9. Space charge layers at boundaries

A difference of the electric potential between the crystal bulk and interface with another medium (including surface) redistributes free carriers, forming a space charge layer. The layer screens the electric field that would be observable in the situation with no free carriers. The equilibrium distribution of charge depends on the difference of electric potential at the interface, on the bulk density of free charges, on static permittivity of the crystal, and on temperature. The equilibrium reflects the counteraction between the attraction/repulsion of free carriers by the electric field towards/from the interface, and the tendency of the free carrier gas to be dispersed homogeneously in the whole volume of the crystal.

Let us describe qualitatively the following situation:
- the difference of the potential is produce by an infinitely thin layer of positive charge of the areal density η,
- the bulk contains free electrons. i.e., it is the n-type semiconductor.

The first assumption implies an increase of the potential at the interface compared to its bulk value ; in fact, a positively charged test particle increases its potential energy when approaching the positively charged layer, as the force is repulsive. On the contrary, freely moving (quasi)electrons are attracted by the positive charge at the interface. At zero temperature, an infinitely thin layer of negative charge with the areal density $-\eta$ would be formed at the interface, screening totally the field of the positive charge. The thermal movement at finite temperatures broadens this layer. The following figure describes schematically this situation, showing the dependence of the energies of the bottom of conduction band, E_c, and of the top of valence band, E_v, on the coordinate z. The chemical potential, denoted E_F, is independent of z (in equilibrium).
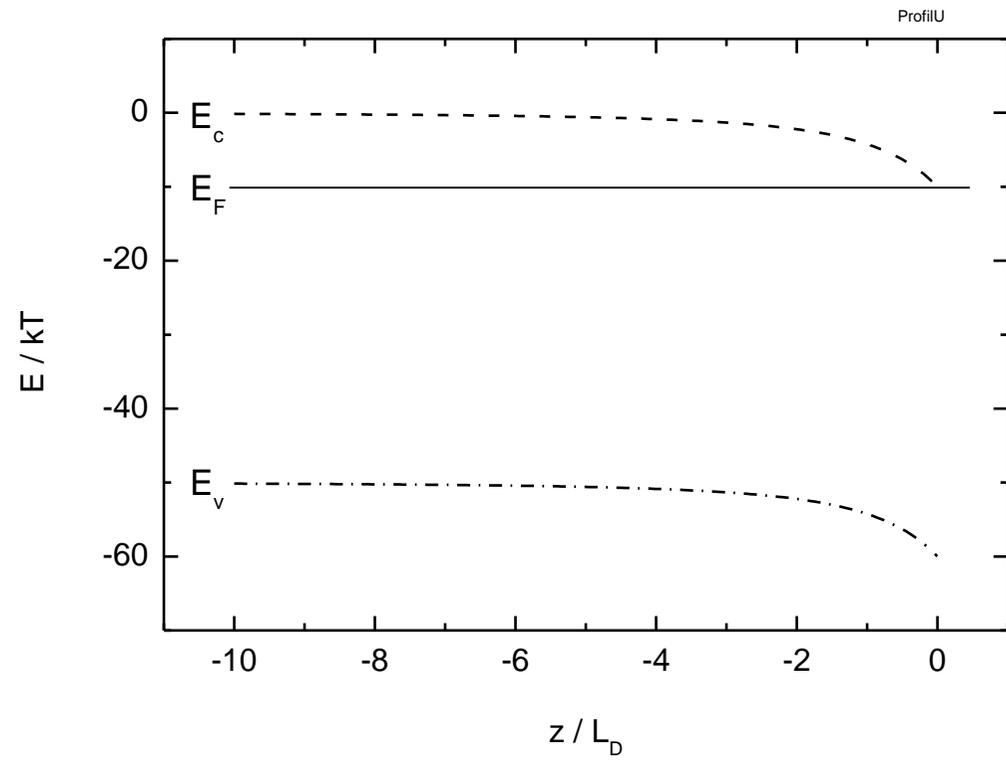
Band energies at a charged interface.

Space charge layer in equilibrium

Thee quantitative treatment of the energy profiles has to involve the relation of the potential, $\varphi(z)$, to the charge density, $\rho(z)$, given by the Poisson equation,

$$\frac{d^2\varphi(z)}{dz^2} = -\frac{4\pi}{\varepsilon}\rho(z) \ , \tag{9.1}$$

where ε is the static dielectric constant of the crystal. Equation (9.1) uses the centimeter-gram-second (cgs) system of units; switching to SI requires the static permittivity to be replaced by the product $4\pi\varepsilon_o\varepsilon_r$, where ε_r is dimensionless relative permittivity, and ε_o the permittivity of vacuum (8.854E-12 F/m):

$$\frac{d^2\varphi(z)}{dz^2} = -\frac{1}{\varepsilon_o\varepsilon_r}\rho(z) \ . \tag{9.1 SI}$$

In a homogeneous insulating slab of the thickness d, and the applied voltage U, the Poisson equation leads to the constant electric field intensity, $U/(d\varepsilon_o\varepsilon_r)$, and a quadratic dependence of the potential on the position within the slab. The capacitance C (charge per unit voltageí) of a capacitor with the area S is $\varepsilon_o\varepsilon_r S/d$; the relative static permittivity of silicon is about 11.4; for the area of 1 cm^2 and the thickness of 1 mm, the capacitance is roughly 10.4 pF in the absence of noticeable free carrier density.

