Notes on the
Solution of the Poisson-Boltzmann Equation
for MOS Capacitors and MOSFETs

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1. Introduction

These notes are intended to complement the discussion on pp. 63 – 68 in *Fundamentals of Modern VLSI Devices* by Yuan Taur and Tak H. Ning [1]. (Another good reference is *Semiconductor Device Fundamentals* by R.F. Pierret [2].) The objective is to understand how to treat MOS electrostatics without making the δ-depletion approximation.

2. MOS Electrostatics: Electric Field vs. Position

We begin with Poisson's equation:

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\varepsilon_{Si}}[p(x) - n(x) + N_D^+ - N_A^-] \tag{2.147}$$

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 $p_o - n_o - N_A = 0$, which means

$$N_A = p_o - n_o\,, \tag{1}$$

so Poisson's equation becomes

$$\frac{d^2\psi}{dx^2} = \frac{-q}{\varepsilon_{s_i}}[p(x) - n(x) + n_o - p_o], \tag{2}$$

where

$$\begin{aligned} p_o &\cong N_A \\ n_o &\cong n_i^2 / N_A \end{aligned}. \tag{3}$$

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

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

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

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

and

$$n(x) = \frac{n_i^2}{N_A} e^{+q\psi(x)/k_B T}, \tag{6}$$

which are eqns. (2.149) and (2.150) in [1]. Finally, using eqns. (5) and (6) in (4), we find the *Poisson-Boltzmann equation*,

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

which we need to integrate twice to find $\psi(x)$. Equation (7) is eqn. (2.151) in [1].

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

$$p\frac{dp}{d\psi} = \frac{-q}{\varepsilon_{s_i}}\left[N_A(e^{-q\psi/k_BT}-1) - \frac{n_i^2}{N_A}(e^{q\psi/k_BT}-1)\right]. \tag{8}$$

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

$$pdp = \frac{-q}{\varepsilon_{s_i}}\left[N_A(e^{-q\psi/k_BT}-1) - \frac{n_i^2}{N_A}(e^{q\psi/k_BT}-1)\right]d\psi$$

$$\int_0^p p'dp' = \frac{-q}{\varepsilon_{s_i}}\int_o^\psi\left[N_A(e^{-q\psi/k_BT}-1) - \frac{n_i^2}{N_A}(e^{+q\psi/k_BT}-1)\right]d\psi$$

$$\frac{p^2}{2} = \frac{-q}{\varepsilon_{s_i}}\left[N_A\left\{\left(\frac{-kT}{q}\right)e^{-q\psi/k_BT}\Big|_o^\psi - \psi\right\} - \frac{n_i^2}{N_A}\left\{\left(\frac{kT}{q}\right)e^{q\psi/k_BT}\Big|_o^\psi - \psi\right\}\right]$$

$$p^2 = \frac{2k_BTN_A}{\varepsilon_{s_i}}\left[\left(e^{-q\psi/k_BT} + \frac{q\psi}{k_BT} - 1\right) + \frac{n_i^2}{N_A^2}\left(e^{q\psi/k_BT} - \frac{q\psi}{k_BT} - 1\right)\right].$$

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

$$E(x) = \frac{-d\psi(x)}{dx} = \pm\sqrt{\frac{2k_BTN_A}{\varepsilon_{Si}}}\,F(\psi), \tag{9}$$

where

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

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. Equations (9) and (10) should be compared to eqn. (2.153) in [1].

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, ψ_S, we find the surface electric field as

$$E_s = \pm\sqrt{\frac{2k_BT N_A}{\varepsilon_{Si}}}\, F(\psi_s) \ . \tag{11}$$

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

$$\boxed{Q_s(\psi_s) = -\varepsilon_{Si} E_s = \mp\sqrt{2\varepsilon_{Si} k_B T N_A}\, F(\psi_s)} \,, \tag{12}$$

which is an important and frequently-used result. Eqn. (12) is just eqn. (2.154) in [1] and was used to produce Fig. 2.25 in [1]. For the assumed p-type semiconductor, the + sign is used when $\psi_S > 0$ and the – sign when $\psi_S < 0$.

Now let's examine eqn. (12) more closely. Consider accumulation ($\psi_s < 0$) first. In this case, we have from eqn. (12)

$$Q_{s_i} = +\sqrt{2\varepsilon_{Si} k_B T N_A}\, F(\psi_s)$$

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

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

so

$$Q_{s_i} \approx +\sqrt{2\varepsilon_{Si}k_BTN_A}\; e^{-q\psi_s/2k_BT}$$

which agrees with Fig. 2.25.

