

**Notes on the  
Solution of the Poisson-Boltzmann Equation  
for MOS Capacitors and MOSFETs  
2<sup>nd</sup> Edition**

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## **1. Introduction**

These notes are intended to complement discussions in standard textbook such as *Fundamentals of Modern VLSI Devices* by Yuan Taur and Tak H. Ning [1] and *Semiconductor Device Fundamentals* by R.F. Pierret [2].) The objective here is to understand how to treat MOS electrostatics without making the so-called  $\delta$ -depletion approximation. We assume a bulk MOS structure, but a similar approach could be used for SOI structures.

## **2. MOS Electrostatics: Electric Field vs. Position**

We begin with Poisson's equation:

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\epsilon_{Si}} [p(x) - n(x) + N_D^+ - N_A^-] \quad (0)$$

and assume a p-type semiconductor for which  $N_D = 0$ . Complete ionization of dopants will be assumed ( $N_A^- = N_A$ ). In the bulk, we have space charge neutrality, so  $p_B - n_B - N_A = 0$ , which means

$$N_A = p_B - n_B, \quad (1)$$

so Poisson's equation becomes

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\epsilon_{Si}} [p(x) - n(x) + n_B - p_B], \quad (2)$$

where

$$\begin{aligned} p_B &\cong N_A \\ n_B &\cong n_i^2 / N_A \end{aligned} \quad (3)$$

Using eqn. (3), we can express eqn. (2) as

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\epsilon_{Si}} [p(x) - N_A - n(x) + n_i^2 / N_A]. \quad (4)$$

The energy bands vary with position when the electrostatic potential varies with position. For example, a positive gate voltage bends the bands down, and a negative gate voltage bends the bands up (because a positive potential lowers the electron energy). If we assume equilibrium, then the equilibrium carrier densities in the semiconductor can be related to the electrostatic potential by

$$p(x) = N_A e^{-q\psi(x)/k_B T_L} \quad (5)$$

and

$$n(x) = \frac{n_i^2}{N_A} e^{+q\psi(x)/k_B T_L}. \quad (6)$$

Finally, using eqns. (5) and (6) in (4), we find the *Poisson-Boltzmann equation*,

$$\boxed{\frac{d^2\psi}{dx^2} = \frac{-q}{\epsilon_{Si}} \left[ N_A (e^{-q\psi/k_B T_L} - 1) - \frac{n_i^2}{N_A} (e^{q\psi/k_B T_L} - 1) \right]} \quad (7)$$

which we need to integrate twice to find  $\psi(x)$ .

To integrate eqn. (7), we begin with

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx} \times \left( \frac{d\psi}{dx} \right)$$

and use the chain rule,

$$\frac{d^2\psi}{dx^2} = \frac{d}{d\psi} \times \left( \frac{d\psi}{dx} \right) \times \frac{d\psi}{dx}.$$

If we let  $p = \frac{d\psi}{dx}$ , then

$$\frac{d^2\psi}{dx^2} = p \frac{dp}{d\psi},$$

and eqn. (7) becomes

$$p \frac{dp}{d\psi} = \frac{-q}{\epsilon_{Si}} \left[ N_A (e^{-q\psi/k_B T_L} - 1) - \frac{n_i^2}{N_A} (e^{q\psi/k_B T_L} - 1) \right]. \quad (8)$$

