

## **4. The p-n junction**

### **4.1 Electrostatic solution of the p-n homojunction**

#### 4.1.1. Approximate solution using the full depletion approximation

##### a) Abrupt p-n junction

An easy way to derive the depletion layer widths in a p-n diode is to treat it as a combination of two Schottky diodes, one with an n-type semiconductor and an other with a p-type semiconductor. The metal between the two semiconductors is assumed to be infinitely thin. We can then express the potential difference between the two semiconductors as:

$$\phi_n + \phi_p = \phi_i - V_a = \frac{1}{q} [E_i - E_{fp} - (E_i - E_{fn})] - V_a = V_t \ln \left[ \frac{N_d N_a}{n_i^2} \right] - V_a \quad [4.1.1]$$

where  $\phi_n$  and  $\phi_p$  are the potentials across the n respectively the p-type material. These potentials can be expressed as a function of the depletion layer widths just like for the Schottky barrier diode, assuming the full depletion approximation.

$$\phi_n = \frac{q N_d x_n^2}{2 \epsilon_s} \text{ and } \phi_p = \frac{q N_a x_p}{2 \epsilon_s} \quad [4.1.2]$$

To solve [4.1.1] and [4.1.2] we need an additional relation between  $x_n$  and  $x_p$ , which is obtained by observing that the positive charge in the n-type semiconductor equals the negative charge in the p-type semiconductor, again assuming full depletion.

$$q N_a x_p = q N_d x_n \quad [4.1.3]$$

Solving for  $x_n$  and  $x_d$  then yields:

$$x_d = x_n + x_p = \sqrt{\frac{2 \epsilon_s}{q} \left( \frac{1}{N_a} + \frac{1}{N_d} \right) (\phi_i - V_a)} \quad [4.1.4]$$

##### b) Linearly graded junction

For a linearly graded junction the impurity concentration is given by:

$$N_d - N_a = ax \quad [4.1.5]$$

where  $a$  is a proportionality constant with units  $[\text{cm}^{-4}]$ . Equations [4.1.1], [4.1.2] and [4.1.3] then take the following form:

$$\phi_n + \phi_p = \phi_i - V_a = \frac{1}{q} [E_i - E_{fp} - (E_i - E_{fn})] - V_a = 2 V_t \ln\left[\frac{ax_n}{n_i}\right] - V_a \quad [4.1.6]$$

$$\phi_n = \frac{q a x_n^3}{3\epsilon_s} \text{ and } \phi_p = \frac{q a x_p^3}{3\epsilon_s} \quad [4.1.7]$$

$$q a x_p^2 = q a x_n^2 \quad [4.1.8]$$

Both depletion layer widths are the same and are obtained by solving the following transcendental equation:

$$x_n = \left[ \frac{3\epsilon_s}{2 q a} (2 V_t \ln\left[\frac{ax_n}{n_i}\right] - V_a) \right]^{1/3} \quad [4.1.9]$$

### c) Abrupt p-i-n junction

For a p-i-n junction the above expressions take the following modified form:

$$\phi_n + \phi_p + \phi_u = \phi_i - V_a \quad [4.1.10]$$

$$\phi_n = \frac{q N_d x_n^2}{2\epsilon_s}, \phi_p = \frac{q N_a x_p^2}{2\epsilon_s} \text{ and } \phi_u = \frac{q N_a x_p d}{\epsilon_s} \quad [4.1.11]$$

$$q N_a x_p = q N_d x_n \quad [4.1.12]$$

Where  $\phi_u$  is the potential across the middle undoped region of the diode, which has a thickness  $d$ . Equations [4.2.11] through [4.2.13] can be solved for  $x_n$  yielding:

$$x_n = \frac{\sqrt{d^2 + \frac{2\epsilon_s(\phi_i - V_a)(N_a + N_d)}{q N_d N_a}} - d}{\left(1 + \frac{N_d}{N_a}\right)} \quad [4.1.14]$$

From  $x_n$  and  $x_p$ , all other parameters of the p-i-n junction can be obtained. The potential throughout the structure is given by:

$$\phi(x) = -\frac{qN_d}{2\epsilon_s}(x + x_n)^2 \quad -x_n < x < 0 \quad [4.1.15]$$

$$\phi(x) = -\phi_n - \frac{qN_d x_n}{\epsilon_s} x \quad 0 < x < d \quad [4.1.16]$$

$$\phi(x) = -(\phi_i - V_a) + \frac{qN_a}{2\epsilon_s}(x - d - x_p)^2 \quad d < x < d + x_p \quad [4.1.17]$$

where the potential at  $x = -x_n$  was assumed to be zero.

