Band-bending

In the *p*-*n* junction and BJT, we saw that the semiconductor band edges were bent in the depletion layers. We used the depletion approximation and Poisson's equation to relate the band-bending (barrier height) to the electric field to the depletion layer width. In the case of depletion, our treatment is reasonably accurate. However, we need to look at the case when the bands bend the other way, creating an accumulation layer or when they bend so much in depletion that they create an inversion layer. To handle these cases, we need a more complete theory.

In dealing with general band-bending problems, we will find it useful to look at bending in *p*- and *n*-type material independently. Once we have solutions to the band-bending in the different layers, we can combine the separate into a complete solution.



Upward band bending: electrons depleted. holes increasing.

 $E_{C}(x)$ E_{Fn} $E_{i}(x)$

Downward band bending: electrons *accumulate*. holes decreasing. Downward band bending: holes depleted. electrons increasing.



Upward band bending: holes *accumulate*. electrons decreasing.

Poisson-Boltzmann equation

Consider the *n*-type side of a *p*-*n* junction. We can simplify the upcoming math by assuming that:

1) the donor concentration is position-independent (uniform doping)

- 2) all donors are fully ionized, and
- 3) $N_D \ll N_C$ (the semiconductor is non-degenerate).

Start with Poisson's equation

 $\frac{d^{2}\phi\left(x\right)}{dx^{2}} = -\frac{\rho\left(x\right)}{\varepsilon_{s}}$

Recall the electrostatic potential is related to the band-edge energy by

 $q\phi(x) = -E_C(x) + \text{constant}$

Then we can re-write Poisson's equation in terms of the conductionband energy:

$$\frac{d^{2}E_{C}\left(x\right)}{dx^{2}} = \frac{q\rho\left(x\right)}{\varepsilon_{s}}$$

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Using the stated assumptions, we can write the charge density at any x:

$$\rho\left(x\right) = q\left[N_D - n\left(x\right)\right]$$

To relate the electron concentration to the band-banding, recall that

$$n(x) = N_C \exp\left[-\frac{E_C(x) - E_F}{kT}\right]$$

Note that in the neutral region, where there is no band-bending $(x \rightarrow -\infty)$

$$n(x \to -\infty) = N_C \exp\left[-\frac{E_C(\to -\infty) - E_F}{kT}\right] = n_{no} = N_D$$

$$n(x) = N_C \exp\left[-\frac{E_C(x) - E_C(x \to -\infty) + E_C(x \to -\infty) - E_F}{kT}\right]$$

$$= N_C \exp\left[-\frac{E_C(x) - E_C(x \to -\infty)}{kT}\right] \exp\left[-\frac{E_C(x \to -\infty) - E_F}{kT}\right]$$

$$n(x) = N_D \exp\left[-\frac{E_C(x) - E_C(x \to -\infty)}{kT}\right]$$

Define a normalized "band-bending parameter"

$$\psi_n(x) = \frac{E_C(x) - E_C(x \to -\infty)}{kT}$$
 (No units.)

Then

$$n(x) = N_D \exp\left[-\psi_n(x)\right]$$

and the charge density can be written

$$\rho\left(x\right) = N_D \left|1 - e^{-\psi_n(x)}\right|$$

These relations should make some intuitive sense – as the band bends up in an *n*-type depletion region (ψ is positive), the electron concentration decreases, leaving just the exposed dopant charge. However, if we have a situation where the band bends down (ψ is negative), then the electron concentration increases exponentially! (We call this accumulation.) We can re-write Poisson's equation using this new band-bending parameter:

$$\frac{d^2\psi_n(x)}{dx^2} = \frac{q\rho(x)}{\varepsilon_s kT} \quad -\text{the general form.}$$

Inserting the $\rho(x)$ for uniformly doped *n*-type semiconductor:

$$\frac{d^2\psi_n\left(x\right)}{dx^2} = \frac{qN_D}{\varepsilon_s kT} \left[1 - e^{-\psi(x)}\right]$$

This is the Poisson-Boltzmann equation for a uniformly doped *n*-type semiconductor. Unfortunately, this is a non-linear differential equation. Yuck.

$$E_C(x) - E_C(\text{flat}) = kT \cdot \psi_n(x)$$

review:
$$\phi(x) - \phi(\text{flat}) = \frac{E_C(x) - E_C(\text{flat})}{q} = \frac{kT}{q} \cdot \psi_n(x)$$

$$\mathcal{E} = -\frac{d\phi}{dx} = \frac{kT}{q}\frac{d\psi_n}{dx}$$

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The limit of small band-bending: the Debye length

Consider the limit of small band-bending, ($\psi << 1$). In that case:

$$e^{-\psi_n} pprox 1 - \psi_n$$

and

$$\frac{d^{2}\psi_{n}\left(x\right)}{dx^{2}} = \frac{qN_{D}}{\varepsilon_{s}kT}\psi\left(x\right)$$

This has solutions of the form:

$$\psi_n(x) \propto \exp\left(\pm \frac{x}{L_D}\right)$$

where

$$L_D = \sqrt{\frac{\varepsilon_s kT}{q^2 N_D}}$$

is the "Debye length".

