig. 15. As \( Q_G \) is fixed, the oxide drop, \( V_{ox} \), will remain constant at all body thickness. This means, surface potential \( \psi_s \) will also remain constant for all the cases, which is also obtained numerically (Fig. 14). But the voltage drop inside silicon which is mainly due to the depletion charge will reduce for thinner silicon body. Which means the potential at the middle of the silicon body \( \psi_c \), where electric field is zero will increase for thinner body. The relationship is

\[
\psi_s - \psi_c = \frac{qN_a t_{si}^2}{8\varepsilon_{si}} = \frac{Q_b t_{si}}{8\varepsilon_{si}}.
\]

But as Fermi-level is constant in all cases, increased \( \psi_c \) means increased electron concentration at the middle of the body. This is clearly demonstrated in Fig. 15. Thus, the inversion charge comes from the whole body in thin films, in contrast to the bulk or thick DGMOSCs where the inversion is mainly at the surface. This is known as volume inversion. Although the actual distribution of inversion charge is different which will be shown in example 3 (quantum mode simulation), the qualitative nature of the above argument remains essentially valid. For further discussion reference [1] and [2] can be consulted.
REFERENCES


Example 2: Variation of inversion charge with gate voltage in DG-MOSC.

**Objective**

1. The objective of this example is to demonstrate how the inversion charge builds up in a DG-MOSC.

2. Also some qualitative features of the electrostatic will be addressed, which can serve as useful information.

**Figures and Discussion**

Fig. 17. Variation of band-diagram with applied bias. Top three curves show that only the band at the surface varies while band center does not vary much. The bottom curve shows a complete shift of along with the center of the conduction band.
Fig. 18. DG-MOSC classical mode simulation. $t_{in}=75\text{nm}$, $N_A=1.0\times10^{17}\text{cm}^{-3}$, $t_{ox}=55\text{nm}$. (a) Surface potential w.r.t. bulk versus gate voltage. (b) ($\phi_s-\phi_c$) verses gate voltage. (c) Total inversion charge with gate voltage. (d) Total inversion charge with surface potential.

Fig. 19. Charge distribution inside the silicon at various gate voltages.
In the case of a bulk MOSC, if the gate voltage is increased, the substrate starts to deplete and the same time the conduction band edge comes closer to the Fermi level (in other words the surface potential with respect to bulk conduction band edge starts increasing). As the gate voltage increases, the conduction band edge crosses the Fermi level, and the minority carrier concentration becomes important. At sufficiently high gate voltage, the band bending at the surface introduces so many electrons near the interface that any further introduction of gate charge (that is further increase of gate voltage) are screened out almost totally so that the flux lines from gate cannot penetrate into the substrate, which means the depletion region width becomes fixed and the surface potential increases very slowly (logarithmically) beyond that point. Thus any increase of gate voltage appears across the oxide.

Now, what is the picture for DG-MOSC? When the gate voltage starts increasing from the flat band voltage, the silicon film starts depleting from both sides, the conduction band edge gets closer to the Fermi level and the conduction band edge at the center of the silicon body remains at 0K

$$\varphi_{co} = \frac{E_g}{2q} + \psi_B$$

from the Fermi level. In this range of gate voltages the DG-MOSC behaves like a bulk MOSC, as shown by the top two curves of Fig. 17, where increasing the gate voltage from –0.4v to –0.3v only changes $\varphi_s$, leaving $\varphi_c$ at the bulk value $\varphi_{co}$. Further increase in gate voltage eventually causes the silicon film to be fully depleted when the width of the depletion layer becomes equal to half the silicon body thickness. Normally the doping of the silicon film is low and the thickness of the body is small, as a result at a very small gate voltage the silicon body gets fully depleted. Now if the gate voltage is increased beyond this value, no more depletion charge is available, so to balance the gate charge, inversion charge has to increase. To do this the band-edge at the surfaces will move towards to wards the Fermi level, but the difference between $\varphi_c$ and $\varphi_s$ is determined by the total charge inside the silicon, while the minority carrier contribution is still negligible, it is primarily determined by the depletion charge which has become fixed at this stage (as fully depleted). This means the difference between $\varphi_s - \varphi_c$ becomes constant for a range of voltage until sufficient minority carrier is generated, as shown in Fig. 18b, which means now the whole band will move towards the Fermi level as shown by the bottom two curves of
Fig. 17. This effect leads to volume inversion, as can be seen in Fig. 19. The constant difference in the sub-threshold region is approximately equals to [1]

$$ (\varphi_s - \varphi_c) = \frac{qN_s t_{ox}^2}{8\varepsilon_{si}} = \frac{Q_D}{8C_{si}}. $$

Once sufficient inversion charge generates, surface potential increases rapidly due to drop caused by the inversion charge (Fig. 18a and 18b).

**Schred Input file**

`scl.in`

```
*title EXAMPLE 2: $-----------------------------------------------------$
device bulk=no
params temp[K]=300, tox1[nm]=55.0, tox2[nm]=55.0,
  + kox1=3.9, kox2=3.9,
body uniform=true, t_b[nm]=75.0, N[bcm-3]=1.e17
gate metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
  + N1[bcm-3]=-1.e20, N2[bcm-3]=-1.e20
ionize ionize=no, Ea[meV]=45, Ed[meV]=45
voltage dual=yes, Vmin[V]=-0.5, Vmax[V]=1.5, Vstep[V]=0.1,
  + V2min[V]=-0.5
charge quantum=no, Fermi=yes
calc CV_curve=yes, file_cv=cv.dat
save charges=yes, file_ch=chrg.dat,
  + wavefunc=no, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
```

After executing this file the chrg.dat and av_dist.dat file are copied to the working directory. Then using the Matlab script `ex2f1.m` Fig. 17, 18 and 19 are generated. It is to be noted that, when Schred 2.0 gives the value of surface potential, it refers it with respect to the bulk case.

**Reference**

Example 3: Quantum mechanical distribution of inversion charge and effect of centroid on DG-MOSC.

**Objective**
1. To see how the quantum mechanical charge distribution inside silicon film changes with body thickness.
2. To see how to calculate the centroid in case DG-MOSC.
3. To examine the effect of centroid and charge distribution of very thin body DG-MOSC on the CV curve.

**Discussion**
The method that is used in the calculation of the charge centroid for bulk MOSCs, cannot be used directly for DG case due to its symmetric charge distribution. The centroid plays an important role determining the voltage drop inside the silicon body, thus it has a direct consequence on the gate capacitance. Based on Poisson’s equation, it has been shown that a modified definition for the centroid,

\[
z_t = \frac{\int_0^{r_n/2} zn(z)dz}{\int_0^{r_n/2} n(z)dz}
\]  

(1)

can be used [1]. Based on this definition, it can be shown that

\[
\Psi_s = \Psi_c + \frac{z_t}{2\varepsilon_{si}}Q_i + \frac{Q_n}{8C_{si}},
\]

(2)

Where the second term represents the voltage drop inside the semiconductor due to the inversion charge, which is important if

\[
\frac{\varepsilon_{ox} z_t}{\varepsilon_{si} t_{ox}} \approx 1.
\]

(3)

Figure 20 shows the charge distribution inside the body for various body thicknesses. Figure 21 shows the same charge distribution (other half truncated), due to top gate only.
Two cases are presented; Fig. 21a is for a gate voltage in sub-threshold region, while Fig. 21b is for a gate voltage in strong inversion region.