#### d) Capacitance of a p-i-n junction diode

The capacitance of a p-i-n diode can be obtained from the series connection of the capacitances of each region, simply by adding both depletion layer widths and the width of the undoped region:

$$C_j = \frac{\epsilon_s}{x_n + x_p + d} = \frac{\epsilon_s}{x_d} \quad [4.1.18]$$

#### 4.1.2 Exact solution for the p-n diode

Applying Gauss's law one finds that the total charge in the n-type depletion region equals minus the charge in the p-type depletion region:

$$Q_n = \epsilon_s |\mathcal{E}(x=0)| = -Q_p \quad [4.1.19]$$

Poisson's equation can be solved separately in the n and p-type region as was done in section 3.1.1 yielding an expression for  $\mathcal{E}(x=0)$  which is almost identical to equation [3.1.4]:

$$|\mathcal{E}(x=0)| = \frac{V_t}{L_{Dn}} \sqrt{2 \left( \exp\left(\frac{\phi_n}{V_t}\right) - \frac{\phi_n}{V_t} - 1 \right)} = \frac{V_t}{L_{Dp}} \sqrt{2 \left( \exp\left(\frac{\phi_p}{V_t}\right) - \frac{\phi_p}{V_t} - 1 \right)} \quad [4.1.20]$$

where  $\phi_n$  and  $\phi_p$  are assumed negative if the semiconductor is depleted. Their relation to the applied voltage is given by:

$$\phi_n + \phi_p = V_a - \phi_i \quad [4.1.21]$$

Solving the transcendental equations one finds  $\phi_n$  and  $\phi_p$  as a function of the applied voltage. In the special case of a symmetric doping profile, or  $N_d = N_a$  these equations can easily be solved yielding

$$\phi_n = \phi_p = \frac{V_a - \phi_i}{2} \quad [4.1.22]$$

The depletion layer widths also equal each other and are given by

$$x_n = x_p = \left| \frac{Q_n}{qN_d} \right| = \left| \frac{Q_p}{qN_a} \right| = \left| \frac{\epsilon_s \mathcal{E}(x=0)}{qN_d} \right| \quad [4.1.23]$$

Using the above expression for the electric field at the origin we find:

$$x_n = x_p = L_D \sqrt{2 \exp\left(\frac{V_a - \phi_i}{2V_t}\right) + \frac{\phi_i - V_a - V_t}{V_t}} \quad [4.1.24]$$

where  $L_D$  is the extrinsic Debye length. The relative error of the depletion layer width as obtained using the full depletion approximation equals

$$\frac{\Delta x_n}{x_n} = \frac{\Delta x_p}{x_p} = \frac{1 - \sqrt{1 - \frac{V_t}{\phi_i - V_a} + \frac{V_t}{2(\phi_i - V_a)} \exp\left(\frac{V_a - \phi_i}{2V_t}\right)}}{\sqrt{1 - \frac{V_t}{\phi_i - V_a} + \frac{V_t}{2(\phi_i - V_a)} \exp\left(\frac{V_a - \phi_i}{2V_t}\right)}} \quad [4.1.25]$$

for  $\frac{\phi_i - V_a}{V_t} = 1, 2, 5, 10, 20$  and  $40$  one finds the relative error to be 45, 23, 10, 5.1, 2.5 and 1.26%.

## 4.2 Currents in a p-n homojunction

### 4.2.1 Ideal diode characteristics

Currents in a p-n junction could in principle be calculated by combining all the semiconductor equations and solving with the appropriate boundary conditions. This process is not only very tedious, it also requires numerical techniques since no closed-form analytic solution can be obtained. Therefore it is more instructive to make some simplifying assumptions which do enable an analytical solution. First of all we will assume that the electron and hole quasi Fermi levels are constant throughout the depletion region and that they equal the Fermi level in the n-type respectively p-type region. This assumption implies that no current is flowing across the junction which is clearly inaccurate since we plan to calculate the currents through the junction. But compared to the large drift and diffusion currents which flow under thermal equilibrium, the net current flowing is small, so that to first order the quasi Fermi level can be considered constant. This enables to determine the minority carrier concentration at the edges of the depletion region as a function of the potential across the region.

$$n_p(x = x_p) = N_d e^{-(\phi_i - V_a)/V_t} = \frac{n_i^2}{N_a} e^{V_a/V_t} \quad [4.1.19]$$

$$p_n(x = -x_n) = N_a e^{-(\phi_i - V_a)/V_t} = \frac{n_i^2}{N_d} e^{V_a/V_t} \quad [4.1.20]$$

To calculate the current one has to recognize that the recombination processes affect the total current: suppose no recombination would take place, the minority carrier concentration in the quasi-neutral region would be constant and no current would flow. Recombination of carriers causes a gradient of the carrier density, yielding a diffusion current. We will therefore set up the diffusion equations in the quasi-neutral regions under steady-state conditions:

$$0 = D_n \frac{d^2 n}{dx^2} - \frac{n_p - n_{p0}}{\tau_n} \quad , x > x_p \quad [4.1.21]$$

$$0 = D_p \frac{d^2 p}{dx^2} - \frac{p_n - p_{n0}}{\tau_p} \quad , x < -x_n \quad [4.1.22]$$

Solutions to the diffusion equations for different types of boundary conditions are derived below.

