The basic MOS structure

Here we analyze the relationships between band-bending, charge, and electric field for a MOS capacitor on a p-type substrate (which would be the starting point for making an n-channel MOSFET). The analysis for an n-substrate MOS capacitor is similar, with obvious changes for different doping type, etc.

1. Band Diagram

Consider the band diagram in the figure above, showing the MOS structure with a positive bias (i.e. $V_{GS} > 0$). From the diagram, we see that

$$qV_G = qF_M + qF_{ox} - qF_S + qF_S - E_G + d_p = qF_M - qF_S - E_G + d_p$$

(1)

The bracketed terms represent the flat-band potential,

$$qF_{FB} = qF_M - qF_S - E_G + d_p$$

(2)

and the last two terms are the total band-bending in the oxide and the semiconductor.

The flat-band potential is analogous to the built-in potential of a p-n diode, being equal to external bias that would be required in order to make the bands flat.

Exercise: Draw the diagram for PMOS structure (i.e. one using an n-type substrate). Show that the flat band potential for a PMOS could be defined as

$$qF_{FB} = qF_M - qF_S - d_n$$

(3)
A key part of the flat-band potential is the difference in the two barrier heights. We recall that theoretical calculations of barrier heights for Schottky diodes and heterojunctions have been elusive. The story is similar for metal-oxide and semiconductor-oxide barrier heights. However, these quantities are fairly easy to measure. Unfortunately, most textbooks seem to be a bit lax in that they don’t bother giving those values! A brief survey of several textbooks, of which Pierret appears to be the most complete, suggest the following values for the barrier height differences:

- Al: -0.03 eV
- n+ polysilicon: -0.18 eV
- p+ polysilicon: 1.22 eV

Of the three choices, n+ polysilicon is most widely used. Of course, Al and an assortment of other metals were used in early MOS structures. But a word of caution is needed: In order to get to the bottom of the issue on barrier height differences, it will be necessary to scour the relevant research literature. For our purposes, the values given above will suffice.

2. Initial calculation of threshold voltage

Using the band diagram and equation (1) above, we can take a crack at determining the threshold voltage of the MOS structure. Recall that our definition of threshold voltage is when the total amount of band-bending in the semiconductor is twice the separation between the intrinsic level and the Fermi level in the bulk semiconductor:

$$q\varphi_b = 2\left(E_F - E_i\right)_{bulk}$$

$$= 2kT \ln \frac{N_A}{n_i}$$

Inserting into the first equation above

$$qV_T = q\varphi_{FB} + q\varphi_{ox} + 2kT \ln \frac{N_A}{n_i}$$

We see that we are close but still need to determine the change in potential in the oxide. We can get at that by noting that the normal components of the fields on the two sides of the oxide-semiconductor interface are related by

$$D_{ox} = D_s$$

$$\mathbf{n}\cdot \mathbf{E}_{ox} = \mathbf{n}\cdot \mathbf{E}_s$$

and, if there are no charges in the oxide,
\[ \Box_{ax} = E_{ax}t_{ox}. \]  

(7)

But we don’t appear to be any closer to our goal since all we’ve done is shifted from not knowing the potential change in the oxide to not knowing the electric field in the semiconductor. However, we do have a means for estimating the electric field in a depletion layer -- the depletion approximation. (The depletion approximation gives us a good estimate because, even at threshold, most of the negative charge in the semiconductor is in the form of acceptor ions. The electron concentration in the just-formed inversion layer is at least a factor 10 less than the acceptor charge. We can justify this below when we do the exact analysis.) From the depletion approximation, the electric field at the interface is

\[ E_S(0) = \sqrt{\frac{2qN_A\Box_k}{\Box_k}}. \]  

(8)

Using (6), (7), and (8) together:

\[ \Box_{ox} = \frac{t_{ox}}{t_{ox}} \Box \Box_S(0) \]

\[ = \frac{t_{ox}}{t_{ox}} \sqrt{2q\Box N_A\Box_k} \]

\[ = \frac{t_{ox}}{t_{ox}} \sqrt{4kT\Box N_A \ln \frac{N_A}{n_i}} \]  

(9)

Putting it all together gives the threshold voltage:

\[ V_T = \Box_{FB} + \frac{2kT}{q} \ln \frac{N_A}{n_i} + \frac{t_{ox}}{t_{ox}} \sqrt{4kT\Box N_A \ln \frac{N_A}{n_i}} \]  

(10)

We note that the threshold voltage can be increased by increasing the substrate doping -- higher p-type doping means that more bias is required to invert the semiconductor -- or by increasing the oxide thickness -- more of the applied bias is “used up” across the wider oxide layer.

Exercise: Show that the threshold voltage for a PMOS structure is given by

\[ V_T = \Box_{FB} \Box \frac{2kT}{q} \ln \frac{N_D}{n_i} + \frac{t_{ox}}{t_{ox}} \sqrt{4kT\Box N_D \ln \frac{N_D}{n_i}} \]  

(11)

where the flat-band potential for the PMOS is given by equation (3) above.
3. Exact Analysis

In order to do an exact analysis of the band-bending at the MOS interface, we need an exact expression for the charge density.