Now integrate eqn. (8) with respect to  $d\psi$ ,

$$\begin{aligned} p dp &= \frac{-q}{\epsilon_{Si}} \left[ N_A (e^{-q\psi/k_B T_L} - 1) - \frac{n_i^2}{N_A} (e^{q\psi/k_B T_L} - 1) \right] d\psi \\ \int_0^p p' dp' &= \frac{-q}{\epsilon_{Si}} \int_0^\psi \left[ N_A (e^{-q\psi/k_B T_L} - 1) - \frac{n_i^2}{N_A} (e^{+q\psi/k_B T_L} - 1) \right] d\psi \\ \frac{p^2}{2} &= \frac{-q}{\epsilon_{Si}} \left[ N_A \left\{ \left( \frac{-k_B T_L}{q} \right) e^{-q\psi/k_B T_L} \Big|_0^\psi - \psi \right\} - \frac{n_i^2}{N_A} \left\{ \left( \frac{k_B T_L}{q} \right) e^{q\psi/k_B T_L} \Big|_0^\psi - \psi \right\} \right] \\ p^2 &= \frac{2k_B T_L N_A}{\epsilon_{Si}} \left[ \left( e^{-q\psi/k_B T_L} + \frac{q\psi}{k_B T_L} - 1 \right) + \frac{n_i^2}{N_A^2} \left( e^{q\psi/k_B T_L} - \frac{q\psi}{k_B T_L} - 1 \right) \right]. \end{aligned}$$

Recall that  $p = \frac{d\psi}{dx}$ , so we can take the square root of the final result to find

$$\mathcal{E}(x) = -\frac{d\psi(x)}{dx} = \pm \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} F(\psi), \quad (9)$$

where

$$F(\psi) = \sqrt{\left( e^{-q\psi/k_B T_L} + \frac{q\psi}{k_B T_L} - 1 \right) + \frac{n_i^2}{N_A^2} \left( e^{+q\psi/k_B T_L} - \frac{q\psi}{k_B T_L} - 1 \right)}. \quad (10)$$

If  $\psi > 0$ , choose the “+” sign (for a p-type semiconductor), and if  $\psi < 0$ , choose the “-“ sign. Equations (9) and (10) give the position-dependent electric field within the semiconductor *if* we know the position-dependent electrostatic potential.

The surface electric field is an important quantity in MOS electrostatics. From eqn. (9) evaluated at the surface ( $x = 0$ ) where the electrostatic potential,  $\psi(x=0)$ , is the surface potential,  $\psi_s$ , we find the surface electric field as

$$\mathcal{E}_s = \pm \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} F(\psi_s). \quad (11)$$

From eqn. (11) and Gauss’s Law, we find the total charge in the semiconductor as a function of the surface potential as

$$\boxed{Q_s(\psi_s) = -\epsilon_{Si} \mathcal{E}_s = \mp \sqrt{2\epsilon_{Si} k_B T_L N_A} F(\psi_s)}, \quad (12)$$

which is **an important and frequently-used result**. For the assumed p-type semiconductor, the - sign in front of the square root is used when  $\psi_s > 0$  and the + sign when  $\psi_s < 0$ .

### Example 1: Semiconductor Charge vs. Surface Potential

Consider a p-type, silicon MOS capacitor at room temperature with  $N_A = 5 \times 10^{17} \text{ cm}^{-3}$ . Plot  $|Q_s/q|$  vs. surface potential,  $\psi_s$ .

A Matlab script to perform this calculation is included in the appendix. The result is shown below in Fig. 1.