### a) "Long" diode case

Equations [4.1.13] and [4.1.14] can be solved using the carrier concentration at the edge of the depletion region as one boundary condition and the requirement to have a finite solution at  $x = \infty$  as the other boundary condition. This set of boundary conditions is generally related to a "long" diode, where the width of the quasi-neutral region is much longer than the diffusion length. The diffusion length is defined as  $L_n = \sqrt{D_n \tau_n}$  for the electrons in the p-type region and  $L_p = \sqrt{D_p \tau_p}$  for the holes in the n-type region. The solutions to the diffusion equations are:

$$n_p(x) = n_{p0} + n_{p0} (e^{V_a/V_t} - 1) e^{-(x-x_p)/L_n}, \quad x > x_p \quad [4.1.23]$$

$$p_n(x) = p_{n0} + p_{n0} (e^{V_a/V_t} - 1) e^{(x+x_n)/L_p}, \quad x < -x_n \quad [4.1.24]$$

and the corresponding diffusion currents are:

$$J_n(x) = q D_n \frac{dn}{dx} = -q \frac{D_n n_{p0}}{L_n} (e^{V_a/V_t} - 1) e^{-(x-x_p)/L_n}, \quad x > x_p \quad [4.1.25]$$

$$J_p(x) = -q D_p \frac{dp}{dx} = -q \frac{D_p p_{n0}}{L_p} (e^{V_a/V_t} - 1) e^{(x+x_n)/L_p}, \quad x < -x_n \quad [4.1.26]$$

The total current is the sum of the electron and hole current at any point within the junction. Provided one can ignore the change of either current across the depletion region one can express the total current as the sum of the electron current at  $x = x_p$  and the hole current at  $x = -x_n$ , yielding:

$$J_t = -J_n(x = x_p) - J_p(x = x_n) = q \left( \frac{D_n n_{p0}}{L_n} + \frac{D_p p_{n0}}{L_p} \right) (e^{V_a/V_t} - 1) \quad [4.1.27]$$

where the minus sign was added so that a positive current is associated with a positive applied voltage.

### b) "Short" diode case

For a "short" diode one generally assumes the excess carrier density to be zero at a distance  $W'$  from the edge of the depletion region, where  $W'$  is much smaller than the diffusion length. The boundary condition corresponds to an infinite recombination rate at that point which is often assumed to be valid for an ohmic contact. Solving the diffusion equations with this modified set of boundary conditions yields:

$$J_t = q \left( \frac{D_n n_{p0}}{W_p'} + \frac{D_p p_{n0}}{W_n'} \right) (e^{V_a/V_t} - 1) \quad [4.1.28]$$

where  $W_n'$  and  $W_p'$  are the widths of the quasi-neutral regions in the n-type respectively p-type semiconductor.

### c) General cases

The diffusion equations can also be solved for a finite width of the quasi-neutral region with either an infinite or a constant recombination rate at the interface between semiconductor and metal contact. For an ***infinite recombination rate*** one finds the electron concentration in the p-type region to be:

$$n_p(x) = n_{p0} + n_{p0} (e^{V_a/V_t} - 1) \{ \cosh[(x-x_p)/L_n] - \coth[W_p'/L_n] \sinh[(x-x_p)/L_n] \} \quad [4.1.29a]$$

and the corresponding current density evaluated at  $x = x_p$  is:

$$J_n = - \frac{q D_n n_{p0}}{L_n} (e^{V_a/V_t} - 1) \coth[W_p'/L_n] \quad [4.1.29b]$$

Whereas for a ***constant recombination rate***,  $s$ , at the surface one obtains:

$$n_p(x) = n_{p0} + n_{p0} (e^{V_a/V_t} - 1) \{ \cosh[(x-x_p)/L_n] - \frac{1 + D_n/sL_n \tanh[W_p'/L_n]}{D_n/sL_n + \tanh[W_p'/L_n]} \sinh[(x-x_p)/L_n] \} \quad [4.1.30a]$$

with  $s$  being the surface recombination velocity. The current density becomes:

$$J_n = - \frac{q D_n n_{p0}}{L_n} (e^{V_a/V_t} - 1) \left\{ \frac{1 + D_n/sL_n \tanh[W_p'/L_n]}{D_n/sL_n + \tanh[W_p'/L_n]} \right\} \quad [4.1.30b]$$

## 4.2.2 Recombination in the depletion region

Ignoring the change of the current across the depletion region requires more justification: The change in current is caused by recombination of electrons and holes through trap-assisted (SHR) or band-to-band recombination within the depletion region. It will be shown below that the recombination rate is actually higher in the depletion region compared to the recombination rate in the quasi-neutral regions. Therefore the recombination within the depletion region can only be ignored if the depletion region with

is much smaller than the diffusion length of the minority carriers in the quasi-neutral region or the actual width of the quasi-neutral region, whichever is shorter.

#### a) Band-to-band recombination

In the case of band-to-band recombination the recombination rate is constant throughout the depletion region where it reaches its maximum value and tapers off into both quasi-neutral regions. The total change in current due to band-to-band recombination within the depletion region with width  $x_d$  is given by:

$$-\Delta J_n = \Delta J_p = q U_{b-b} x_d = q x_d (np - n_i^2) v_{th} \sigma = q x_d n_i^2 (e^{V_a/V_t} - 1) v_{th} \sigma \quad [4.1.31]$$

#### b) Trap-assisted recombination

If the recombination is trap-assisted the expression is more complex, namely:

$$-\Delta J_n = \Delta J_p = q \int_{-x_n}^{x_p} U_{SHR} dx = q \int_{-x_p}^{x_n} \frac{(pn - n_i^2)}{[n + p + 2 n_i \cosh((E_i - E_t)/kT)] \tau_0} dx \quad [4.1.32]$$