Considering free carriers (let us select electrons), we have to use the statistical relation of their density, $n(z)$, and the energy relative to the bottom of the conduction band,

$$E_c(z) = E_{cB} - e\varphi(z) \ , \tag{9.2}$$

and the Fermi energy, E_F. We have introduced the symbol for the limit vale of E_c in the bulk ($z\rightarrow$-∞), E_{cB}. For a parabolic dispersion with the effective mass m^*, the electron density is determined by the density of states,

$$D(E) = V \frac{\sqrt{2}}{\pi^2} \frac{(m^*)^{3/2}}{\hbar^3} \sqrt{E - E_c} \quad \text{for} \quad E > E_c ,$$

$$D(E) = 0 \quad \text{for} \quad E < E_c ,$$

(9.3)

and the Fermi-Dirac statistics,

$$f_{FD}(E) = \frac{1}{\exp\left(\dfrac{E - E_F}{kT}\right) + 1} .$$

(9.4)

Including the spin degeneracy, the density of free electrons is

$$n = \frac{\sqrt{2}}{\pi^2} \frac{(m^*)^{3/2}}{\hbar^3} \int_{E_c}^{\infty} \frac{\sqrt{E - E_c}}{\exp\dfrac{E - E_F}{kT} + 1} dE .$$

(9.5)

Using the symbol for Fermi-Dirac integrals, the concentration can be written down in the following form,

$$n(z) = N_c F_{1/2}\left(\frac{E_F - E_{cB} - e\varphi(z)}{kT}\right) ,$$

(9.6)

where

$$N_c = \frac{\sqrt{2}}{\pi^2} \frac{(m^* kT)^{3/2}}{\hbar^3} .$$

(9.7)

Note: in the limit of classical statistics, we can use Eq. (8.19) to obtain the following approximate form of Eq. (9.6),

$$n(z) = 2 \frac{(2\pi m^* kT)^{3/2}}{8\pi^3 \hbar^3} \exp\left(\frac{E_F - E_{cB} - e\varphi(z)}{kT} \right) ,$$

(9.6a)

which is a modified form of Eq. (8.21) including the positional dependence of the potential.

The development can be simplified by introducing two dimensionless quantities,

$$u(z) = \frac{e\varphi(z)}{kT} , \quad \alpha = \frac{E_F - E_{cB}}{kT} ,$$

(9.8)

and denoting the bulk density of electrons by n_B. The Poisson equation (9.1) leads to

$$\frac{d^2 u}{dz^2} = -\frac{4\pi}{\varepsilon} \frac{e}{kT} e[n_B - n(z)] = -\frac{4\pi e^2}{\varepsilon kT} N_c \left[F_{1/2}(\alpha) - F_{1/2}(\alpha + u) \right]$$

$$= -\frac{4\pi e^2 N_c F_{1/2}(\alpha)}{\varepsilon kT} \left[1 - \frac{F_{1/2}(\alpha + u)}{F_{1/2}(\alpha)} \right] = -\frac{1}{L_D^2} \left[1 - \frac{F_{1/2}(\alpha + u)}{F_{1/2}(\alpha)} \right] ,$$

(9.9)

where

$$L_D = \sqrt{\frac{\varepsilon kT}{4\pi e^2 N_c F_{1/2}(\alpha)}} = \sqrt{\frac{\varepsilon kT}{4\pi e^2 n_B}}$$

(9.10)

means the Debye screening length in the volume of our crystal.

In the SI units,

$$L_D = \sqrt{\frac{\varepsilon_o \varepsilon_r kT}{e^2 n_B}} \ .$$

(9.10 SI)

Using a simple trick, the nonlinear differential equation (9.9) of the second order for the reduced potential $u(z)$ can be transformed into the equation of the first order:

$$2 \frac{du}{dz} \frac{d^2 u}{dz^2} dz = d\left[\left(\frac{du}{dz}\right)^2\right] = 2 \frac{du}{dz} \left\{ -\frac{1}{L_D^2} \left[1 - \frac{F_{1/2}(\alpha + u)}{F_{1/2}(\alpha)} \right] \right\} dz \ ,$$

(9.11)

i.e.,

$$\left(\frac{du}{dz}\right)^2 = \frac{2}{L_D^2} \int_{-\infty}^{u(z)} \left[-1 + \frac{F_{1/2}(\alpha + t)}{F_{1/2}(\alpha)} \right] dt = \frac{2}{L_D^2} \left[-u + \frac{2}{3} \frac{F_{3/2}(\alpha + u) - F_{3/2}(\alpha)}{F_{1/2}(\alpha)} \right] \ .$$

(9.12)