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

$$Q_{s_i} = -\sqrt{2\varepsilon_{Si}k_BTN_A}\; F(\psi_s),$$

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

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

so

$$Q_{s_i} \approx Q_i \approx +\sqrt{\frac{2\varepsilon_{Si}k_BT\,n_i^2}{N_A}}\; e^{+q\psi_s/2k_BT} \quad ,$$

which is eqn. (2.164) of [1] and also agrees with Fig. 2.25. Taur and Ning point out that the electron density at the surface is

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

so we can write the charge density per cm^2 as

$$Q_{s_i} \approx +\sqrt{2\varepsilon_{Si}k_BT\,n(0)} \quad ,$$

which is eqn. (2.166) of [1]. Taur and Ning also point out that this gives us a simple way to estimate the thickness of the inversion layer. Since

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

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

$$t_{inv} \approx \frac{2\varepsilon_{Si}k_BT}{q|Q_i|}.$$

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),

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

which, according to eqn. (12) gives

$$E_s \cong \sqrt{\frac{2qN_A}{\varepsilon_{Si}}(\psi_s - k_B T / q)} \ .$$

The "exact" result is just like depletion approximation (eqn. (2.161) in [1]) <u>except</u> for $k_B T/q$ correction.

3. The Semiconductor Capacitance

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

$$C_{Si} = \frac{-dQ_s}{d\psi_s} = \sqrt{2q\varepsilon_{Si}N_A} \times$$

$$\left[\frac{\left(1 - e^{-q\psi_s/kT}\right) + \frac{n_i^2}{N_A}\left(e^{q\psi_s/kT} - 1\right)}{2\sqrt{\left(\frac{k_B T}{q}e^{-q\psi_s/k_B T} + \psi_s - \frac{k_B T}{q}\right) + \left(\frac{n_i}{N_A}\right)^2\left(\frac{k_B T}{q}e^{q\psi_s/k_B T} - \psi_s - \frac{k_B T}{q}\right)}} \right]. \qquad (13)$$

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

$$C_{Si} = \frac{-dQ_s}{d\psi_s} = \sqrt{\frac{q\varepsilon_{Si}N_A}{2(\psi_S - k_B T/q)}} = \frac{\varepsilon_{Si}}{W_d} \ ,$$

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

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

$$C_{Si}(FB) = \frac{\varepsilon_{Si}}{L_D} \tag{14}$$

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 ψ_s, we need to integrate again. Recall that

$$\frac{d\psi}{dx} = \mp\sqrt{\frac{2k_BT N_A}{\varepsilon_{Si}}} F(\psi)\,. \tag{9}$$

We can integrate eqn. (9) to find

$$\int_{\psi_s}^{\psi(x)} \frac{d\psi}{F(\psi)} = \mp\sqrt{\frac{2k_BT\ N_A}{\varepsilon_{s_i}}}\ x$$

or

$$x = \sqrt{\frac{\varepsilon_{s_i}}{2k_BT\ N_A}} \int_{\psi(x)}^{\psi_s} \frac{d\psi}{F(\psi)}\,.$$

Finally, it is convenient to write the result as

$$x = L_D \int_{\psi(x)}^{\psi_s} \frac{d\psi}{\frac{k_BT}{q} F(\psi)}\ , \tag{15}$$

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

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

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

so

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

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

$$Q_i = q\frac{n_i^2}{N_A}\int_0^{\infty}\frac{e^{q\psi/k_BT}}{\sqrt{2k_BTN_A/\varepsilon_{Si}}\,F(\psi)}d\psi \ . \qquad (16)$$

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

$$Q_d = -q\int_0^{\infty}[N_A - p(x)]dx = -qN_A\int_0^{\infty}\left(1 - e^{-q\psi/k_BT}\right)dx \ ,$$

which we can change the variable of integration to find.

$$Q_d = -qN_A\int_0^{\psi_s}\frac{1 - e^{-q\psi/k_BT}}{\sqrt{2k_BTN_A/\varepsilon_{Si}}\,F(\psi)}d\psi \ . \qquad (17)$$

5. "Exact" Solution of the MOSFET:

Taur and Ning discuss the "exact" solution for a long channel MOSFET on pp. 112 – 115 of [1]. These notes amplify on their discussion. Let's begin by reviewing the derivation of eqn. (6), which applies only equilibrium.