Unlike for band-to-band recombination where the recombination rate is constant throughout the depletion region, the trap-assisted recombination is the highest for  $n=p=n_i e^{V_a/2V_t}$ , namely:

$$U_{SHRmax} = \frac{n_i (e^{V_a/2V_t} - 1)}{2 \tau_0} \quad [4.1.33]$$

where we assumed the energy of the recombination center to equal the intrinsic Fermi level, or  $E_i = E_t$ . We therefore approximate the integral by multiplying this maximum recombination rate with an effective recombination width  $x'$  which is smaller than the total depletion width yielding:

$$\Delta J_n = -\Delta J_p = q U_{SHRmax} x' = q x' n_i (e^{V_a/2V_t} - 1)/2\tau_0 \quad [4.1.34]$$

where  $\tau_0^{-1} = N_t \sigma v_{th}$  is the carrier lifetime and the effective recombination width  $x'$  is defined as

$$x' = \int_{-x_p}^{x_n} U_{SHR} dx / U_{SHRmax} < x_d \quad [4.1.35]$$



### c) Total diode current

Using these corrections the total current is given by:

$$J_t = q \left( \frac{D_n n_{p0}}{L_n} + \frac{D_p p_{n0}}{L_p} + x_d n_i^2 v_{th} \sigma \right) (e^{V_a/V_t} - 1) + \frac{q x' n_i}{2\tau_0} (e^{V_a/2V_t} - 1) \quad [4.1.36]$$

From this analysis we conclude that the recombination in the depletion region can only be ignored if the width of the depletion region is much smaller than the diffusion length of the minority carriers in the quasi-neutral regions, or the actual width of the quasi-neutral region, whichever is shortest.

### 4.2.3 High injection

High injection of carriers<sup>1</sup> causes to violate one of the approximations made in the derivation of the ideal diode characteristics, namely that the majority carrier density equals the thermal equilibrium value. Excess carriers will dominate the electron and hole concentration and can be expressed in the following way:

$$n_p p_p = n_i^2 e^{V_a/V_t} \cong n_p (p_{p0} + n_p) \quad [4.1.37]$$

$$n_n p_n = n_i^2 e^{V_a/V_t} \cong p_n (n_{n0} + p_n) \quad [4.1.38]$$

where all carrier densities with subscript n are taken at  $x = x_n$  and those with subscript p at  $x = -x_p$ . Solving the resulting quadratic equation yields:

$$n_p = \frac{N_a}{2} \left( \sqrt{1 + \frac{4 n_i^2 e^{V_a/V_t}}{N_a^2}} - 1 \right) \cong n_i e^{V_a/2V_t}$$

$$p_n = \frac{N_d}{2} \left( \sqrt{1 + \frac{4 n_i^2 e^{V_a/V_t}}{N_d^2}} - 1 \right) \cong n_i e^{V_a/2V_t} \quad [4.1.39]$$

where the second terms are approximations for large  $V_a$ . From these expressions one can calculate the minority carrier diffusion current assuming a "long" diode. We also ignore carrier recombination in the depletion region.

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<sup>1</sup>A more complete derivation can be found in R.S. Muller and T.I. Kamins, "Device Electronics for Integrated Circuits", Wiley and sons, second edition p. 323-324.

$$J_n + J_p = q \left( \frac{D_n}{L_n} + \frac{D_p}{L_p} \right) n_i e^{V_a/2V_t} \quad [4.1.40]$$

This means that high injection in a p-n diode will reduce the slope on the current-voltage characteristic on a semi-logarithmic scale to 119mV/decade.

High injection also causes a voltage drop across the quasi-neutral region. This voltage can be calculated from the carrier densities. Let's assume that high injection only occurs in the (lower doped) p-type region. The hole density at the edge of the depletion region ( $x = x_p$ ) equals:

$$p_p(x = x_p) = N_a e^{V_1/V_t} = N_a + n_p(x = x_p) = N_a + n_{p0} e^{(V_a - V_1)/V_t} \quad [4.1.40]$$

where  $V_1$  is the voltage drop across the p-type quasi-neutral region. This equation can then be solved for  $V_1$  yielding

$$V_1 = V_t \ln \left[ \left( \sqrt{1 + \frac{4 n_i^2 e^{V_a/V_t}}{N_a^2}} - 1 \right) / 2 \right] \quad [4.1.40]$$

#### 4.2.4 Resistive drop

At high currents one should incorporate the potential drop across the quasi-neutral regions in the current-voltage characteristics. The total resistance of a diode with area  $A$  can be expressed as:

$$R_d = \frac{W_n'}{A q \mu_n N_d} + \frac{W_p'}{A q \mu_p N_a} \quad [4.1.41]$$

and the total voltage  $V_a^*$  is given by:

$$V_a^* = V_a + R_d (J_n + J_p) A \quad [4.1.42]$$

Where the relation between the current density and the internal voltage  $V_a$  (equation [4.1.28]) remains unchanged.