Fig. 20. Inversion carrier distribution inside the DGMOSC, for various body thickness, with $t_{ox}=10\text{nm}$, $N_a=1.17\text{cm}^{-3}$, $V_G=0.5\text{v}$.

Fig. 21a. Inversion carrier distribution inside the body for various body thickness and with fixed $N_{inv} = 0.196\times10^{14} \text{ cm}^{-2}$.

“Quantum” mode calculation
It is seen that at the smaller gate voltage no-matter what the thickness of the body is, the charge profile is peaked at the middle. Where as at the high gate voltage the peaks shift toward the interface, and the whole distribution looks similar to that of the classical calculation (see Fig. 18). The change in charge profile can be understood in this way. At low gate voltages, the two oxide interfaces create a quantum box whose eigenstates are far shifted from one another (as contrast to the bulk quantum case), so only the lowest subband remains occupied, which have a wavefunction peaked at the middle of the well. As the voltage is increased the other subbands get closer to the Fermi level and begin to be occupied. Their wave functions have more than one peak. For example, the second subband has two peaks and so on. Thus when these wavefunctions are mixed with first subband wavefunction, the overall shape of charge distribution changes, which shifts the centroid from near the center of the body towards the interface. Note that in the case when only the first subband is occupied, the centroid remains close to the middle. The centroid can be calculated using eq. (1) and the data of Fig. 21a. It is clear that, changing gate voltage has very little effect on the centroid if only the first subband is occupied. However, when the other subbands become occupied, the centroid becomes sensitive to the gate voltage, as shown in Fig. 21.
Fig. 22. Quantum calculation, $t_{ox}=5\text{nm}$, $t_{si}=10\text{nm}$, $N_A=1.\text{e}17\text{cm}^{-3}$. (a) variation of centroid with gate voltage, rest three are electron distribution inside silicon film at gate voltage: (b) –0.4v, (c) 0.1v, (d) 1.2v.

Fig. 23. C-V characteristics of ultra-thin body DG-MOSC. $t_{si}=2.0\text{nm}$, $t_{ox}=1.5\text{nm}$ and $N_A=1.\text{E}15$. 
The C-V curve for an ultra-thin, 2nm body with gate oxide thickness of 1.5nm is shown in Fig. 23. The gate capacitance is significantly degraded because eq. (3) is satisfied in this case. The kink near 1.5V is due to the change of centroid as discussed above. At lower gate voltages when only the lowest subband is populated, the centroid varies very slowly with gate voltage and its value is near the middle of the silicon body. However, when the gate voltage exceeds 1.5V the charge distribution changes shape from that of Fig. 22b to Fig. 22c then to Fig. 22d.

**SCHRED INPUT FILES**

**soi.in**

```
*title   EXAMPLE 3, Fig. 1: DG-SOI CHARGE DISTRIBUTION STUDY
-----------------------------------------------------$
$ VARY t_b[nm]: 5, to 20
$-----------------------------------------------------$
device    bulk=no
params     temp[K]=300, tox1[nm]=10.0, tox2[nm]=10.0,
+          kox1=3.9, kox2=3.9,
body       uniform=true, t_b[nm]=20.0, Nb[cm-3]=1.e17
+          metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
+          N1[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize     ionize=no, Ea[meV]=45, Ed[meV]=45
voltage    dual=yes, Vmin[V]=0.5, Vmax[V]=0.5, Vstep[V]=0.1,
+          V2min[V]=0.5
charge     quantum=yes, Fermi=yes, exchange=no, e_nsub1=9, e_nsub2=5,
+          h_nsub1=9, h_nsub2=5
calc       CV_curve=no, file_cv=cv.dat
save       charges=yes, file_ch=chrg.dat,
+          wavefunc=no, file_wf=wfun.dat
converge   toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
```

For each of the values of $t_b[nm]=20nm$, 15nm, 10nm and 5nm, the above file is executed, and after each simulation the chrg.dat file is saved as qs20.dat, qs15.dat, qs10.dat and qs05.dat respectively in a separate directory. Then the Matlab script, fig1.m, is executed from that directory to produce Fig. 20.

**soivgts.in**

```
*title   EXAMPLE 3: Fig. 2a and 2b SOI SIMULATION.
-----------------------------------------------$
$ VARY t_b[nm]: 4, 8 and 30 on both Fig. 2a and 2b. 
$ for Fig. 2a, use: vg=-0.19v, for tsi=4nm
$ vg=-0.24v, for tsi=8nm
$ vg=-0.28v, for tsi=30nm to get
```

```
```
The above file is executed for each of the values of $t_b[nm] = 20nm, 15nm, 10nm$ and $5nm$. For the sub-threshold case (Fig. 21a) the chrg.dat file is saved as csoi4.dat, csoi8.dat, and csoi30.dat respectively. For the strong inversion case (Fig. 21b), the chrg.dat file is saved as sq4.dat, sq8.dat and sq30.dat respectively after each simulation. Then the Matlab scripts, fig2a.m and fig2b.m, are executed to generate Fig. 21a and 21b.

soizi.in

*title EXAMPLE 3: Fig. 3 DG-SOI CENTROID STUDY
$-----------------------------------------------------$

device   bulk=no
params   temp[K]=300, tox1[nm]=5.0, tox2[nm]=5.0,
+  kox1=3.9, kox2=3.9,
body     uniform=true, t_b[nm]=10.0, Nb[cm-3]=1.e17
gate     metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
+  N1[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize   ionize=no, Ea[meV]=45, Ed[meV]=45
voltage  dual=yes, Vmin[V]=-0.5, Vmax[V]=1.5, Vstep[V]=0.1,
+  V2min[V]=-0.5
charge   quantum=yes, Fermi=yes, exchange=no, e_nsub1=11, e_nsub2=7,
+  h_nsub1=11, h_nsub2=7
calc     CV_curve=yes, file_cv=cv.dat
save     charges=yes, file_ch=chrg.dat,
+  wavefunc=no, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
In this case `chrg.dat` and `av_dist.dat` these two files are necessary to generate Fig. 22. These two files have been dumped into a separate folder and then Matlab script `fig3.m` is executed on them to generate Fig. 22.

**sicv.in**

```plaintext
*title   EXAMPLE 3: Fig. 4, C-V curve
$-----------------------------------------------------$
device   bulk=no
params   temp[K]=300, tox1[nm]=1.5, tox2[nm]=1.5,
         + kox1=3.9, kox2=3.9,
body     uniform=true, t_b[nm]=2.0, Nb[cm-3]=1.e15
gate     metall1=true, metall2=true, phi1[eV]=4.05, phi2[eV]=4.05,
         + N1[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize   ionize=no, Ea[meV]=45, Ed[meV]=45
voltage  dual=yes, Vmin[V]=-5, Vmax[V]=5, Vstep[V]=0.1,
         + V2min[V]=-5
charge   quantum=yes, Fermi=yes, exchange=no, e_nsub1=11, e_nsub2=7,
         + h_nsub1=11, h_nsub2=7
calc     CV_curve=yes, file_cv=cv.dat
save     charges=no, file_ch=chrg.dat,
         + wavefunc=no, file_wf=wfun.dat
converge toleranc=5.e-6, max_iter=2000
$-----------------------------------------------------$
```

Executing the Matlab script, `fig4.m`, on the `chrg.dat` file will produce Fig. 23.