We have used the following property of the Fermi-Dirac integrals, which can be verified directly from their definition:

$$\frac{d}{dt} F_j(t) = j F_{j-1}(t) \ .$$

(9.13)

The first derivative of the reduced potential from Eq. (9.12) is

$$\frac{du}{dz} = \frac{\sqrt{2}}{L_D} F(u, \alpha) \ ,$$

(9.14)

6

where

$$F(u,\alpha) = \pm\sqrt{-u + \frac{2}{3}\frac{F_{3/2}(\alpha+u) - F_{3/2}(\alpha)}{F_{1/2}(\alpha)}}$$

(9.15)

with the + sign for positive, and the − sign for the negative values of u, respectively. Rewriting Eq. (9.14) in the following form,

$$\frac{du}{F(u,\alpha)} = \frac{\sqrt{2}}{L_D}dz \ ,$$

(9.16)

the sought dependence of the potential on the coordinate results, in an implicit form, from another integration:

$$\frac{1}{\sqrt{2}}\int_{u(0)}^{u(z)}\frac{dt}{F(t,\alpha)} = \frac{z}{L_D} \ .$$

(9.17)

A suitable assessment of the monotonic dependence $u(z)$ can be obtained by the exponential,

$$u(z) \approx u(0)\exp\left(\frac{z}{L}\right) ,$$

(9.18)

setting its slope at $z = 0$ to the correct value from Eq. (9.14); this means the correct value of the electric field intensity at the interface. This condition is fulfilled by using the (effective screening) length

$$L = L_D\frac{1}{\sqrt{2}}\frac{u(0)}{F[u(0),\alpha]} \ .$$

(9.19)

The Debye screening length of Eq. (9.10) is a good basis for a quick orientation. It is plotted in the following figure for a broad range of free carrier concentrations; with the relative permittivity of 10 at room temperature, the value of 10 nm is achieved for the carrier density of about 1E17 cm^{-3}.
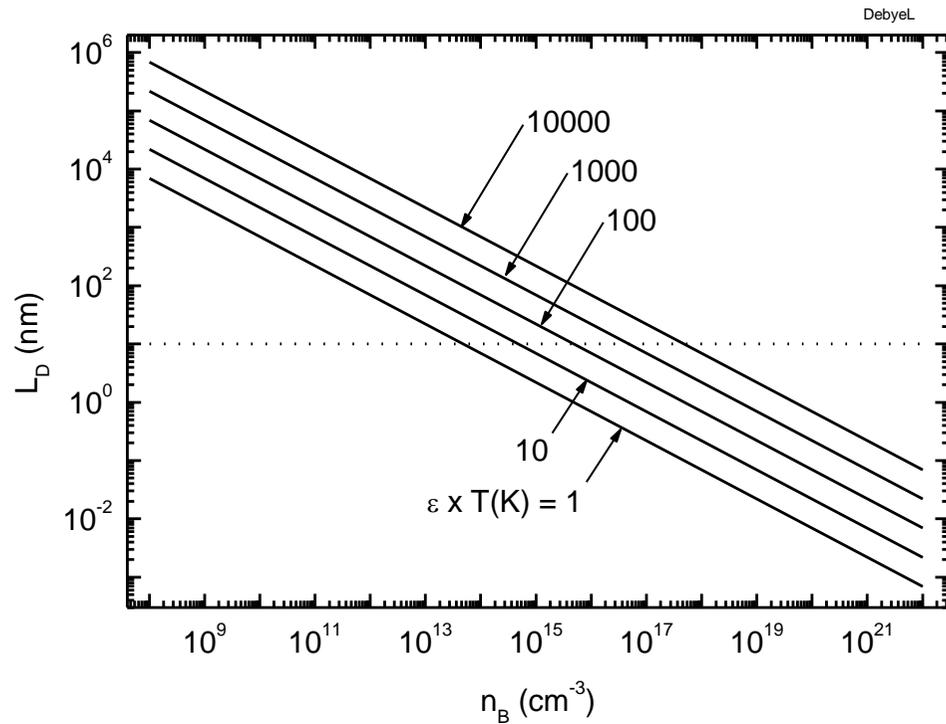
Debye screening length as the function of free carrier density, for several values of the product of relative permittivity and temperature.

Effective screening length of Eq. (9.19) is shown in the following two figures in the form of the ration to the Debye length, on linear and logarithmic scale.

For the positive values of the reduced potential, with accumulated electrons, the thickness of the space charge layer diminishes. This is expected, as the screening ability of the gas increases with its density. The value of α specifies the position of the Fermi energy relative to the bottom of conduction band; it becomes negative for the Fermi energy within the forbidden band.