### 4.3 Quasi-Fermi levels in a p-n diode

Quasi-fermi levels in a p-n junction can be related to the electron and hole concentration under non-equilibrium conditions through the following equations:

$$n = n_i e^{(F_n - E_i)/kT} = N_C e^{(F_n - E_C)/kT} \quad [4.3.1]$$

$$p = n_i e^{(E_i - F_p)/kT} = N_v e^{(E_v - F_p)/kT} \quad [4.3.2]$$

These equations are a generalization of the expressions under thermal equilibrium where two quasi-Fermi levels replace the equilibrium fermi level. Under non-equilibrium conditions we can postulate that the quasi-Fermi level is constant provided no recombination of carriers occurs. This way we can determine the electron (hole) density at the edge of the depletion layer in the p-type (n-type) semiconductor:

$$n(x_p) = \frac{n_i^2}{N_a} e^{V_a/V_t} \quad [4.3.3]$$

$$p(-x_n) = \frac{n_i^2}{N_d} e^{V_a/V_t} \quad [4.3.4]$$

More physical insight into the meaning of a constant quasi-fermi level can be obtained by relating it to the current density:

$$J_n = \mu_n n \frac{dF_n}{dx} = 0 = q \mu_n n \mathcal{E} + q D_n \frac{dn}{dx} \quad [4.3.5]$$

which can be rewritten as:

$$q \mathcal{E} = -q V_t \frac{d(\ln n)}{dx} \quad [4.3.6]$$

Or postulating a constant quasi-Fermi level implies that the electrostatic force equals the diffusion force.

## 4.4 The heterojunction p-n diode

The heterojunction p-n diode is in principle very similar to a homojunction. The main problem that needs to be tackled is the effect of the bandgap discontinuities and the different material parameters which make the actual calculations more complex even though the p-n diode concepts need almost no changing. An excellent detailed treatment can be found in Wolfe et al.<sup>2</sup>.

### 4.4.1 Band diagram of a heterojunction p-n diode under Flatband conditions

The flatband energy band diagram of a heterojunction p-n diode is shown in the figure below. As a convention we will assume  $\Delta E_c$  to be positive if  $E_{cn} > E_{cp}$  and  $\Delta E_v$  to be positive if  $E_{vn} < E_{vp}$ .

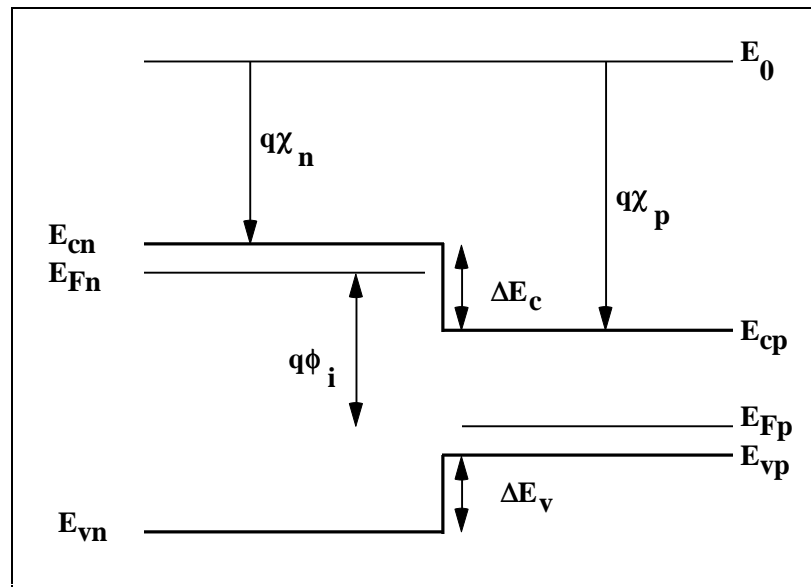


Fig.4.1 Flat-band energy band diagram of a p-n heterojunction

### 4.4.2 Calculation of the contact potential (built-in voltage)

The built-in potential is defined as the difference between the Fermi levels in both the n-type and the p-type semiconductor. From the energy diagram we find:

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<sup>2</sup>Wolfe, C. Holonyak, N. Stillman, G. Physical properties of semiconductors, Prentice Hall, Chapter 9.

$$q \phi_i = E_{Fn} - E_{Fp} = E_{Fn} - E_{cn} + E_{cn} - E_{cp} + E_{cp} - E_{Fp} \quad [4.4.1]$$

which can be expressed as a function of the electron concentrations and the effective densities of states in the conduction band:

$$q \phi_i = \Delta E_c + kT \ln \left( \frac{n_{n0} N_{cp}}{n_{p0} N_{cn}} \right) \quad [4.4.2]$$

The built-in voltage can also be related to the hole concentrations and the effective density of states of the valence band:

$$q \phi_i = -\Delta E_v + kT \ln \left( \frac{p_{p0} N_{vn}}{p_{n0} N_{vp}} \right) \quad [4.4.3]$$

Combining both expressions yields the built-in voltage independent of the free carrier concentrations:

$$q \phi_i = \frac{\Delta E_c - \Delta E_v}{2} + kT \ln \left( \frac{N_d N_a}{n_{in} n_{ip}} \right) + \frac{kT}{2} \ln \left( \frac{N_{vn} N_{cp}}{N_{cn} N_{vp}} \right) \quad [4.4.4]$$

where  $n_{in}$  and  $n_{ip}$  are the intrinsic carrier concentrations of the n and p-type region, respectively.  $\Delta E_c$  and  $\Delta E_v$  are positive quantities if the bandgap of the n-type region is smaller than that of the p-type region. The above expression reduces to that of the built-in junction of a homojunction if the material parameters in the n-type region equal those in the p-type region. If the effective densities of states are the same the expression reduces to:

$$q \phi_i = \frac{\Delta E_c - \Delta E_v}{2} + kT \ln \left( \frac{N_d N_a}{n_{in} n_{ip}} \right) \quad [4.4.5]$$