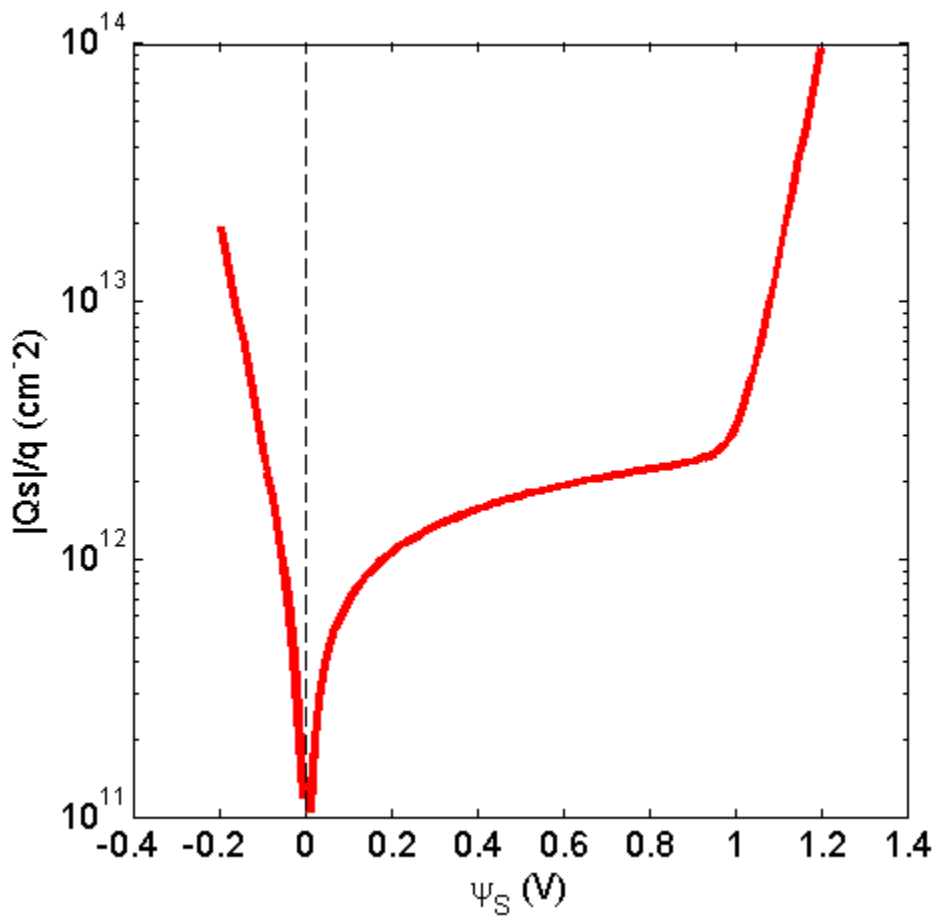


Fig. 1 Magnitude of the charge per square cm (divided by  $q$ ) vs. surface potential in volts. (See the appendix for the Matlab® script that produced this plot.)

Figure 1 shows the accumulation of holes for  $\psi_s < 0$ , the depletion of the p-type semiconductor for  $\psi_s > 0$ , and inversion for  $\psi_s > 2\psi_B$ . To understand the result, let's examine eqn. (12) more closely. Consider accumulation ( $\psi_s < 0$ ) first. In this case, we have from eqn. (12)

$$Q_s = +\sqrt{2\epsilon_{Si}k_B T_L N_A} F(\psi_s)$$

and according to eqn. (10), for strong accumulation

$$F(\psi_s) \rightarrow e^{-\psi_s/2k_B T_L},$$

so

$$Q_s \approx +\sqrt{2\epsilon_{Si}k_B T_L N_A} e^{-q\psi_s/2k_B T_L}.$$

Next, consider inversion ( $\psi_s > 2\psi_B$ ) next. In this case, we have from eqn. (12)

$$Q_s = -\sqrt{2\epsilon_{Si}k_B T_L N_A} F(\psi_s),$$

and according to eqn. (1), for strong inversion

$$F(\psi_s) \rightarrow \frac{n_i}{N_A} e^{+q\psi_s/2k_B T_L},$$

so

$$Q_s \approx Q_n \approx +\sqrt{\frac{2\epsilon_{Si}k_B T_L n_i^2}{N_A}} e^{+q\psi_s/2k_B T_L}.$$

The electron density at the surface is

$$n(0) = \frac{n_i^2}{N_A} e^{+q\psi_s/k_B T_L} \text{ cm}^{-3},$$

so we can write the charge density per  $\text{cm}^2$  as

$$Q_s \approx +\sqrt{2\epsilon_{Si}k_B T_L n(0)}.$$

Taur and Ning [1] point out that this gives us a simple way to estimate the thickness of the inversion layer. Since

$$Q_n \approx qn(0)t_{inv},$$

we get the following estimate for the thickness of the inversion layer,

$$t_{inv} \approx \frac{2\epsilon_{Si}k_B T_L n(0)}{q|Q_n|}.$$

Finally, consider the case of depletion ( $0 < \psi_s < 2\psi_B$ ). In this case, we can ignore electrons and holes to find from eqn. (10),

$$F(\psi_s) \cong \sqrt{\frac{q\psi_s}{k_B T_L} - 1},$$

which, according to eqn. (12) gives

$$\mathcal{E}_s \cong \sqrt{\frac{2qN_A}{\epsilon_{Si}}(\psi_s - k_B T_L / q)}.$$

The “exact” result is just like depletion approximation (eqn. (2.161) in [1]) except for  $k_B T_L / q$  correction.