**REFERENCE**

Example 4: Threshold voltage variation with thickness.

Objective

1. To study the trend of threshold voltage with body thickness.

Definition of Threshold Voltage

How the threshold voltage should vary with body thickness in a DG-MOSC is the topic of this example. However, before anything else it is important to define the threshold voltage. There is some arbitrariness in defining the threshold voltage. Normally it is defined as that gate voltage for which the silicon band bending is $2\Phi_B$ [1]. However this definition is not applicable when quantum effects are significant. An useful definition, which will take the familiar textbook form in classical limit but will work as well in the quantum mechanical regime is [2]

$$\frac{\partial Q_{inv}}{\partial V_G} \bigg|_{V_T} = \frac{\partial Q_{depl}}{\partial V_G} \bigg|_{V_T}. \quad (1)$$

However this is not applicable for the fully depleted (FD) double gate case as $Q_{depl}$ is independent of gate voltage. One method could be to use a linearly extrapolated value in the $N_{inv} \sim V_G$ curve. In this example the threshold voltage will be defined as the gate voltage for which the total inversion charge equals the depletion charge [3]. This may not be the best choice but simple enough to serve the purpose of this example.

Figures and Discussion

According to the definition above, the threshold voltage of a DG-MOSC should be smaller for thinner silicon body. However, if the body thickness becomes thinner than a certain critical value, the threshold voltage starts to increase instead of decreasing [4]. This is due to the fact that the potential well formed by the two oxide interfaces introduces energy quantization, which becomes important when the body thickness gets thinner than some critical value. The thinner the body thickness is, the wider is the separation between the eigenenergies and also higher is the value of the lowest subband energy. As the subband energies, more importantly the lowest
subband energy, gets shifted away from the Fermi level, the total number of inversion carriers decrease from that predicted by classical calculations.

Thus to achieve a given inversion layer density, larger gate voltage will be required.

For the same $V_G$, \( (Q_i)_{cl} > (Q_i)_{qm} \), \( (2) \)

but \( (Q_{depl})_{cl} = (Q_{depl})_{qm} = \frac{qN_iT_{si}}{2} \), \( (3) \)

so \( (Q_s = Q_i + Q_{depl})_{cl} > (Q_s = Q_i + Q_{depl})_{qm} \) \( (4) \)

that is, \( \left( \frac{V_{ox}}{2\varepsilon_{ox}} \right)_{cl} > \left( \frac{V_{ox}}{2\varepsilon_{ox}} \right)_{qm} \) \( (5) \)

which leads to \( (\Delta\phi_s)_{cl} < (\Delta\phi_s)_{qm} \). \( (6) \)

Thus, at the same gate voltage, quantum theory predicts a higher semiconductor potential drop than a classical calculation does. The explanation for this is
The bracketed term in the above expression is the depletion drop which is the same in either classical or quantum mechanical treatment. However, according to inequality (6), the second term of eq. (7) must be higher for quantum mechanical calculations. Thus, electrostatics requires that, although $Q_i$ decreases from the classical value, the inversion layer charge has to distribute in such a way so that $z_i$ increases sufficiently to make the second term of eq. (7) larger than classically calculated value. This is consistent because as the separation between lowest subband and Fermi level increases, only the lowest subband becomes primarily occupied, for which the charge centroid $z_i$ has larger value (see, Fig. 22a) and thus leading to higher semiconductor drop. Variation of threshold voltage with thickness is shown in Fig. 24.

**Schred input files**

The following Schred 2.0 files have been simulated to generate $N_{inv}$, $V_G$ data, which are stored in the `av_dist.dat` file. The Matlab script, `fig1.m` extracts the threshold voltage from these data based on the definition discussed above. Schred files, `scl.in`, have been used to calculate the threshold voltage classically for thickness 300nm to 5nm. The file, `soi.in`, has been used for quantum calculation for body thickness 15nm to 3nm. Simulations involving voltage sweeps in finer steps normally require longer times. In these cases it is helpful to know how the simulation progressing. The output file, `DEBUG` is continuously updated by Schred 2.0 and contains information about the current simulation as it progresses.

**scl.in**

```
*title EXAMPLE 4: CLASSICAL THRESHOLD EXTRACTION
$-----------------------------------------------$
$ VARY t_b[nm]: from 300 to 5       $
$-----------------------------------------------$

device      bulk=no
params      temp[K]=300, tox1[nm]=10.0, tox2[nm]=10.0,
+           kox1=3.9, kox2=3.9,
body        uniform=true, t_b[nm]=5.0, Nb[cm-3]=1.e17
gate        metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
+           N1[cm-3]=-1.e20, N2[cm-3]=-1.e20
ionize      ionize=no, Ea[meV]=45, Ed[meV]=45
voltage     dual=yes, Vmin[V]=-2.0, Vmax[V]=-0.07, Vstep[V]=0.01,
+           V2min[V]=-2.0
```

\[
\Delta \phi_s = \left\{ \frac{qN_i t_i^2}{\varepsilon_{si}} \right\} + \frac{Q_i z_i}{2\varepsilon_{si}}, \tag{7}
\]
**soi.in**

*title EXAMPLE 4: QUANTUM THRESHOLD EXTRACTION

$-----------------------------------------------$

$ VARY t_b[nm]: from 15 to 3 $  

$-----------------------------------------------$

device bulk=no

params  
  temp[K]=300, tox1[nm]=10.0, tox2[nm]=10.0,  
  kox1=3.9, kox2=3.9, 

body  
  uniform=true, t_b[nm]=2.0, Nb[cm-3]=1.e17

gate  
  metal1=true, metal2=true, phi1[eV]=4.05, phi2[eV]=4.05,
  N1[cm-3]=-1.e20, N2[cm-3]=-1.e20

ionize  
  ionize=no, Ea[meV]=45, Ed[meV]=45

voltage  
  dual=yes, Vmin[V]=-0.07, Vmax[V]=-0.01, Vstep[V]=0.0031,
  V2min[V]=-0.07

charge  
  quantum=yes, Fermi=yes, exchange=no, e_nsub1=9, e_nsub2=5,
  h_nsub1=9, h_nsub2=5

calc  
  CV_curve=yes, file_cv=cv.dat

save  
  charges=yes, file_ch=chrg.dat,
  wavefunc=no, file_wf=wfun.dat

converge  
  toleranc=5.e-6, max_iter=2000

$-----------------------------------------------$

**REFERENCES**


Appendix
**Syntax of Input File**

The input file is composed of the following ten tokens

```
    device, params, body, gate, ionize,
    voltage, charge, calc, save, converge
```

And we will now discuss how these tokens specify a bulk MOS capacitor for Schred simulation. Double gate MOS capacitors will be discussed in the next section.