### 4.4.3 Electrostatics

#### a) Abrupt p-n junction

For the calculation of the charge, field and potential distribution in an abrupt p-n junction we follow the same approach as for the homojunction. First of all we use the full depletion approximation and solve Poisson's equation. The expressions derived in section 4.1.1 then still apply.

$$\phi_n + \phi_p = \phi_i - V_a \quad [4.4.6]$$

$$\phi_n = \frac{q N_d x_n^2}{2\epsilon_{sn}} \text{ and } \phi_p = \frac{q N_a x_p^2}{2\epsilon_{sp}} \quad [4.4.7]$$

$$q N_a x_p = q N_d x_n \quad [4.4.8]$$

The main differences are the different expression for the built-in voltage and the discontinuities in the field distribution (because of the different dielectric constants of the two regions) and in the energy band diagram. However the expressions for  $x_n$  and  $x_p$  for a homojunction can still be used if one replaces  $N_a$  by  $N_a \frac{\epsilon_{sp}}{\epsilon_s}$ ,  $N_d$  by  $N_d \frac{\epsilon_{sn}}{\epsilon_s}$ ,  $x_p$  by  $x_p \frac{\epsilon_s}{\epsilon_{sp}}$ , and  $x_n$  by  $x_n \frac{\epsilon_s}{\epsilon_{sn}}$ . Adding  $x_n$  and  $x_p$  yields the total depletion layer width  $x_d$ :

$$x_d = x_n + x_p = \sqrt{\frac{2\epsilon_{sn}\epsilon_{sp}}{q} \frac{(N_a + N_d)^2 (\phi_i - V_a)}{N_a N_d (N_a \epsilon_{sp} + N_d \epsilon_{sn})}} \quad [4.4.9]$$

The capacitance per unit area can be obtained from the series connection of the capacitance of each layer:

$$C_j = \frac{1}{x_n/\epsilon_{sn} + x_p/\epsilon_{sp}} = \sqrt{\frac{q\epsilon_{sn}\epsilon_{sp}}{2} \frac{N_a N_d}{(N_a \epsilon_{sp} + N_d \epsilon_{sn}) (\phi_i - V_a)}} \quad [4.4.10]$$

#### b) Abrupt P-i-N junction

For a P-i-N junction the above expressions take the following modified form:

$$\phi_n + \phi_p + \phi_u = \phi_i - V_a \quad [4.4.11]$$

$$\phi_n = \frac{q N_d x_n^2}{2\epsilon_{sn}}, \phi_p = \frac{q N_a x_p^2}{2\epsilon_{sp}} \text{ and } \phi_u = \frac{q N_a x_p d}{\epsilon_{su}} \quad [4.4.12]$$

$$q N_a x_p = q N_d x_n \quad [4.4.13]$$

Where  $\phi_u$  is the potential across the middle undoped region of the diode, having a thickness  $d$ . The depletion layer width and the capacitance are given by:

$$x_d = x_n + x_p + d \quad [4.4.14]$$

$$C_j = \frac{1}{x_n/\epsilon_{sn} + x_p/\epsilon_{sp} + d/\epsilon_{su}} \quad [4.4.15]$$

Equations [4.2.11] through [4.2.13] can be solved for  $x_n$  yielding:

$$x_n = \frac{\sqrt{\left[\frac{d \epsilon_{sn}}{\epsilon_{su}}\right]^2 + \frac{2\epsilon_{sn}(\phi_i - V_a)}{qN_d} \left(1 + \frac{N_d}{N_a}\right)} - \frac{d \epsilon_{sn}}{\epsilon_{su}}}{\left(1 + \frac{N_d}{N_a}\right)} \quad [4.4.16]$$

A solution for  $x_p$  can be obtained from [4.2.16] by replacing  $N_d$  by  $N_a$ ,  $N_a$  by  $N_d$ ,  $\epsilon_{sn}$  by  $\epsilon_{sp}$ , and  $\epsilon_{sp}$  by  $\epsilon_{sn}$ . Once  $x_n$  and  $x_p$  are determined all other parameters of the P-i-N junction can be obtained. The potential throughout the structure is given by:

$$\phi(x) = -\frac{qN_d}{2\epsilon_{sn}}(x+x_n)^2 \quad -x_n < x < 0 \quad [4.4.17]$$

$$\phi(x) = -\phi_n - \frac{qN_d x_n}{\epsilon_{su}} x \quad 0 < x < d \quad [4.4.18]$$

$$\phi(x) = -(\phi_i - V_a) + \frac{qN_a}{2\epsilon_{sp}}(x-d-x_p)^2 \quad d < x < d + x_p \quad [4.4.19]$$

where the potential at  $x=-x_n$  was assumed to be zero.