## Example 2: Surface Potential vs. Gate Voltage

Figure 1 is in terms of the surface potential; we vary the surface potential with the gate voltage according to:

$$V_G = V_{FB} + \psi_s - \frac{Q_s}{C_{ox}}$$

where  $V_{FB}$  is the “flat band voltage”. Consider a p-type, silicon MOS capacitor at room temperature with  $N_A = 5 \times 10^{17} \text{ cm}^{-3}$ . Assume  $V_{FB} = 0$ ,  $t_{ox} = 2 \text{ nm}$ , and  $\kappa_{ox} = 4$ . Plot the surface potential,  $\psi_s$  vs. gate voltage on the x-axis.

A Matlab script to perform this calculation is included in the appendix. The result is shown below in Fig. 2.

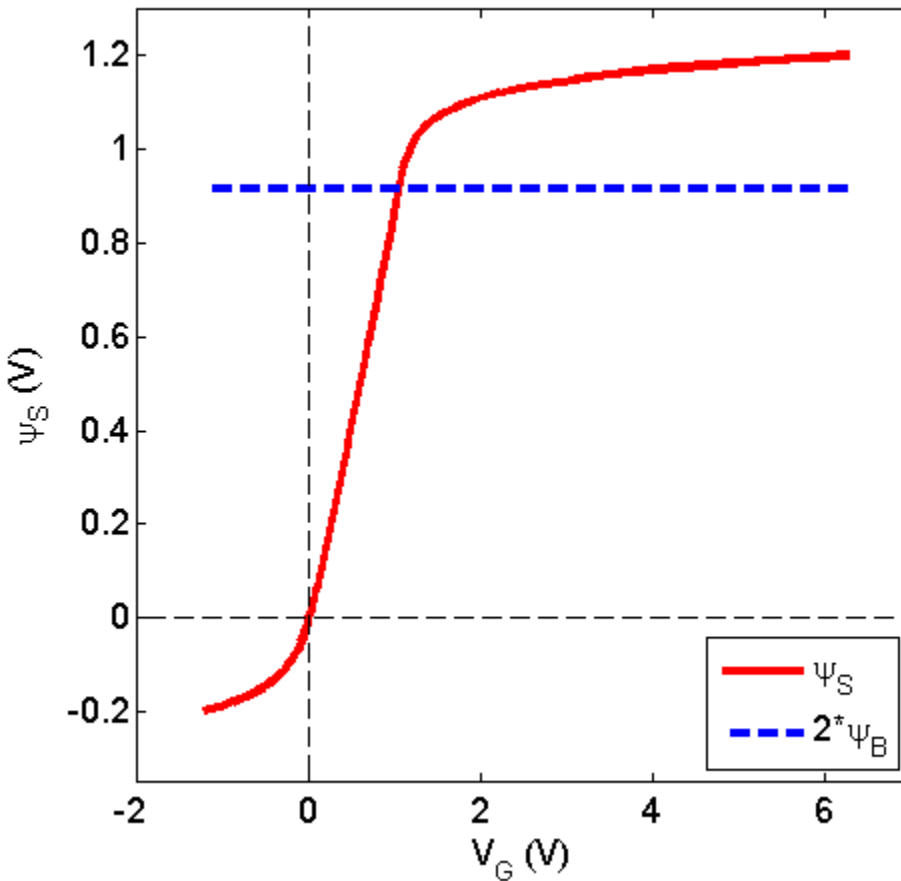


Fig. 2 Surface potential vs. gate voltage. (See the appendix for the Matlab® script that produced this plot.)

Figure 2 shows that no matter how large the gate voltage is, it is hard to push the surface potential very much beyond  $2\psi_B$ .