For the negative values of the reduced potential, with depleted electrons, the thickness of the space charge layer increases; the reason is the decreased screening ability of the gas. Within the range of validity of classical statistics ("far from degeneracy"), the Fermi-Dirac integrals can be approximated by exponentials (for negative z of large absolute values),

$$F_{1/2}(z) \approx \frac{\sqrt{\pi}}{2} \exp(z) \, , \; F_{3/2}(z) \approx \frac{3\sqrt{\pi}}{4} \exp(z) \, ,$$

(9.20)

and the function F of Eq. (9.15) reduces to

$$F(u, \alpha) \approx -\sqrt{-u + \frac{\exp(\alpha + u) - \exp(\alpha)}{\exp(\alpha)}} = -\sqrt{-u + \exp(u) - 1} \, .$$

(9.21)

Effective screening length of Eq. (9.19) becomes

$$L = L_D \sqrt{\frac{-u(0)}{2}} \quad \text{pro} \quad -u(0) \gg 1 \, .$$

(9.22)

On the contrary, for small values of $|u|$, the following simplification takes place:

$$F(u, \alpha) \approx -\sqrt{-u + 1 + u + \frac{u^2}{2} - 1} = -\frac{|u|}{\sqrt{2}} \quad \Rightarrow \quad L \approx L_D \, .$$

(9.23)
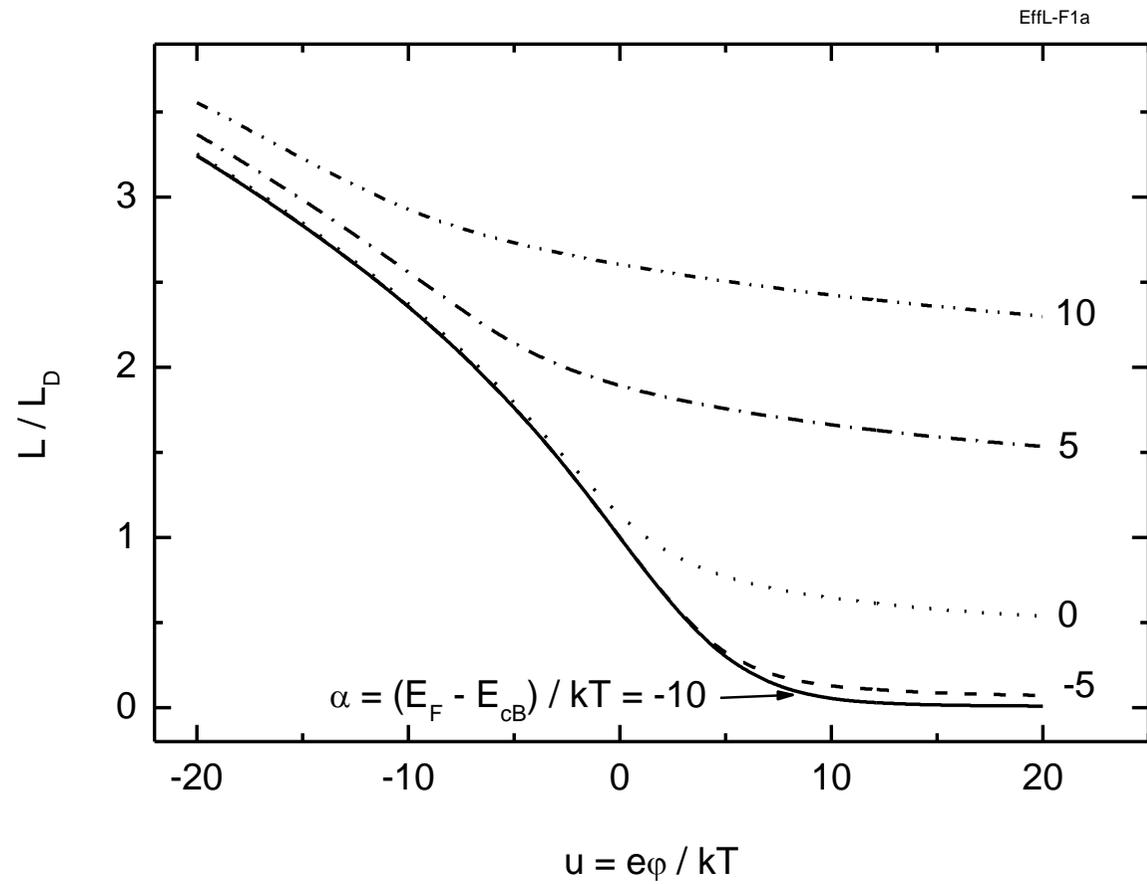
EffL-F1a

$\alpha = (E_F - E_{cB}) / kT = -10$

$u = e\varphi / kT$

Effective screening length (relative to the Debye length) as the function of the reduced potential, for several values of the relative position of the bottom of the conduction band and Fermi energy in the bulk.