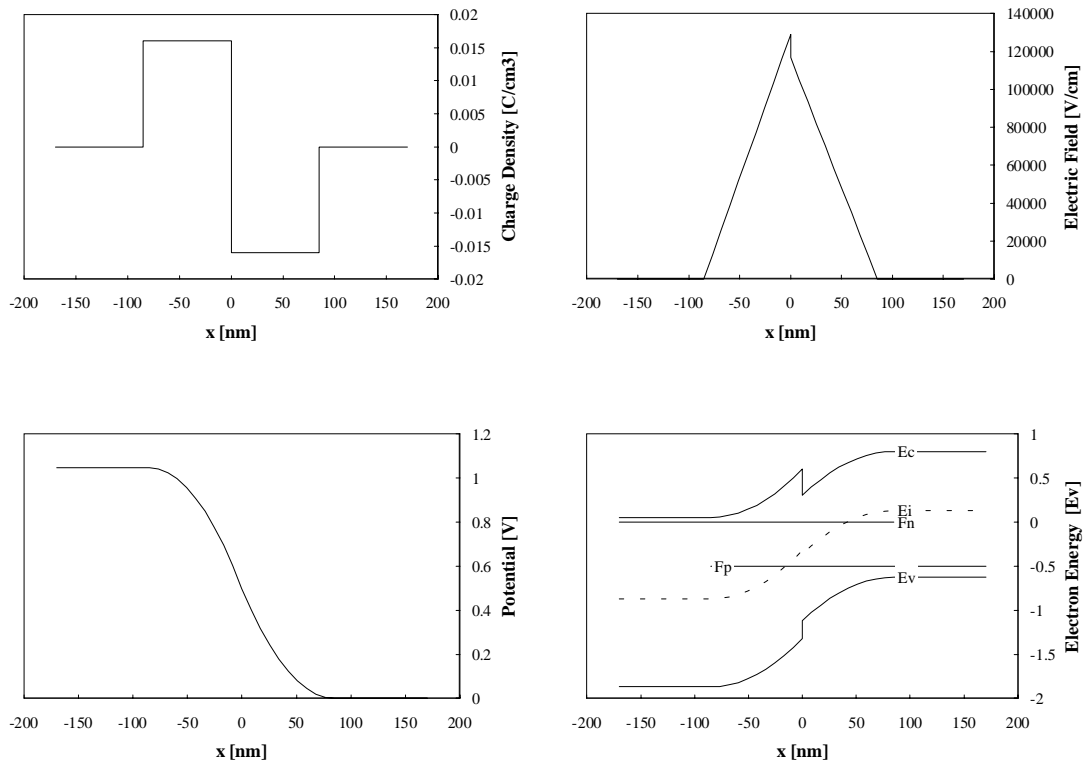


Fig.4.2 Charge distribution, electric field, potential and energy band diagram of an AlGaAs/GaAs p-n heterojunction with  $V_a = 0.5V$ ,  $x = 0.4$  on the left and  $x = 0$  on the right.  $N_d = N_a = 10^{17}cm^{-3}$

The above derivation ignores the fact that, because of the energy band discontinuities, the carrier densities in the intrinsic region could be substantially larger than in the depletion regions in the n- and p-type semiconductor. Large amounts of free carriers imply that the full depletion approximation is not valid and that the derivation has to be repeated while including a possible charge in the intrinsic region.

#### c) A P-M-N junction with interface charges

Real P-i-N junctions often differ from their ideal model which was described in section b). The intrinsic region could be lightly doped, while a fixed interface charge could be present between the individual layers. Assume the middle layer to have a doping concentration  $N_m = N_{dm} - N_{am}$  and a dielectric constant  $\epsilon_{sm}$ . A charge  $Q_1$  is assumed between the N and M layer, and a charge  $Q_2$  between the M and P layer. Equations [4.2.11] through [4.2.13] then take the following form:

$$\phi_n + \phi_p + \phi_m = \phi_i - V_a \quad [4.4.20]$$

$$\phi_n = \frac{qN_dx_n^2}{2\epsilon_{sn}}, \phi_p = \frac{qN_ax_p^2}{2\epsilon_{sp}} \text{ and } \phi_m = (qN_ax_p + Q_1) \frac{d}{\epsilon_{sm}} + \frac{qN_md^2}{2\epsilon_{sm}} \quad [4.4.21]$$

$$qN_dx_n + Q_1 + Q_2 + qN_md = qN_ax_p \quad [4.4.22]$$

These equations can be solved for  $x_n$  and  $x_p$  yielding a general solution for this structure. Again it should be noted that this solution is only valid if the middle region is indeed fully depleted.

Solving the above equation allows to draw the charge density, the electric field distribution, the potential and the energy band diagram.