The general solution

To find a general solution, we make use of the fact that the charge density depends on position only implicitly through the band-bending.

$$\frac{d^{2}\psi_{n}\left(x\right)}{dx^{2}} = \frac{q\rho\left(x\right)}{\varepsilon_{s}kT}$$

Start by multiplying both sides by $2\frac{d\psi_n(x)}{dx}$

 $2\frac{d^2\psi_n}{dx^2}\frac{d\psi_n}{dx} = \frac{2q\rho\left(\psi_n\right)}{\varepsilon_s kT}\frac{d\psi_n}{dx}$ Note the subtle shift in ρ — it is now treated as a function of ψ_n , not x.

Then we integrate the equation, with the boundary conditions that both ψ_n and $d\psi_n/dx$ go to zero as $x \rightarrow -\infty$. (i.e. There is no band-bending far from the junction and consequently no electric field, either.)

$$\left(\frac{d\psi_n}{dx}\right)^2 = \frac{2q}{\varepsilon_s kT} \int_0^{\psi_n} \rho\left(\psi'\right) d\psi'$$

But, $d\psi_n/dx$ is proportional to electric field:

$$\mathcal{E} = -\frac{d\phi}{dx} = \frac{kT}{q}\frac{d\psi_n}{dx}$$

Re-writing the P-B solution in terms of the electric field:

$$\mathcal{E}^{2}(x) = \frac{2kT}{q\varepsilon_{s}} \int_{0}^{\psi_{n}(x)} \rho(\psi') d\psi'$$

$$\mathcal{E}(x) = \pm \sqrt{\frac{2kT}{q\varepsilon_s}} \int_0^{\psi_n(x)} \rho(\psi') d\psi'$$

For the case of the uniformly doped n-type region, where

 $\rho(\psi_n) = qN_D[1 - \exp(-\psi_n]]$, the integral is easy to do.

$$\mathcal{E}(x) = \pm \sqrt{\frac{2kTN_D}{q\varepsilon_s}} \left[\psi_n(x) + e^{-\psi_n(x)} - 1\right]^{1/2}$$

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Because of the square-root, the direction of the electric field is not specified by the above equations. It is easy (using the *p*-*n* diode for instance) to show that the following rule applies: If the semiconductor extends to the right of the interface in question, the sign of \mathcal{E} is opposite that of ψ , while for a semiconductor extending to the left, \mathcal{E} and ψ have the same sign.

Strong depletion: the depletion approximation returns

In the case of strong depletion, ($\psi_n > 3$ or so) and so $\exp(-\psi_n) \approx 0$. Then

$$\mathcal{E}(x) = \pm \sqrt{\frac{2kTN_D}{q\varepsilon_s}} \left[\psi_n(x) - 1\right]^{1/2}$$

Recalling that: $\phi(x) = \frac{kT}{q}\psi_n(x)$

On the *n*-side, the maximum band-bending corresponds to the total electrostatic potential change on the n-side.

$$\phi_n = \frac{kT}{q}\psi_n \left(0\right)$$

This also corresponds to the location of the maximum electric field.

$$\mathcal{E}_{max} = \sqrt{\frac{2qN_D}{\varepsilon_s}} \left[\phi_n - \frac{kT}{q}\right]^{1/2}$$

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This is nearly identical to the result obtained using the depletion approximation. The only difference is the kT/q term. This is known as the *Gummel correction*, and it represents the gradual transition at the depletion-layer edge that was assumed to be abrupt in the depletion approximation. This is a relatively minor correction and shows us (finally) that the depletion approximation was really pretty accurate.

Then the depletion layer width is

$$w_n = \frac{\varepsilon_s \mathcal{E}_{max}}{qN_D} = \sqrt{\frac{2\varepsilon_s \left(\phi_n - \frac{kT}{q}\right)}{qN_D}}$$

including the Gummel correction.



The p-type case

Define the band-bending in a p-type region.

$$\psi_{p}(x) = -\frac{E_{V}(x) - E_{V}(x \to -\infty)}{kT}$$

In the *p*-type case, positive ψ_p corresponds to *downward* band bending. This is consistent with the n-type case in that positive ψ_p represents *depletion*. Given that, all of the equations for the *p*-type case will have the same form as the *n*-type case.

$$\rho(x) = -qN_A + p(x) = -qN_A \left[1 - e^{-\psi_p(x)}\right]$$