EffL-F1b
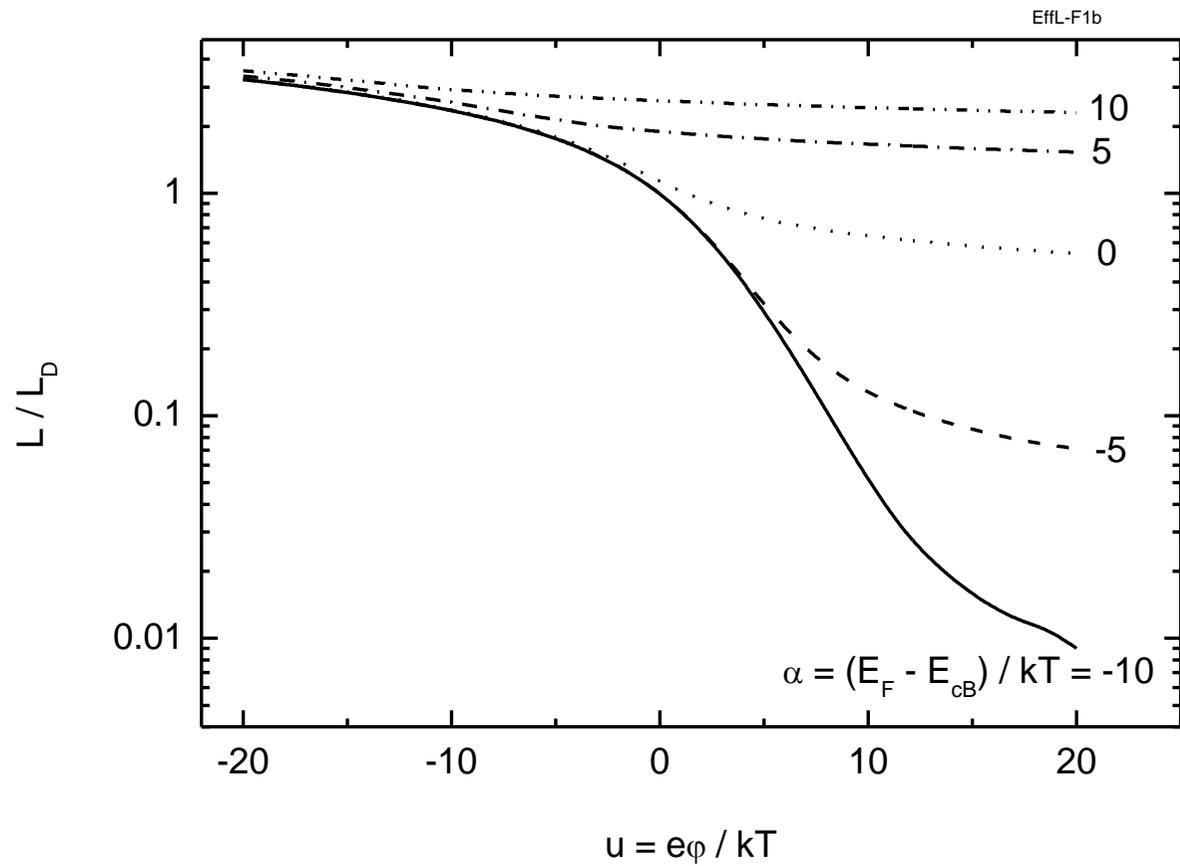
Effective screening length (relative to the Debye length) as the function of the reduced potential, for several values of the relative position of the bottom of the conduction band and Fermi energy in the bulk.

Another simple description of the depleted layer concerns the case of strong degeneracy of the gas (large concentration of the free carriers and/or low temperatures). Making use of the approximation of the Fermi-Dirac integrals for large positive z (replacing the integrand in Eq. (8.17) by the function t^j for $t < z$ and zero for $t > z$):

$$F_j(z) \approx \frac{z^{j+1}}{j+1} \; .$$

(9.24)

This leads to the approximate form of the function F of Eq. (9.15),

$$F(u,\alpha) \approx -\sqrt{-u + \frac{2}{5}\frac{(\alpha+u)^{5/2} - \alpha^{5/2}}{\alpha^{3/2}}} \; .$$

(9.25)

When calculating the effective screening length of Eq. (9.19), special care is needed in the neighborhood of the vanishing value of u; for example, the Taylor expansion in Eq. (9.25) up to the second order in u results in

$$L = L_D\sqrt{\frac{2\alpha}{3}} \quad \text{pro} \quad u(0) = 0 \; .$$

(9.26)

With the Fermi energy of 100 meV inside the conduction band and the temperature of 4 K, the value of α is roughly 300, the effective screening length for the potential of 300 meV at the edge of the depleted layer is about 25-times larger than the Debye length.