**device**: This token specifies the type of the MOS capacitor; whether it is a bulk device or a double gate device. Syntax is:

```
    device     bulk=yes
```

For double gate MOS capacitors, we had to use ‘bulk=no’.

**params**: This token specifies temperature (in kelvin), oxide thickness and oxide dielectric constant. Syntax is:

```
    params     temp[K]=300, tox[nm]=4, kox=3.9
```

**body**: This is to specify the body doping. Schred can handle both uniform as well as non-uniform doping. Syntax for uniform and non-uniform doping are shown separately:

**Uniform doping**

```
    body     uniform=true, Nb[cm-3]=1.e17
```

Note the binary tag **uniform**. If it is ‘true’, then the **Nb[cm-3]** variable needs to be specified.

**Non-uniform doping**

```
    body     uniform=false, dop_prof=dopingp, Ns[cm-3]=2e16
    +        Nb[cm-3]=1e18
```

Here ‘**uniform=false**’ specifies, non-uniform doping profile. The doping data have to come from a file, whose name is given to the variable **dop_prof**. The file must be in the working folder where the input file resides. **Ns[cm-3]** specifies the substrate doping and **Nb[cm-3]** specifies the bulk doping.
Note that, a +ve doping concentration means Acceptors and –ve doping concentration means Donors.

gate: This token is used to specify the gate material. The gate either may be of metal or of polysilicon. Either one can be selected using the tag – metal. Both metal gate and polysilicon gate syntax is shown below

**Metal gate**

gate metal=true, phi[eV]=4.00

‘metal=true’ specifies metal gate. In case metal gate, work function of the metal needs to be specified, which is given to the variable phi[eV]

**Polysilicon gate**

gate metal=false, Ng[cm-3]=-1.e20

Here ‘metal=false’ means polysilicon gate. Ng[cm-3] specifies the doping of polysilicon gate. As before, -ve concentration means Donors, and +ve concentration means Acceptors.

**ionize:** This token is used to specify whether the full ionization of the impurity atoms will used or not. This is set by the binary tag ionize which may be yes or no. In addition to this the donors and acceptors energy levels are specified by Ed[meV] and Ea[meV] respectively.

\[
\text{ionize} \quad \text{ionize=no, Ea[meV]=45, Ed[meV]=45}
\]

**voltage:** Specifies voltage sweep applied to the gate. The start voltage, end voltage and sweep step, these three variables are specified under this token.

\[
V_{\text{min}}[V]=0.5, \quad V_{\text{max}}[V]=3.0, \quad V_{\text{step}}[V]=0.5
\]

**charge:** Here the charge calculation method is specified. Binary tag quantum determines whether quantum calculation or semi-classical calculation have to be performed. If quantum mode is chosen, then 5 variables exchange, e_nsub1, e_nsub2, h_nsub1 and h_nsub2 needs to be specified along with the variable Fermi, which must be specified both for quantum and semi-classical mode.
**Quantum Calculation**

charge quantum=yes, Fermi=yes, exchange=no, e_nsub1=4, e_nsub2=2

`quantum=yes` means quantum calculation. `exchange=no` means exchange co-relation correction is not used. However, if used this variable is to be set `yes`. `Fermi=yes` says, Fermi-Dirac statistics is to be used, other wise, Boltzman statistics is used. `e_nsub1` is used to specify number sub-bands to be used from unprimed ladder and `e_nsub2` specified number of sub-bands from primed ladder. Similarly `h_nsub1`, and `h_nsub2` specifies number of sub-bands from heavy hole and light hole valence band.

**Semi-Classical Calculation**

Just use `quantum=no` along with `Fermi` variable.

charge quantum=no, Fermi=yes

calc: This token is used to turn on or off the CV calculation. Syntax is:

calc      CV_curve=yes, file_cv=cv.dat

If CV curve is not needed then the syntax should look like:

calc      CV_curve=no, file_cv=cv.dat

save: Specifies whether or not the wave function and the charge data will be saved.

save      charges=yes, file_ch=chrg.dat,
+         wavefunc=yes, file_wf=wfun.dat

converge: Converge related parameters, `toleranc` and `max_iter` are specified. `toleranc` is the maximum difference between the last two solution of the Possion’s equation. And `max_iter` is the maximum number of iterations to be performed.

converge toleranc=5.e-6, max_iter=2000
**MATLAB Scripts**

### Part II

**Example 1**

**ex1.m:**

```matlab
%-----------------------------------------------------------% 
% ex1.m                   %
% plots fig1 and fig2 for example 1 of schred tutorial    %
% inputs: ex1qms.dat          %
%         ex1cl.dat          %
%-----------------------------------------------------------% 

clear all; clc;
load ex1qms.dat; qms=ex1qms;
load ex1cl.dat;  cl=ex1cl;
[N,M]=size(qms); qm=qms(1:N/2,:); qm2=qms(N/2+1:N,:);
xcl =cl(:,1);  ecl =cl(:,2);  ncl =cl(:,4);
xqm =qm(:,1);  eqm =qm(:,2);  nqm =qm(:,4);
xqm2=qm2(:,1); eqm2=qm2(:,2); nqm2=qm2(:,4);

% fig 1a: band diagram
%-----------------------------------------------------------
figure(1);
subplot(2,2,1); h1=plot(xqm,eqm);
set(h1, 'linewidth', [2.0]);
xlabel('Distance into semiconductor [nm]');
ylabel('E_c [eV]');
title('(a) : V_G = 0v');
axis([-10, 130, -3.1, 3.5]);

subplot(2,2,2); h1=plot(xqm2,eqm2);
set(h1, 'linewidth', [2.0]);
xlabel('Distance into semiconductor [nm]');
ylabel('E_c [eV]');
title('(b) : V_G = 3v');
axis([-10, 130, -3.1, 3.5]);

subplot(2,2,3); h1=plot(xqm,eqm, xqm2,eqm2);
set(h1, 'linewidth', [2.0]);
xlabel('Distance into semiconductor [nm]');
ylabel('E_c [eV]');
axis([-0.1, 120, -0.3, 1.1]);
gtext('V_G = 0v');
gtext('V_G = 3v');
title('(c)');

subplot(2,2,4); h1=plot(xqm,eqm, xqm2,eqm2);
set(h1, 'linewidth', [2.0]);
xlabel('Distance into semiconductor [nm]');
ylabel('E_c [eV]');
```

62
axis([0.0, 5, -0.3, 0.5]);
gtext('V_G = 0v');
gtext('V_G = 3v');
title('(d)');

% fig 2: electron density
%-----------------------------------------
figure(2);
h2=plot(xcl,nc1, xqm,nqm, 'r.-');
set(h2, 'linewidth', [2.0]);
xlabel('Distance into semiconductor [nm]');
ylabel('Electron density [cm-3]');
v=axis; v(1)=0.0; v(2)=20.0; axis(v);
legend('Classical', 'Quantum');
%-----------------------------------------------------------%