The most general expression for charge density would have the following form:

\[ \mathcal{J}(x) = q \left[ n_D^*(x) \cdot N_A + p(x) \cdot n(x) \right]. \tag{12} \]

However, this is probably too general. Including doping variations and doping ionization would make the analysis unduly messy at the outset. So assume the doping is constant and the impurities are fully ionized, so that (11) simplifies to

\[ \mathcal{J}(x) = q \left[ n_D \cdot N_A + p(x) \cdot n(x) \right]. \tag{13} \]

Assuming that Boltzmann statistics are applicable everywhere, the hole concentration is

\begin{align*}
p(x) &= n_i \exp \left[ \frac{E_i(x) - E_F}{kT} \right] \\
&= n_i \exp \left[ \frac{E_i(x) - E_F}{kT} \right] \exp \left[ \frac{E_i(x) - E_F}{kT} \right] \\
&= p_o \exp \left[ \frac{E_i(x) - E_F}{kT} \right]. \tag{14}
\end{align*}

The last expression in brackets is simply the band-bending parameter for the p-type material. (Recall that downward band-bending is defined as positive for a p-type semiconductor.) So,

\[ p(x) = p_o \exp \left[ \mathcal{J}(x) \right]. \tag{15} \]

Similarly, the electron concentration can be expressed as

\[ n(x) = n_o \exp \left[ \mathcal{J}(x) \right]. \tag{16} \]

As seen before, the electron and hole concentrations depend on position only through the band-bending, so these quantities can be viewed as functions of band-bending. Consequently, the charge density can be viewed as a function of band bending,

\[ \mathcal{J}(\mathcal{J}) = q \left[ n_D \cdot N_A + p_o \exp(\mathcal{J}) \cdot n_o \exp(\mathcal{J}) \right]. \tag{17} \]

As a final step, we can simplify (17) slightly by noting that in the bulk semiconductor, far from the interfaces, the band-bending and the charge density are both zero. Thus,
Of course, the electron and hole concentrations in the bulk are related by mass-action law, \( n_o p_o = n_i^2 \).

\[ N_D N_A = n_o p_o. \tag{18} \]

Using the Poisson-Boltzmann equation, we can determine the electric field as a function of position.

\[ E_S(y) = \pm \frac{2kT}{q} \int_0^y \left[ p_o \left[ \exp (\frac{y}{kT}) + 1 \right] - n_o \left[ \exp (\frac{y}{kT}) - 1 \right] \right] dy. \tag{20} \]

Re-arranging slightly and taking the square-root,

\[ E_S(y) = \pm \sqrt{\frac{2kT p_o}{q} \left[ \exp (\frac{y}{kT}) + 1 \right] - \frac{n_o p_o}{p_o} \left[ \exp (\frac{y}{kT}) - 1 \right]} \tag{21} \]

Equation (21) requires us to make a choice between the positive and negative root. A moment’s reflection leads to the conclusion that, for the current geometry with the semiconductor occupying the positive half-plane, we should choose the positive root if the band-bending is positive and the negative root if the band-bending is negative. Equation (20) is particularly useful when evaluated at the interface, where the semiconductor band-bending is maximum,

\[ \frac{t_{ox}}{t_{as}} E_S(0) = V_G - V_{FB}. \tag{22} \]
\[
\frac{Q_{ox}}{t_{ox}} \left( V_G - V_{FB} \right) \frac{kT}{q} \left( 0 \right) = \pm \sqrt{\frac{2kT_p}{k} \ln \left[ \exp \left( \sqrt{\frac{kT_p}{q} \ln \left( n_i \right) + \sqrt{0} \right) \right] + \frac{n_o}{p_o} \left\{ \exp \left[ \sqrt{0} \right] \sqrt{0} \right\} - n_o - p_o + n_i - p_i \right)}
\]

Equation (23) does not have a particularly user-friendly form, but calculating the band bending for a given applied bias is a straightforward exercise in finding the zeroes of an equation. Note that the reverse operation — calculating the gate voltage corresponding to a given amount of band-bending — is quite easy.

4. Threshold voltage redux

Equation (23) can be used to re-examine the threshold voltage given in equation (10) above. Our established criterion says that threshold occurs when the total band-bending is equal to twice the value of \( E_i - E_F \) in the bulk of the semiconductor.

\[
kT \sqrt{0} = 2 \left[ E_i (x \nabla ) - E_F \right]
\]

Inserting the condition (24) into equation (23), and solving for \( V_G = V_T \), (with a decent dose of algebra thrown in)

\[
V_T = \sqrt{0} + \frac{2kT}{q} \ln \frac{p_o}{n_i} + \frac{t_{ox}}{Q_{ox}} \sqrt{4kT_p \ln \left( p_o \right) n_i - p_o} \ln \left( n_o \right) + 4kT_p \ln \left( p_o \right) n_i - p_o
\]

Note that this is exactly the result obtained above in equation (10) using the depletion approximation.

Exercise: Fill in the steps that are missing in the derivation of (25).

The figures below show the threshold voltage for NMOS (p-substrate) and PMOS (n-substrate) structures, using n+ polysilicon as the gate material. The different lines in each graph are for different oxide thicknesses.
The electron concentration in the inversion layer

The electron concentration at the interface is

\[ n(0) = n_s \exp(\Box). \]

However, for the FET calculations, we may be more interested in the total electron sheet concentration, defined as

\[ n_s = \int n(x) dx \]
\[ = \int_0^n(\Box) d\Box. \]

In principle, we can always use equation (23) along with some numerical integration to obtain the sheet concentration. However, we can also note that

\[ D_S(0) = Q_S \]
\[ \Box E_S(0) = qn_s + qN_A W_p \]

Using equation (22),

\[ \frac{\Box}{t_{ox}} (V_G \Box V_{FB} \Box V_S) = qn_s + qN_A W_p. \]
\[ qn_s = C_{ox} (V_G \Box V_{FB} \Box V_S) qN_A W_p. \]