The situation of the strongly degenerate depleted layer is depicted in the following figure.
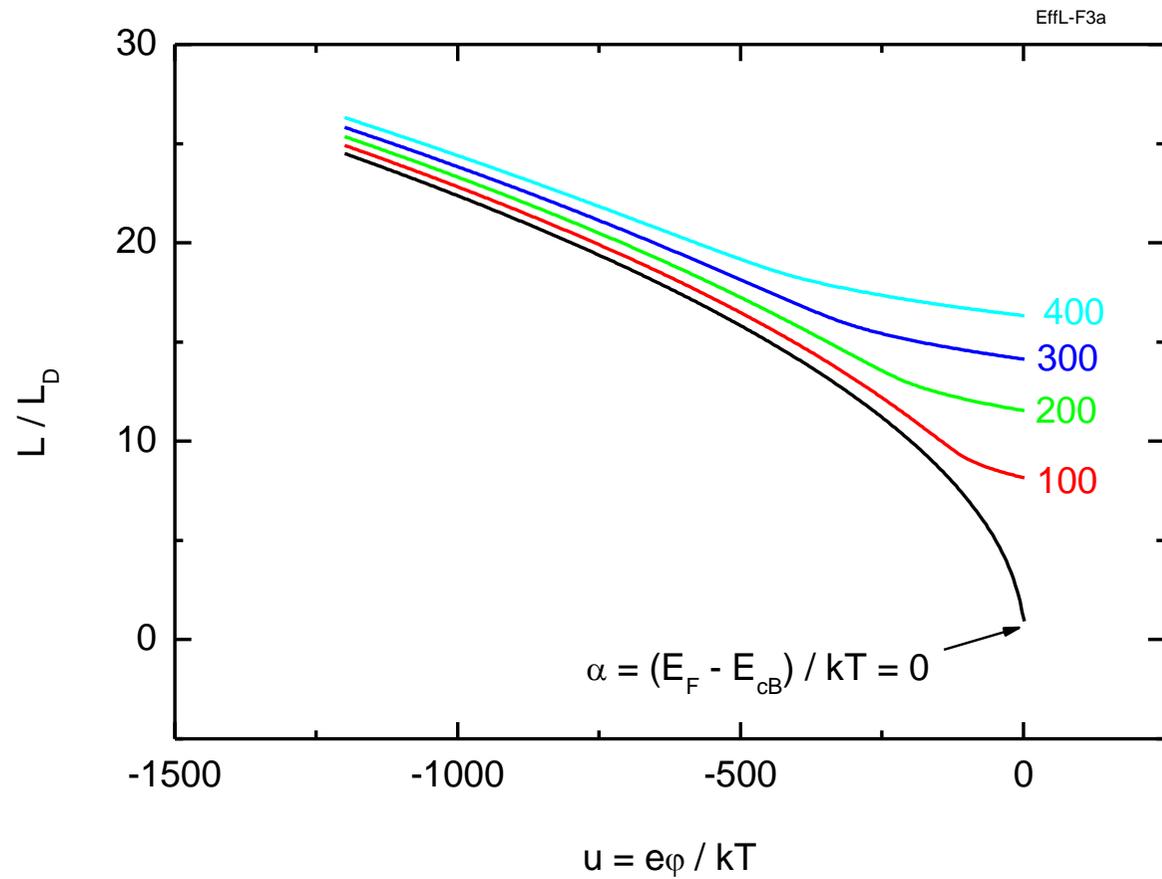
EffL-F3a

L / L_D

30

20

10

0

400

300

200

100

$\alpha = (E_F - E_{cB}) / kT = 0$

-1500   -1000   -500   0

$u = e\varphi / kT$

Effective screening length (relative to the Debye length) as the function of the reduced potential, for several values of the relative position of the bottom of the conduction band and Fermi energy in the bulk.

Capacitance of the space charge layer

The space charge layer is evidently behaving as a capacitor, with a rather tricky behavior. For estimating its capacitance, we can use the Poisson equation (9.1), rewritten for the charge density:

$$\rho(z) = -\frac{\varepsilon}{4\pi}\frac{d^2\varphi(z)}{dz^2} = -\frac{\varepsilon}{4\pi}\frac{kT}{e}\frac{d^2u(z)}{dz^2} \quad . \tag{9.27}$$

The second derivative of the reduced potential is given by Eq. (9.9), leading to

$$\rho(z) = \frac{\varepsilon kT}{4\pi e L_D^2}\left[1 - \frac{F_{1/2}\left[\alpha + u(z)\right]}{F_{1/2}(\alpha)}\right] \quad . \tag{9.28}$$

A simplification results when taking the exponential dependence of u on the position from Eqs. (9.18) and (9.19); we arrive at

$$\rho(z) = -\frac{\varepsilon kT}{4\pi e L^2}u(0)\exp\left(\frac{z}{L}\right) \quad . \tag{9.29}$$

The charge per unit area results from the integration over z up to the position of the reduced potential $u(0)$:

$$Q_s = \int_{-\infty}^{0}\rho(z)dz = -\frac{\varepsilon kT}{4\pi e L}u(0) = -\frac{\varepsilon}{4\pi L}\varphi(0) \quad . \tag{9.30}$$

The capacitance per unit area is therefore

$$C_s = \left|\frac{Q_s}{\varphi(0)}\right| = \frac{\varepsilon}{4\pi L} \quad ; \tag{9.31}$$

it depends on the potential, via the variability of the length L. For small band curvature (close to the "flat-band" condition), Eqs. (9.23), (9.10) and (9.6a) predict the capacitance nearly independent of the surface potential:

$$C_{s0} = \frac{\varepsilon}{4\pi L_D} = \sqrt{\frac{\varepsilon e^2 n_B}{4\pi kT}} = \sqrt{\frac{\varepsilon e^2 (m^*)^{3/2} (2\pi kT)^{1/2}}{8\pi^3 \hbar^3}} \exp\left(\frac{E_F - E_{cB}}{2kT}\right) .$$

(9.32)

Consequently, the capacitance per unit area depends only on the static permittivity and the Debye screening length; in the SI units:

$$C_{s0} = \frac{\varepsilon_o \varepsilon_r}{L_D} .$$

(9.32 SI)

With the relative permittivity of silicon, 11.4, and the Debye length of 10 nm, the capacitance of the area of 1 μm^2 is about 10.1 pF.