### 3. The Semiconductor Capacitance

Capacitance is the derivative of charge with respect to voltage, so we find the semiconductor capacitance as



$$C_{Si} = \frac{-dQ_s}{d\psi_s} = \sqrt{2q\epsilon_{Si}N_A} \times \left[ \frac{(1 - e^{-q\psi_s/kT_L}) + \frac{n_i^2}{N_A}(e^{q\psi_s/kT_L} - 1)}{2\sqrt{\left(\frac{k_B T_L}{q} e^{-q\psi_s/k_B T_L} + \psi_s - \frac{k_B T_L}{q}\right) + \left(\frac{n_i}{N_A}\right)^2 \left(\frac{k_B T_L}{q} e^{q\psi_s/k_B T_L} - \psi_s - \frac{k_B T_L}{q}\right)}} \right]. \quad (13)$$

Under depletion conditions,  $0 < \psi_s < 2\psi_B$  and eqn. (13) simplifies to

$$C_{Si} = \frac{-dQ_s}{d\psi_s} = \sqrt{\frac{q\epsilon_{Si}N_A}{2(\psi_s - k_B T_L / q)}} = \frac{\epsilon_{Si}}{W_D},$$

which is the standard depletion approximation result (eqn. (2.174) of [1]) except for the  $k_B T_L / q$  correction, which is often neglected.

We can also take the limit of eqn. (13) as  $\psi_s \rightarrow 0$ , to find the flat band capacitance as

$$C_{Si}(FB) = \frac{\epsilon_{Si}}{L_D} \quad (14)$$

Equation (13) can be used to evaluate the low frequency MOS CV characteristic. With a little more care, it can also be adapted to evaluate the high frequency CV characteristic too.

#### 4. MOS Electrostatics II (potential vs. position)

So far, we have only integrated Poisson's equation, eqn. (7), once. To get  $\psi(x)$  for a given  $\psi_s$ , we need to integrate again. Recall that

$$\frac{d\psi}{dx} = \mp \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} F(\psi). \quad (9)$$

We can integrate eqn. (9) to find

$$\int_{\psi_s}^{\psi(x)} \frac{d\psi}{F(\psi)} = \mp \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} x$$

or

$$x = \sqrt{\frac{\epsilon_{Si}}{2k_B T_L N_A}} \int_{\psi(x)}^{\psi_s} \frac{d\psi}{F(\psi)}.$$

Finally, it is convenient to write the result as

$$x = L_D \int_{\psi(x)}^{\psi_s} \frac{d\psi}{\frac{k_B T_L}{q} F(\psi)}, \quad (15)$$

where  $L_D$  is the extrinsic Debye length. Equation (15) cannot be integrated analytically, so, for a given  $\psi_s$ , select  $0 < \psi(x) < \psi_s$ , then numerically integrate (15) to get  $x$ .

The next question is: ‘‘How do we compute  $Q_n(\psi_s)$ ?’’ Well above threshold,  $Q_s \approx Q_n$ , so we can get it from eqn. (12), but how would we do it exactly for all bias conditions? First, recall that

$$n(x) = \frac{n_i^2}{N_A} e^{q\psi(x)/k_B T_L},$$

so

$$Q_n = q \int_0^\infty n(x) dx = q \int_{\psi_s}^0 \frac{n_i^2}{N_A} e^{q\psi(x)/k_B T_L} \frac{dx}{d\psi} d\psi.$$

Since we know the electric field as a function of  $y$  from eqn. (9), we find

$$Q_n = q \frac{n_i^2}{N_A} \int_0^{\psi_s} \frac{e^{q\psi/k_B T_L}}{\sqrt{2k_B T_L N_A / \epsilon_{Si}} F(\psi)} d\psi. \quad (16)$$

Consider another question: ‘‘How do we compute the depletion layer charge?’’ We know how to compute it using the depletion approximation, but how to we do it exactly. We begin with

$$Q_D = -q \int_0^{\infty} [N_A - p(x)] dx = -q N_A \int_0^{\infty} (1 - e^{-q\psi/k_B T_L}) dx,$$

which we can change the variable of integration to find.