$$n = n_i e^{(E_F - E_i)/k_BT} \qquad (18)$$

let

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

and choose

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

The result is eqn. (6),

$$n = n_i e^{q\psi(x)/k_BT}. \tag{21}$$

Out of equilibrium, we have

$$n = n_i e^{\left[F_n(x) - E_i(x)\right]/k_BT} \tag{22}$$

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

$$n(x) = n_i e^{q\left[\psi(x) + F_n(x) - E_F\right]/k_BT} \tag{23}$$

If we define

$$q\phi_n \equiv E_F - F_n \tag{24}$$

then

$$n(x) = n_i e^{q\left[\psi(x) - \phi_n(x)\right]/k_BT} \tag{25}$$

which is eqn. (3.1) in Taur and Ning (but note that Taur and Ning use V for ϕ_n).

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

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

which can be integrated to find

$$E(\psi,\phi_n) = \pm\sqrt{\frac{2k_BT\ N_A}{\varepsilon_{Si}}}\ F(\psi,\phi_n) \tag{27}$$

where

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

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

$$Q_i = -q\int_o^\infty n(x)dx = -q\int n(x)\frac{dx}{d\psi}d\psi$$

$$= -q\int_{\psi_B}^{\psi_s} \frac{n(x)}{E(\psi,\phi_n)}d\psi$$

or

$$Q_i(\phi_n) = -q\frac{n_i^2}{N_A}\int_{\psi_B}^{\psi_S} \frac{e^{q(\psi-\phi_n)/k_BT}}{E(\psi,\phi_n)}d\psi \tag{29}$$

We should note ψ_S varies along the channel. We determine ψ_S from

$$V_g = V_{fb} + \psi_S - \frac{Q_S}{C_{ox}}$$

or

$$V_g = V_{fb} + \psi_S + \frac{\varepsilon_{Si}E_s(\psi_s,\phi_n)}{C_{ox}} \ , \tag{30}$$

Where 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 ψ_S, given the gate voltage, V_g. Knowing ψ_S, we determine the corresponding inversion layer charge by integrating eqn. (29) numerically.

The next question is: How do we determine I_{ds}?" From

$$J_n = n\mu_n \frac{dF_n}{dy} \tag{31}$$

we find

$$I_{ds} = \mu_{eff} \frac{W}{L} \int_{o}^{V_{ds}} [-Q_n(\phi_n)] d\phi_n \tag{32}$$

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

$$I_{ds} = q\mu_{eff} \frac{W}{L} \int_{0}^{V_{ds}} \left(\int_{\psi_B}^{\psi_S} \frac{(n_i^2 / N_A) e^{q(\psi - \phi_n)/k_B T}}{\mathcal{E}(\psi, \phi_n)} d\psi \right) d\phi_n \tag{33}$$

Equation (33) is just eqn. (3.13) in Taur and Ning, which 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:

$$E_s = \pm \sqrt{\frac{2k_B T N_A}{\varepsilon_{Si}}} F(\psi_s) \tag{11}$$

where

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

2) Semiconductor charge density for a given surface potential:

$$Q_s(\psi_s) = -\varepsilon_{Si} E_s = \mp\sqrt{2\varepsilon_{Si} k_B T N_A}\, F(\psi_s) \qquad (12)$$

In depletion, eqn. (12) reduces to:

$$Q_s \cong \sqrt{2q\varepsilon_{Si} N_A(\psi_s - k_B T / q)}\ ,$$

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

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

$$Q_{s_i} \approx +\sqrt{2\varepsilon_{Si} k_B T N_A}\ e^{-q\psi_s / 2k_B T} \quad \text{(strong accumulation)}$$

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

$$Q_{s_i} \approx Q_i \approx +\sqrt{\frac{2\varepsilon_{Si} k_B T n_i^2}{N_A}}\ e^{+q\psi_s / 2k_B T} \qquad \text{(strong inversion)}$$

which can also be expressed as

$$Q_{s_i} \approx +\sqrt{2\varepsilon_{Si} k_B T\, n(0)}$$

The inversion layer thickness can be estimated as:

$$t_{inv} \approx \frac{2\varepsilon_{Si} k_B T}{q|Q_i|}$$

3) Capacitance:

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

$$C_{Si}(FB) = \frac{\varepsilon_{Si}}{L_D} \qquad (14)$$

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.