More generally, the dependence on the surface potential follows the inverse proportionality to the effective screening length:

$$C_s = \frac{C_{s0}}{L / L_D} .$$

(9.33)

The differential capacitance per unit area is

$$C_{sd} = \left| \frac{dQ_s}{d\varphi(0)} \right| .$$

(9.34)

The basic structure of the capacitor uses all of the three types of materials, a metallic contact (M), an insulating layer (I), and the semiconductor hosting the space charge layer (S). This MIS structure is commonly denoted as MOS, since the insulation is provided by oxides (O).

MOS capacitor
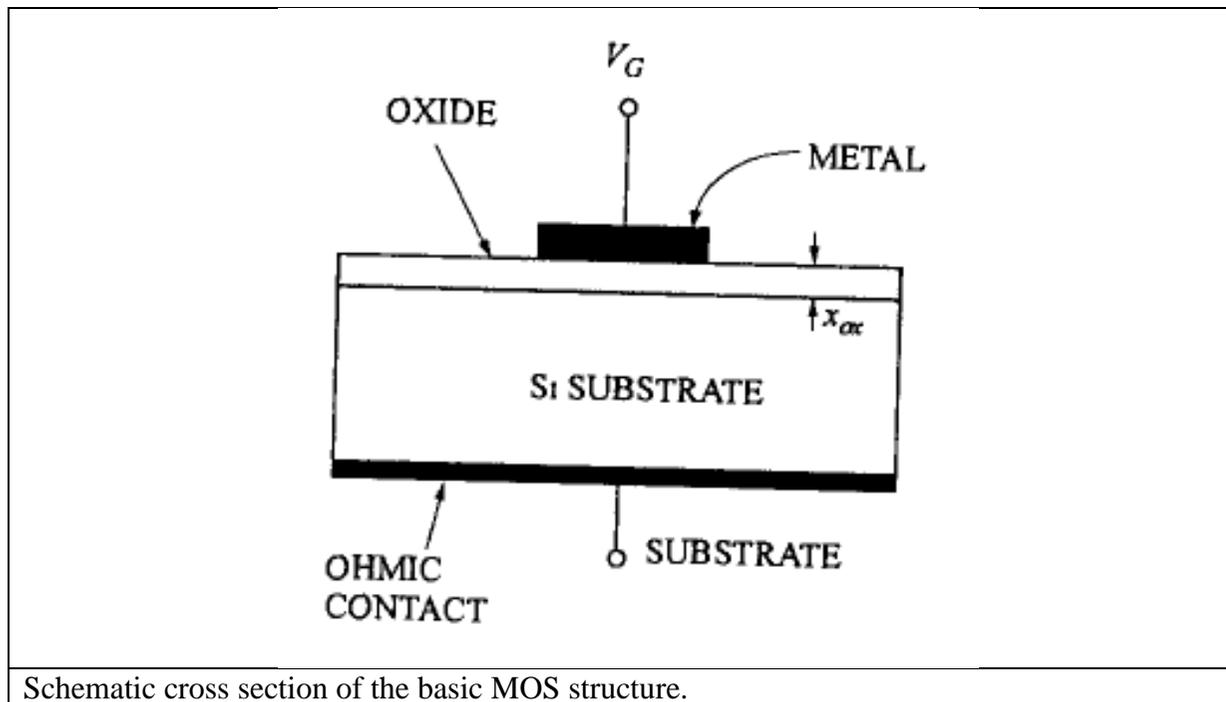
Schematic cross section of the basic MOS structure.
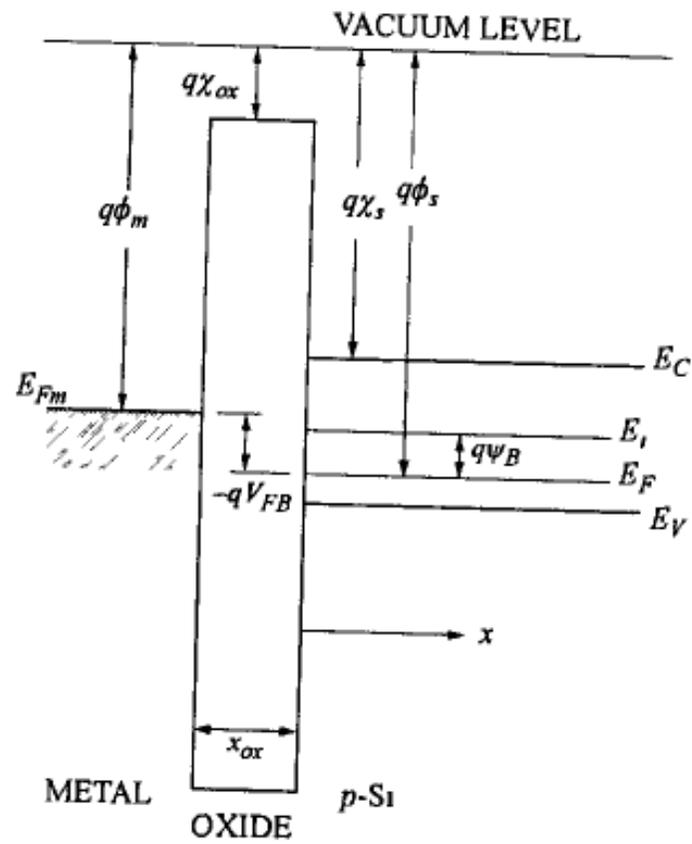
Band energies of the MOS structure, flat-band condition.