$$Q_D = -q N_A \int_0^{\psi_s} \frac{1 - e^{-q\psi/k_B T_L}}{\sqrt{2k_B T_L N_A / \epsilon_{Si}} F(\psi)} d\psi. \quad (17)$$

## 5. “Exact” Solution of the MOSFET:

Taur and Ning discuss the “exact” solution for a long channel MOSFET [1]. These notes amplify on their discussion. Let’s begin by reviewing the derivation of eqn. (6), which applies only equilibrium.

$$n = n_i e^{(E_F - E_i)/k_B T_L} \quad (18)$$

let

$$E_i = -q\psi(x) - q\psi_{REF} \quad (19)$$

and choose

$$q\psi_{REF} = -E_F. \quad (20)$$

The result is eqn. (6),

$$n = n_i e^{q\psi(x)/k_B T_L}. \quad (21)$$

Out of equilibrium, we have

$$n = n_i e^{[F_n(x) - E_i(x)]/k_B T_L} \quad (22)$$

Using eqns. (19) and (20) in eqn. (22), we have

$$n(x) = n_i e^{q[\psi(x) + F_n(x) - E_F]/k_B T_L} \quad (23)$$

If we define

$$q\phi_n \equiv E_F - F_n \quad (24)$$

then

$$n(x) = n_i e^{q[\psi(x) - \phi_n(x)]/k_B T_L}. \quad (25)$$

In a MOSFET, a positive drain bias will pull  $F_n$  down by  $qV_D$  at the drain. If the source is grounded,  $\phi_n(y=0) = 0$  and  $\phi_n(y=L) = V_D$ . The quasi-Fermi potential will vary with distance,  $y$ , along the channel, but we assume that it is constant with  $x$ , at least across the inversion layer. In a MOSFET, the holes will stay in equilibrium, so eqn. (5) continues to apply.

Now, we make the gradual channel approximation, so that a 1D Poisson equation can be solved to find  $E_x(x, y)$ . Equation (7) becomes

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\epsilon_{Si}} \left[ p_o (e^{-q\psi/k_B T_L} - 1) - \frac{n_i^2}{N_A} (e^{q(\psi - \phi_n)/k_B T_L} - 1) \right], \quad (26)$$

which can be integrated to find

$$\mathcal{E}(\psi, \phi_n) = \pm \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} F(\psi, \phi_n) \quad (27)$$

where

$$F(\psi, \phi_n) = \sqrt{\left( e^{-q\psi/k_B T_L} + \frac{q\psi}{k_B T_L} - 1 \right) + \frac{n_i^2}{N_A} \left( e^{-q\phi_n/k_B T_L} (e^{q\psi/k_B T_L} - 1) - \frac{q\psi}{k_B T_L} \right)}. \quad (28)$$

To find the inversion layer density at any point along the channel,

$$\begin{aligned} Q_n &= -q \int_0^\infty n(x) dx = -q \int n(x) \frac{dx}{d\psi} d\psi \\ &= -q \int_{\psi_B}^{\psi_S} \frac{n(x)}{\mathcal{E}(\psi, \phi_n)} d\psi \end{aligned}$$

or

$$Q_n(\phi_n) = -q \frac{n_i^2}{N_A} \int_{\psi_B}^{\psi_S} \frac{e^{q(\psi - \phi_n)/k_B T_L}}{\mathcal{E}(\psi, \phi_n)} d\psi \quad (29)$$

We should note  $\psi_s$  varies along the channel. We determine  $\psi_s$  from

$$V_G = V_{FB} + \psi_s - \frac{Q_s}{C_{ox}}$$

or

$$V_G = V_{FB} + \psi_s + \frac{\epsilon_{Si} \mathcal{E}_s(\psi_s, \phi_n)}{C_{ox}}, \quad (30)$$

Where  $\mathcal{E}_s$  is determined from eqn. (27) with  $\psi = \psi_s$ .