Example 2

ex2f1.m :
%-----------------------------------------------------------%
% ex2f1.m                  %
% plots fig2 for example 2 of schred tutorial     %
% inputs: ex2qm1.dat              %
%         ex2qm2.dat              %
%    ex2cl2.dat              %
%-----------------------------------------------------------%
clear all; clc;
load ex2qm1.dat; qm1=ex2qm1; % for Na=1.e17 quantum
load ex2qm2.dat; qm2=ex2qm2; % for Na=1.e18 quantum
load ex2cl2.dat; cl2=ex2cl2; % for Na=1.e18 classical
load clcv10.dat; cvc10=clcv10;
load clcv2.dat; cvc2=clcv2;
load qmcv10.dat; cvq10=qmcv10;
load qmcv2.dat; cvq2=qmcv2;

vg1=qm1(:,1); us1=qm1(:,2); ni1=qm1(:,4); zi1=qm1(:,5);
vg2=qm2(:,1); us2=qm2(:,2); ni2=qm2(:,4); zi2=qm2(:,5);
vg3=cl2(:,1); us3=cl2(:,2); ni3=cl2(:,4); zi3=cl2(:,5);

qe=1.609e-19; eps=11.7*8.854e-14;
ni=1.4e10; na1=1.e17;
phit=25.9e-3; na2=1.e18;

phib1=phit*log(na1/ni);
phib2=phit*log(na2/ni);
phis11=2.0*phib1*ones(length(vg1),1);
phis21=2.0*phib2*ones(length(vg1),1);
phis12=(2.0*phib1+6*phit)*ones(length(vg1),1);
phis22=(2.0*phib2+6*phit)*ones(length(vg1),1);

ud1=us1-(qe*ni1/eps).*zi1*1.e-7;
ud2=us2-(qe*ni2/eps).*zi2*1.e-7;
ud3=us3-(qe*ni3/eps).*zi3*1.e-7;
nd2=sqrt(2.0*eps*qe*na2*ud2)/qe;
nd3=sqrt(2.0*eps*qe*na2*ud3)/qe;

figure(1);
subplot(2,2,2); h1=plot(vg1,ud1,'r.-', vg1,us1, vg1,phis11,'m--',
vg1,phis12,'k-.' );
set(h1, 'linewidth', [2.0]);
axis([0,8,0.5,1.4]);
xlabel('V_G [v]');
ylabel('U_S [v]');
title('(b) : N_A=10^{17} cm^{-3}');

subplot(2,2,1); h2=plot(vg2,ud2,'r.-', vg2,us2, vg2,phis21,'m--',
vg2,phis22,'k-.' );
set(h2, 'linewidth', [2.0]);
axis([0,8,0,1.5]);
xlabel('V_G [v]');
ylabel('U_S [v]');
title('(a) : N_A=10^{18} cm^{-3}');

subplot(2,2,3); h3=plot(vg2,nd2*qe,'k', vg3,nd3*qe,'b--'); hold on;
set(h3, 'linewidth', [2.0]);
legend('Qntm.', 'Clscl.');
%h4=semilogy(vg2,nd2,'k', vg2,ni2,'k--');
%set(h4, 'linewidth', [2.0]);
xlabel('V_G [v]');
ylabel('Qdep [C/cm^2]');
title('(c)'); hold off;

subplot(2,2,4); h5=plot(vg2,us2,'k', vg3,us3,'b--');
set(h5, 'linewidth', [2.0]);
xlabel('V_G [v]');
ylabel('U_S [v]');
legend('Qntm.', 'Clscl.');
title('(d)');

figure(2);
h5=semilogx(ni1,zi1, ni2,zi2,'kx-', ni3,zi3,':');
set(h5, 'linewidth', [2.0]);
axis([1.e9, 2.e13, 0, 4.0]);
legend('N_A=1E17cm^{-3}', 'N_A=1E18cm^{-3}', 'N_A=1E18cm^{-3}, classical');
xlabel('N_i [cm^{-2}]');
ylabel('Z_i [nm]');

figure(3);
vgc10=cvc10(:,1); ctc10=cvc10(:,2); coc10=cvc10(:,3);
vgc2=cvc2(:,1); ctc2=cvc2(:,2); coc2=cvc2(:,3);
vqg10=cvq10(:,1); ctq10=cvq10(:,2); coq10=cvq10(:,3);
vqg2=cvq2(:,1); ctq2=cvq2(:,2); coq2=cvq2(:,3);

h1=plot(vqg10,ctq10,'k-.', vgc10,ctc10,'r.-', vqg10,coq10,'--');
xlabel('V_G [v]');
ylabel('Capacitance [uF/cm^2]');
title('(a): t_{ox}=10nm');

figure(4);
h2=plot(vqg2,ctq2,'k-.', vgc2,ctc2,'r.-', vqg2,coq2,'--');
xlabel('V_G [v]');
Example 3

**ex3f1.m:**

```matlab
%-------------------------------------------------------------------------%
% ex3f1.m
% plots fig1 for example 3 of schred tutorial
% inputs: ex2qm2.dat
%    ex2cl2.dat
%-------------------------------------------------------------------------%
clear all; clc;
load ex2qm2.dat; qm2=ex2qm2; % for Na=1.e18 quantum
load ex2cl2.dat; cl2=ex2cl2; % for Na=1.e18 classical

vg2=qm2(:,1); us2=qm2(:,2); ni2=qm2(:,4); zi2=qm2(:,5);
vg3=cl2(:,1); us3=cl2(:,2); ni3=cl2(:,4); zi3=cl2(:,5);

qe=1.609e-19; eps=11.7*8.854e-14;
ni=1.4e10; na1=1.e17;
phit=25.9e-3; na2=1.e18;
phib2=phit*log(na2/ni);
phis2v=2.0*phib2*ones(length(vg2),1);

ud2=us2-(qe*ni2/eps).*zi2*1.e-7;
ud3=us3-(qe*ni3/eps).*zi3*1.e-7;
nd2=sqrt(2*eps*qe*na2*ud2)/qe;
nd3=sqrt(2*eps*qe*na2*ud3)/qe;

cd2=diff(nd2)./diff(us2);
ci2=diff(ni2)./diff(us2);

figure(1);
subplot(2,2,1); h1=semilogy(us3,ni3,'r.-', us2,ni2,'k.-');
set(h1, 'linewidth', [2.0]);
legend('Clscl.', 'Qntm.');
xlabel('U_s [v]');
ylabel('Ni [#/cm^2]');
title('(a)');
```

```matlab
deg1=(max(coq10)-max(ctq10))/max(coq10)*100
deg2=(max(coq2)-max(ctq2))/max(coq2)*100
```

```matlab
ylabel('Capacitance [uF/cm^2]');
title('(b): t_{ox}=2nm');
set(h1, 'linewidth', [2.0]);
set(h2, 'linewidth', [2.0]);
```
subplot(2,2,2); h2=semilogy(vd2,qe*cd2,'k', vd2,qe*ci2,'k--', vd3,qe*cd3,'r', vd3,qe*ci3,'r--');
set(h2, 'linewidth', [2.0]);
axis([0,8,1.e-20,1]);
xlabel('V_G [v]');
ylabel('Cinv and Cdep [F/cm^2]');
title('(b)');

subplot(2,2,3); h3=plot(vg3,ni3,'r.-', vg2,ni2,'k.-');
set(h3, 'linewidth', [2.0]);
legend('Clscl.', 'Qntm.');
xlabel('V_G [v]');
ylabel('Ni [#/cm^2]');
title('(c)');

subplot(2,2,4); h4=semilogy(vg3,ni3,'r.-', vg2,ni2,'k.-');
set(h4, 'linewidth', [2.0]);
legend('Clscl.', 'Qntm.');
xlabel('V_G [v]');
ylabel('Ni [#/cm^2]');
title('(d)');