The actual behavior of the MOS capacitors is usually influenced by possible non-equilibrium states of the free-carrier gas due to fast changes of the gate potential. Note the influence of measurement frequency, and also the ramp of the mean value of the gate voltage.
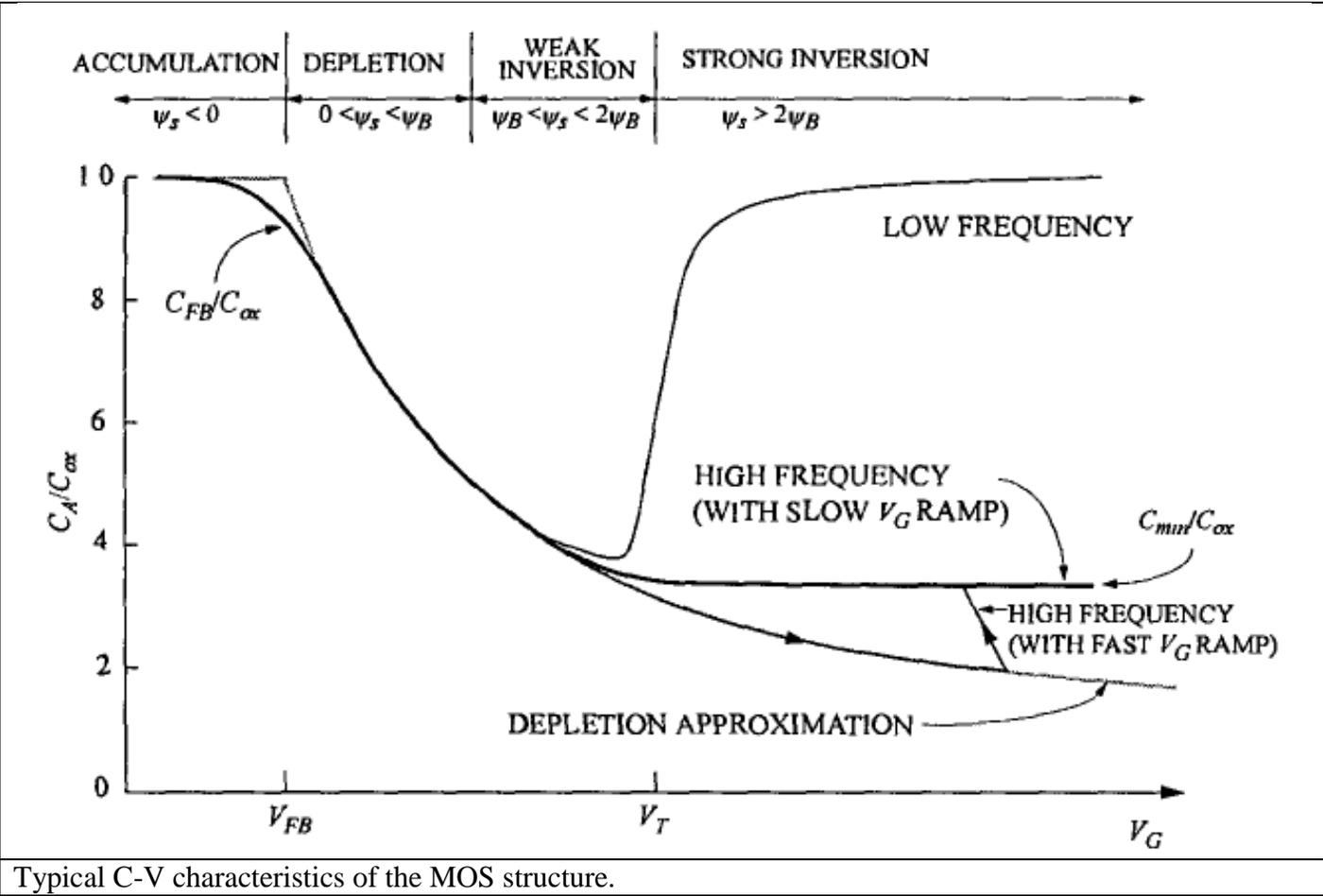
Typical C-V characteristics of the MOS structure.