To summarize, at some location,  $y$ , along the channel there is a corresponding  $\phi_n(y)$ . Equation (30) can be solved iteratively for  $\psi_s$ , given the gate voltage,  $V_G$ . Knowing  $\psi_s$ , we determine the corresponding inversion layer charge by integrating eqn. (29) numerically.

The next question is: “How do we determine  $I_{DS}$ .” From

$$J_n = n\mu_n \frac{dF_n}{dy} \quad (31)$$

we find

$$I_{DS} = \mu_{eff} \frac{W}{L} \int_0^{V_{DS}} [-Q_n(\phi_n)] d\phi_n \quad (32)$$

which is eqn. (3.10) in Taur and Ning (recall that Taur and Ning use  $V$  for  $\phi_n$ ). Using eq. (29) in eqn. (32), we find

$$I_{DS} = q\mu_{eff} \frac{W}{L} \int_0^{V_{DS}} \left( \int_{\psi_B}^{\psi_s} \frac{(n_i^2 / N_A) e^{q(\psi - \phi_n)/k_B T_L}}{\mathcal{E}(\psi, \phi_n)} d\psi \right) d\phi_n \quad (33)$$

Equation (33) is the famous Pao-Sah double integral expression for  $I_{DS}$ .

Equation (33) can be integrated numerically to obtain  $I_{DS}(V_{GS}, V_{DS})$ . Note that we made the gradual channel approximation, so it applies only to long channel transistors. Note also, that it is valid for the entire  $V_{DS}$  range; the drain current saturates automatically without needing to

worry about channel pinch-off. Finally, note that the double integral expression can be converted to a single integral as discussed by Pierret and Shields [2].

## 6. Summary

A few key things to remember (or look up when you need them) are listed below.

### 1) Surface electric field for a given surface potential:

$$\mathcal{E}_s = \pm \sqrt{\frac{2k_B T_L N_A}{\epsilon_{Si}}} F(\psi_S) \quad (11)$$

where

$$F(\psi) = \sqrt{\left( e^{-q\psi/k_B T_L} + \frac{q\psi}{k_B T_L} - 1 \right) + \frac{n_i^2}{N_A^2} \left( e^{+q\psi/k_B T_L} - \frac{q\psi}{k_B T_L} - 1 \right)} \quad (10)$$

### 2) Semiconductor charge density for a given surface potential:

$$Q_S(\psi_S) = -\epsilon_{Si} \mathcal{E}_s = \mp \sqrt{2\epsilon_{Si} k_B T_L N_A} F(\psi_S) \quad (12)$$

In depletion, eqn. (12) reduces to:

$$Q_S \cong \sqrt{2q\epsilon_{Si} N_A (\psi_S - k_B T_L / q)},$$

which is very close to the depletion approximation, except for the  $-k_B T_L / q$  correction.

For strong accumulation, eqn. (12) reduces to:

$$Q_S \approx +\sqrt{2\epsilon_{Si} k_B T_L N_A} e^{-q\psi_S/2k_B T_L} \quad (\text{strong accumulation})$$

For strong inversion, eqn. (12) reduces to:

$$Q_S \approx Q_n \approx +\sqrt{\frac{2\epsilon_{Si} k_B T_L n_i^2}{N_A}} e^{+q\psi_S/2k_B T_L} \quad (\text{strong inversion})$$

which can also be expressed as

$$Q_s \approx +\sqrt{2\epsilon_{Si}k_B T_L n(0)}$$

The inversion layer thickness can be estimated as:

$$t_{inv} \approx \frac{2\epsilon_{Si}k_B T_L}{q|Q_n|}$$

### 3) Capacitance:

An analytical expression for the semiconductor capacitance exists as given by eqn. (13). Under flatband conditions, the semiconductor capacitance becomes:

$$C_{Si}(FB) = \frac{\epsilon_{Si}}{L_D} \quad (14)$$

## References

- [1] Yuan Taur and Tak Ning, *Fundamentals of Modern VLSI Devices*, Cambridge University Press, Cambridge, UK, 1998.
- [2] R.F. Pierret, *Semiconductor Device Fundamentals*, Addison Wesley, Reading, MA, 1996.
- [3] R. F. Pierret and J. A. Shields, "Simplified Long Channel MOSFET Theory," *Solid-State Electronics*, **26**, pp. 143-147, 1983.