%-----------------------------------------------------------%
% ex3f23.m :
%-----------------------------------------------------------%
ex3f23.m :
% ex3.m     
% plots fig2 and fig3 for example 3.     
%-----------------------------------------------------------%
clear all;
load ex3n15cl25.dat; cl1=ex3n15cl25;
load ex3n16cl25.dat; cl2=ex3n16cl25;
load ex3n17cl25.dat; cl3=ex3n17cl25;
load ex3n18cl25.dat; cl4=ex3n18cl25;
load ex3n19cl25.dat; cl5=ex3n19cl25;
load ex3n15qm25.dat; qm1=ex3n15qm25;
load ex3n16qm25.dat; qm2=ex3n16qm25;
load ex3n17qm25.dat; qm3=ex3n17qm25;
load ex3n18qm25.dat; qm4=ex3n18qm25;
load ex3n19qm25.dat; qm5=ex3n19qm25;
load ex3n15cl10.dat; cl6=ex3n15cl10;
load ex3n16cl10.dat; cl7=ex3n16cl10;
load ex3n17cl10.dat; cl8=ex3n17cl10;
load ex3n18cl10.dat; cl9=ex3n18cl10;
load ex3n19cl10.dat; cl10=ex3n19cl10;
load ex3n15qm10.dat; qm6=ex3n15qm10;
load ex3n16qm10.dat; qm7=ex3n16qm10;
load ex3n17qm10.dat; qm8=ex3n17qm10;
load ex3n18qm10.dat; qm9=ex3n18qm10;
load ex3n19qm10.dat; qm10=ex3n19qm10;
qe=1.609e-19; eps=11.7*8.854e-14; phit=25.9e-3; ni=1.4e10;
na=[1.e15, 1.e16, 1.e17, 1.e18, 1.e19];
for n=1:5
    switch n
        case 1,
            qm25=qm1; cl25=cl1;
            qm10=qm6; cl10=cl6;
        case 2,
            qm25=qm2; cl25=cl2;
            qm10=qm7; cl10=cl7;
        case 3,
            qm25=qm3; cl25=cl3;
            qm10=qm8; cl10=cl8;
        case 4,
            qm25=qm4; cl25=cl4;
            qm10=qm9; cl10=cl9;
        case 5,
            qm25=qm5; cl25=cl5;
            qm10=qm10; cl10=cl10;
    end
% Quantum mechanical calculation .......................%-----------------------------------------------------
    vg25=qm25(:,1); us25=qm25(:,2); ni25=qm25(:,4); zi25=qm25(:,5);
    vg10=qm10(:,1); us10=qm10(:,2); ni10=qm10(:,4); zi10=qm10(:,5);
    ud25=us25-(qe*ni25/eps).*zi25*1.e-7;
    nd25=sqrt(2.0*qe*eps*na(n)*ud25)/qe;
    cd25=abs(diff(nd25)./diff(us25)); cd25=[cd25;cd25(length(cd25))];
    ci25=abs(diff(ni25)./diff(us25)); ci25=[ci25;ci25(length(ci25))];
    n1=find(sign(ci25-cd25)>=0); vth25q(n)=vg25(n1(1));
    ud10=us10-(qe*ni10/eps).*zi10*1.e-7;
    nd10=sqrt(2.0*qe*eps*na(n)*ud10)/qe;
    cd10=abs(diff(nd10)./diff(us10)); cd10=[cd10;cd10(length(cd10))];
    ci10=abs(diff(ni10)./diff(us10)); ci10=[ci10;ci10(length(ci10))];
    n1=find(sign(ci10-cd10)>=0); vth10q(n)=vg10(n1(1));
% Classical calculation ..............................%-----------------------------------------------------
    vg25=cl25(:,1); us25=cl25(:,2); ni25=cl25(:,4); zi25=cl25(:,5);
    vg10=cl10(:,1); us10=cl10(:,2); ni10=cl10(:,4); zi10=cl10(:,5);
    ud25=us25-(qe*ni25/eps).*zi25*1.e-7;
    nd25=sqrt(2.0*qe*eps*na(n)*ud25)/qe;
    cd25=abs(diff(nd25)./diff(us25)); cd25=[cd25;cd25(length(cd25))];
    ci25=abs(diff(ni25)./diff(us25)); ci25=[ci25;ci25(length(ci25))];
    n1=find(sign(ci25-cd25)>=0); vth25c(n)=vg25(n1(1));
    ud10=us10-(qe*ni10/eps).*zi10*1.e-7;
    nd10=sqrt(2.0*qe*eps*na(n)*ud10)/qe;
    cd10=abs(diff(nd10)./diff(us10)); cd10=[cd10;cd10(length(cd10))];
    ci10=abs(diff(ni10)./diff(us10)); ci10=[ci10;ci10(length(ci10))];
    n1=find(sign(ci10-cd10)>=0); vth10c(n)=vg10(n1(1));
end
figure(1);
h1=semilogx(na,vth25c,'kx-', na,vth25q,'r.-');
set(h1, 'linewidth', [2.0]);
axis([1.e15,1.e18,-0.3,0.5]);
Part III

Example 1

ex1_f1.m:

%***********************************************************************%
% fig. 1a, and fig. 1b. of example 1.                                 %
%***********************************************************************%

clear all; clc;
load scl250.dat; load scl150.dat;
load scl50.dat;  load bcl.dat;

z250=scl250(:,1); ec250=scl250(:,2); n250=scl250(:,4);
z150=scl150(:,1); ec150=scl150(:,2); n150=scl150(:,4);
z50=scl50(:,1);   ec50=scl50(:,2);   n50=scl50(:,4);
z=zb=0.0;        ecb=zb(:,2);      nb=zb(:,4);

figure(1);
h1=plot(z250,ec250, z150,ec150, z50,ec50,'k', zb,ecb,'r--');
set(h1, 'linewidth', [2.0]);
set(gca, 'xtick', [0,50,150,250]);
xlabel('z [nm]'); ylabel('E_c [eV]');
legend('DG: t_s=250nm', 'DG: t_s=150nm', 'DG: t_s=50nm', 'Bulk');

n=[n]; z=0.50; tsi=250; n=find((z>=0.0)&(z<=tsi));
z=0.50; n1=n250(n);

z=0.50; tsi=150; n=find((z>=0.0)&(z<=tsi));
z=0.50; n2=n150(n);

z=0.50; tsi=50;  n=find((z>=0.0)&(z<=tsi));
z=0.50; n3=n50(n);

z=0.50; tsi=250; n=find((z>=0.0)&(z<=tsi));
z=0.50; n4=nb(n);

figure(2);
h2=semilogy(z1,n1, z2,n2, z3,n3,'k', z4,n4,'r--');
set(h2, 'linewidth', [2.0]);
grid; set(gca, 'xtick', [0,50,150,250]);
xlabel('z [nm]'); ylabel('n [cm^{-3}]');
legend('DG: t_s=250nm', 'DG: t_s=150nm', 'DG: t_s=50nm', 'Bulk');