## Appendix

This appendix contains the Matlab® script that produces Figs. 1 and 2.

```
% Surface potential vs. Gate voltage for MOS Capacitor
% Date: Oct. 23, 2012
% Author: Xingshu Sun and Mark S. Lundstrom(Purdue University)
%
% References

% [1] Mark Lundstrom and Xingshu Sun (2012), "Notes on the
Solution of the Poisson-Boltzmann Equation for MOS Capacitors and
MOSFETs, 2nd Ed." http://nanohub.org/resources/5338.

%Initialize the range of the surface potential
psi = -0.2:0.01:1.2; %[V]
%Specify the physical constants

epsilon_siO2 = 4*8.854*1e-14; %Permittivity of SiO2 [F/cm]
```



```

epsilon_si = 11.68*8.854*1e-14; %Permittivity of Si [F/cm]
k_b = 1.380e-23; %Boltzmann constant [J/K]
q = 1.6e-19; %Elementary charge [C]

%Specify the environmental parameters
TL = 300; %Room temperature[K]
ni = 1e10; %Intrinsic semiconductor carrier density [cm-3]
N_A = 5e17; %Acceptor concentration [cm-3]
tox = 2e-7; %The thickness of SiO2 [cm]
V_FB = 0; %The flat-band voltage [V]

%Calculate the capacitance
cox = epsilon_si/tox; %[F/cm2]

%Calculate the F function (to calculate the total charge) with
respect to different surface potentials. See: eqn. (10) in [1]

F_psi1 = exp(-psi*q/k_b/TL) + psi*q/k_b/TL -1;
F_psi2 = ni^2/N_A^2*(exp(psi*q/k_b/TL) - psi*q/k_b/TL -1);
F_psi = sqrt(F_psi1 + F_psi2);

%Initialize the vectors
psi_length = length(psi);
Qs = zeros(psi_length,1);
V_G = zeros(psi_length,1);
psi_B = zeros(psi_length,1);

```

```

%Calculate the total charges and the corresponding gate voltages.
See eqn. (12) in [1]

for i = 1:psi_length
    if psi(i) <= 0
        Qs(i) = sqrt(2*epsilon_si*k_b*TL*N_A)*F_psi(i);
%Calculate charge when the surface potential is negative

    else
        Qs(i) = -sqrt(2*epsilon_si*k_b*TL*N_A)*F_psi(i);
%Calculate charge when the surface potential is positive
    end

    psi_B(i) = k_b*TL/q*log(N_A/ni); %Get the bulk potential as a
reference and it is a constant with respect to VG

    V_G(i) = V_FB+psi(i)-Qs(i)/cox; %Calculate the gate voltage
end

%Plot total charge vs. surface potential (psi_S)
figure(1)
semilogy(psi,abs(Qs)/q,'r','linewidth',3);
hold on
set(gca, 'xlim', [-0.4 1.4], 'ylim', [1e11 1e14]);
set(gca,'fontsize',13);
xlabel('\psi_S (V)');
ylabel('|Qs|/q (cm^-2)');
%Plot x=0
plot(zeros(1,21),logspace(10,16,21),'k--')

```

```

%Plot surface potential (psi_S) vs. gate voltage with reference
potential 2*psi_B
figure(2)
h1=plot(V_G,psi,'r','linewidth',3);
hold on
h2=plot(V_G,2*psi_B,'--b','linewidth',3);
set(gca, 'xlim', [-3 10], 'ylim', [-0.4 1.4]);
set(gca,'fontsize',13);
legend('\psi_S','2*\psi_B','Location','SouthEast')
xlabel('V_G (V)');
ylabel('\psi_S (V)');

%Plot x=0 and y=0
plot(-10:10, zeros(1,21), 'k--')
plot(zeros(1,21),-10:10, 'k--')

```