%-----------------------------------------------%

ex1_f2.m :
%******************************************%
% Figure 2. of example 1
%******************************************%
clear all; clc;
load ni_l.dat; nil=ni_l;
Na=1.e17;
tsi=2.0*nil(:,3); ni=nil(:,2);
qb=Na*tsi*1.e-7; qt=ni+qb; qb([1:4])=qt(5)-ni([1:4]); qt=ni+qb;

h1=plot(tsi,ni, tsi,qb, tsi,qt); grid;
set(h1, 'linewidth', [2.0]);
set(gca, 'xtick', [0,10,25,50,100,150,170,190,210,230,250]);
xlabel('t_{si} [nm]');
gtext('-Qb/q'); gtext('N_i'); gtext('Qs');
%-----------------------------------------------%

Example 2

ex2f1.m :

clear all;
load chrg.dat;   ch=chrg;
load av_dist.dat; av=av_dist;

M=size(ch);
N=size(av);
T=M(1)/N(1);
m=1:T;
tsi=av(1,3)*2;
mp=[2,3,5,10,18];

for n=1:N(1)
    chv=ch((n-1)*T+m,:);
    n1=find(chv(:,1)>0.0 & chv(:,1)<tsi);
    n1=n1(2:length(n1));
    if (n==mp(1)),
        x1=chv(n1,1); ec1=chv(n1,2); fd1=chv(n1,3); ni1=chv(n1,4);
    elseif (n==mp(2)),
        x2=chv(n1,1); ec2=chv(n1,2); fd2=chv(n1,3); ni2=chv(n1,4);
    elseif (n==mp(3)),
        x3=chv(n1,1); ec3=chv(n1,2); fd3=chv(n1,3); ni3=chv(n1,4);
    elseif (n==mp(4)),
        x4=chv(n1,1); ec4=chv(n1,2); fd4=chv(n1,3); ni4=chv(n1,4);
    elseif (n==mp(5)),
        x5=chv(n1,1); ec5=chv(n1,2); fd5=chv(n1,3); ni5=chv(n1,4);
    end
ecv=chv(n1,2);
    esc(n,1)=max(ecv)-min(ecv);
end

vg=av(:,1); ni=av(:,2); us=av(:,4);

figure(1);
%

h1=plot(x1,ec1, x2,ec2, x3,ec3, x4,ec4); grid
lgd1=[num2str(vg(mp(1))),'v'];
lgd2=[num2str(vg(mp(2))),'v'];
lgd3=[num2str(vg(mp(3))),'v'];
lgd4=[num2str(vg(mp(4))),'v'];
legend(lgd1, lgd2, lgd3, lgd4);
set(h1, 'linewidth', [2.0]);
xlabel('z [nm]'); ylab('E_c inside silicon [eV]');

figure(2);
%

subplot(2,2,1); h1=plot(vg, us); grid
set(h1, 'linewidth', [2.0]);
set(gca, 'xtick', [0,0.25,0.75,1]);
xlabel('V_G [v]'); ylab('U_s [v]');
title('(a)');

subplot(2,2,2); h2=plot(vg, esc); grid
set(h2, 'linewidth', [2.0]);
set(gca, 'xtick', [0,0.25,0.75,1]);
xlabel('V_G [v]'); ylab('(U_s-U_c) [v]');
title('(b)');

subplot(2,2,3); h3=semilogy(vg, ni); grid
set(h3, 'linewidth', [2.0]);
set(gca, 'xtick', [0,0.25,0.75,1]);
xlabel('V_G [v]'); ylab('N_i [cm-2]');
title('(c)');

subplot(2,2,4); h4=semilogy(us, ni); grid
set(h4, 'linewidth', [2.0]);
set(gca, 'xtick', [0,0.25,0.75,1]);
xlabel('U_S [v]'); ylab('N_i [cm-2]');
title('(d)');

figure(3);
%

subplot(2,2,1); h1=semilogy(x2, ni2); grid
set(h1, 'linewidth', [2.0]);
v=axis; v(1)=0.0; v(2)=tsi; axis(v);
xlabel('z [nm]'); ylab('n [cm-3]');
ttl1=num2str(av(mp(2),1)); ttl1 = ['(a) v_g = ', ttl1];
ttl1 = label(ttl1);

subplot(2,2,2); h1=semilogy(x4, ni4); grid
set(h1, 'linewidth', [2.0]);
v=axis; v(1)=0.0; v(2)=tsi; axis(v);
xlabel('z [nm]'); ylab('n [cm-3]');
Example 3

**fig1.m**

```matlab
%****************************************************************************
% Figure 1. of example 3
%****************************************************************************
clear all; clc;

% Load qs20.dat for t_v=20nm ............
%----------------------------------------
load qs20.dat; qs=qs20; tsi=20.0;
x=qs(:,1); ec=qs(:,2); fd=qs(:,3); n=qs(:,4);
n1=find((x>=0.0) & (x<=tsi));
x=x(n1); n=n(n1);
t20=[x,n];

% Load qs15.dat for t_v=15nm ............
%----------------------------------------
load qs15.dat; qs=qs15; tsi=15.0;
x=qs(:,1); ec=qs(:,2); fd=qs(:,3); n=qs(:,4);
n1=find((x>=0.0) & (x<=tsi));
x=x(n1); n=n(n1);
t15=[x,n];

% Load qs10.dat for t_v=10nm ............
%----------------------------------------
load qs10.dat; qs=qs10; tsi=10.0;
x=qs(:,1); ec=qs(:,2); fd=qs(:,3); n=qs(:,4);
n1=find((x>=0.0) & (x<=tsi)); n2=find(((2.0*x)>tsi) & (x<=tsi));
x=x(n1); n=n(n1);
t10=[x,n];

% Load qs05.dat for t_v=05nm ............
%----------------------------------------
load qs05.dat; qs=qs05; tsi=5.0;
```
x=qs(:,1); ec=qs(:,2); fd=qs(:,3); n=qs(:,4);
n1=find((x>=0.0) & (x<=tsi)); n2=find(((2.0*x)>tsi) & (x<=tsi));
x=x(n1); n=n(n1);
t05=[x,n];

figure(1);
h2=plot(t20(:,1),t20(:,2),':.', t15(:,1),t15(:,2),'-.', t10(:,1),t10(:,2),'--', t05(:,1),t05(:,2));
set(h2, 'linewidth', [2.0]);
xlabel('Body thickness [nm]');
ylabel('Inversion carrier distribution [cm^{-3}]');
legend('DG: t_s=20nm', 'DG: t_s=15nm', 'DG: t_s=10nm', 'DG: t_s=5nm');

fig2a.m :
%*****************************************************************************%
% Figure 2a. of example 3 %
%*****************************************************************************%
clear all; clc;
% Load vg-ni data files..............
%----------------------------------------
load csoi4.dat; csoi=csoi4; tsi=4.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
n1=find((x>=0.0) & (x<=tsi)); n2=find(((2.0*x)>tsi) & (x<=tsi));
nt=n(n1); n(n2)=0.0; x=x(n1); n=n(n1);
t4=[x,n,nt];

load csoi8.dat; csoi=csoi8; tsi=8.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
n1=find((x>=0.0) & (x<=tsi)); n2=find(((2.0*x)>tsi) & (x<=tsi));
nt=n(n1); n(n2)=0.0; x=x(n1); n=n(n1);
t8=[x,n,nt];

load csoi30.dat; csoi=csoi30; tsi=30.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
n1=find((x>=0.0) & (x<=tsi)); n2=find(((2.0*x)>tsi) & (x<=tsi));
nt=n(n1); n(n2)=0.0; x=x(n1); n=n(n1);
t30=[x,n,nt];

%load cblk.dat; csoi=cblk;
%x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
%tb=[x,n];

figure(1);
h1=plot(t4(:,1),t4(:,3),'--', t8(:,1),t8(:,3),':.', t30(:,1),t30(:,3));
set(h1, 'linewidth', [2.0]);
xlabel('Body thickness [nm]');
ylabel('Total inversion charge density [cm^{-3}]');
legend('DG: t_s=4nm', 'DG: t_s=8nm', 'DG: t_s=30nm');

figure(2);
%h2=plot(t4(:,1),t4(:,2),'-', t8(:,1),t8(:,2),'-', t30(:,1),t30(:,2),'--',
%tb(:,1), tb(:,2));
h2=plot(t4(:,1),t4(:,2),'-', t8(:,1),t8(:,2),'-', t30(:,1),t30(:,2));
set(h2, 'linewidth', [2.0]);
vaxis; v(1)=0.0; v(2)=6.0; axis(v);
xlabel('Body thickness [nm]');
ylabel('Inversion charge density of one gate[cm-3]');
legend('DG: t_s=4nm', 'DG: t_s=8nm', 'DG: t_s=30nm');

fig2b.m :
%******************************************%
% Figure 2b. of example 3           %
%******************************************%
clear all; clc;

% Load vg-ni data files..............
load sq4.dat; csoi=sq4; tsi=4.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
N1=find((x>=0.0) & (x<=tsi)); N2=find(((2.0*x)>tsi) & (x<=tsi));
n(N2)=0.0; x=x(N1); n=n(N1);
t4=[x,n];

load sq8.dat; csoi=sq8; tsi=8.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
N1=find((x>=0.0) & (x<=tsi)); N2=find(((2.0*x)>tsi) & (x<=tsi));
n(N2)=0.0; x=x(N1); n=n(N1);
t8=[x,n];

load sq30.dat; csoi=sq30; tsi=30.0;
x=csoi(:,1); ec=csoi(:,2); fd=csoi(:,3); n=csoi(:,4);
N1=find((x>=0.0) & (x<=tsi)); N2=find(((2.0*x)>tsi) & (x<=tsi));
n(N2)=0.0; x=x(N1); n=n(N1);
t30=[x,n];

figure(2);
h2=plot(t4(:,1),t4(:,2),':', t8(:,1),t8(:,2),':', t30(:,1),t30(:,2),':',
tb(:,1), tb(:,2));
h2=plot(t4(:,1),t4(:,2),':', t8(:,1),t8(:,2),':', t30(:,1),t30(:,2),':',
set(h2, 'linewidth', [2.0]));
v=axis; v(1)=0.0; v(2)=6.0; axis(v);
xlabel('V_G [V]'); ylabel('N_i [cm^{-2}]');
legend('DG: t_s=4nm', 'DG: t_s=8nm', 'DG: t_s=30nm');

fig3.m :
%******************************************%
% Figure 3 of example 3           %
%******************************************%
clear all;
load chrg.dat; ch=chrg;
load av_dist.dat; av=av_dist;

M=size(ch);
N=size(av);
T=M(1)/N(1);
m=1:T;
ts=av(1,3);
ts=2*tsch;
mp=[2,7,18];
for n=1:N(1)
    chv=ch((n-1)*T+m,:);
    if (n==mp(1)),
        x11=chv(:,1); ni1=chv(:,4);
    elseif (n==mp(2)),
        x12=chv(:,1); ni2=chv(:,4);
    elseif (n==mp(3)),
        x13=chv(:,1); ni3=chv(:,4);
    end
    n1=find(chv(:,1)>0.0 & chv(:,1)<tsi);
    n1=n1(2:length(n1));
    n2=find(chv(:,1)>tsih & chv(:,1)<tsi);
    x1=chv(n1,1);
    el1=chv(n1,4); el1(n2)=0.0; el1=el1(n1);
    zi(n,1) = trapz(x1,x1.*el1)/trapz(x1,el1);
    ecv=chv(n1,2);
    ec(n,1)=max(ecv);
end
vg=av(:,1);
figure(1);
subplot(2,2,1); h1=plot(av(:,1), zi); grid
set(h1, 'linewidth', [2.0]);
xlabel('V_g [v]');
ylabel('z_I [nm]');
title('(a)');

subplot(2,2,2); h1=plot(x11, ni1); grid
set(h1, 'linewidth', [2.0]);
v=axis; v(1)=0.0; v(2)=tsi; axis(v);
xlabel('z [nm]');
ylabel('n_i [cm^{-3}]');
title('(b)');
lgd1=[num2str(vg(mp(1))),'v'];
legend(lgd1);

subplot(2,2,3); h1=plot(x12, ni2); grid
set(h1, 'linewidth', [2.0]);
v=axis; v(1)=0.0; v(2)=tsi; axis(v);
xlabel('z [nm]');
ylabel('n_i [cm^{-3}]');
title('(c)');
lgd2=[num2str(vg(mp(2))),'v'];
legend(lgd2);

subplot(2,2,4); h1=plot(x13, ni3); grid
set(h1, 'linewidth', [2.0]);
v=axis; v(1)=0.0; v(2)=tsi; axis(v);
xlabel('z [nm]');
ylabel('n_i [cm^{-3}]');
title('(d)');
lgd3=[num2str(vg(mp(3))),'v'];
legend(lgd3);

%----------------------------------------

fig4.m :
clear all; clc;
load cv.dat;
vg=cv(:,1); ct=cv(:,3); cox=cv(:,4);
h1=plot(vg,ct, vg,2*cox, 'r--'); grid;
set(h1, 'linewidth', [2.0]);
xlabel('v_g [v]');
ylabel('Capacitance [uf/cm2]');
legend('C_g', '2*C_{ox}');

Example 4

fig1.m :

load av_dist.dat; av=av_dist;

vg=av(:,1); ni=av(:,2); tsi=2*av(1,3);
na=1.0e17; nd=na*1.e-7*tsi;
n1=find(ni>=nd);
vth=vg(n1(1));