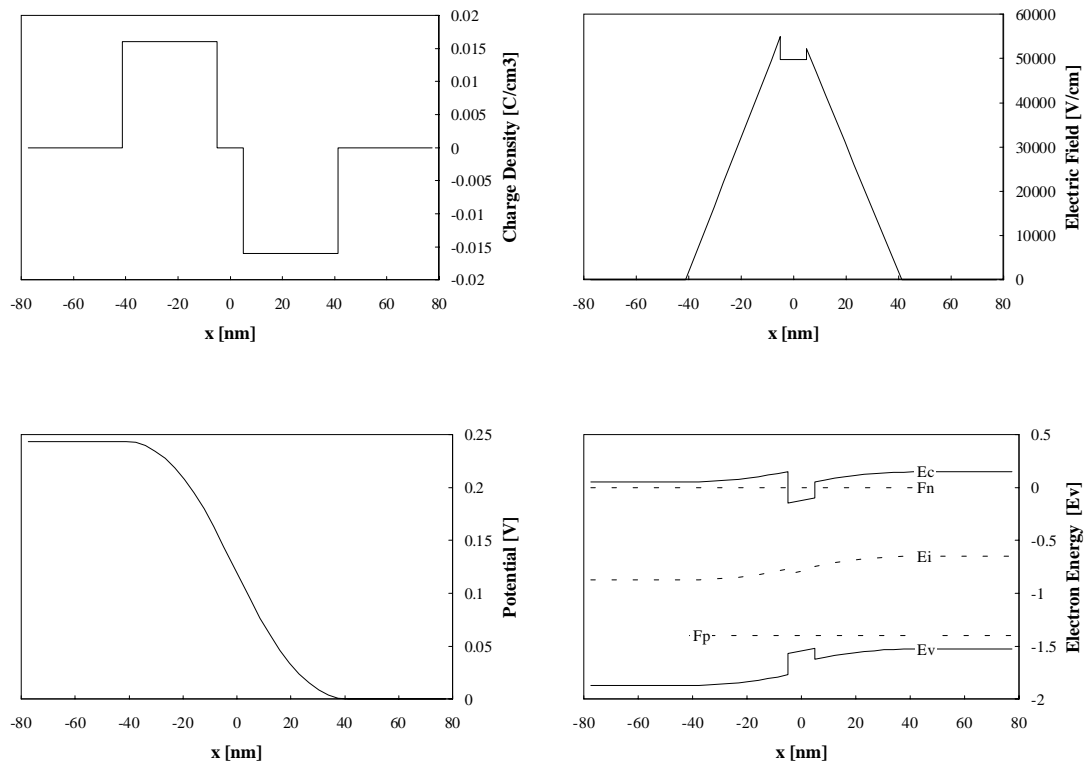


Fig.4.3 Charge distribution, electric field, potential and energy band diagram of an AlGaAs/GaAs p-i-n heterojunction with  $V_a = 1.4$  V,  $x = 0.4$  on the left,  $x = 0$  in the middle and  $x = 0.2$  on the right.  $d = 10$  nm and  $N_d = N_a = 10^{17} \text{cm}^{-3}$

#### d) Quantum well in a p-n junction

Consider a p-n junction with a quantum well located between the n and p region as shown in the figure below.

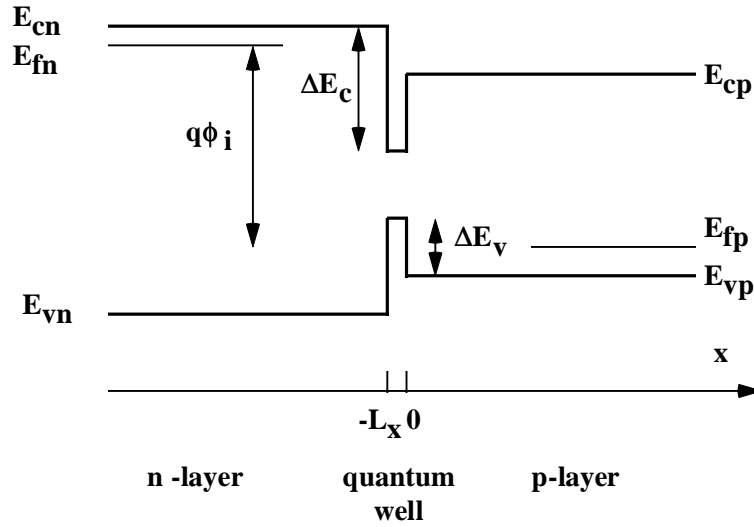


Fig.4.4 Flat-band energy band diagram of a p-n heterojunction with a quantum well at the interface.

Under forward bias charge could accumulate within the quantum well. In this section we will outline the procedure to solve this structure. The actual solution can only be obtained by solving a transcendental equation. Approximations will be made to obtain useful analytic expressions.

The potentials within the structure can be related to the applied voltage by:

$$\phi_n + \phi_{qw} + \phi_p = \phi_i - V_a \quad [4.4.20]$$

where the potentials across the p and n region are obtained using the full depletion approximation:

$$\phi_n = \frac{qN_d x_n^2}{2\epsilon_{sn}}, \text{ and } \phi_p = \frac{qN_a x_p^2}{2\epsilon_{sp}} \quad [4.4.21]$$

The potential across the quantum well is to first order given by:

$$\phi_{qw} = \frac{qN_d x_n L_x}{\epsilon_{sqw}} + \frac{q(P-N)L_x}{2\epsilon_{sqw}} \quad [4.4.22]$$

where P and N are the hole respectively electron densities per unit area in the quantum well. This equation assumes that the charge in the quantum well  $Q=q(P-N)$  is located in the middle of the well. Applying Gauss's law to the diode yields the following balance between the charges:

$$qN_d x_n - qN = -qP + qN_a x_p \quad [4.4.23]$$

where the electron and hole densities can be expressed as a function of the effective densities of states in the quantum well:

$$N = N_{cqw} \sum_{\ell=1}^{\infty} \ln[1 + e^{\Delta E_{\ell n}/kT}] \quad [4.4.24]$$

$$P = N_{vqw} \sum_{\ell=1}^{\infty} \ln[1 + e^{\Delta E_{\ell p}/kT}] \quad [4.4.25]$$

with  $\Delta E_{\ell n}$  and  $\Delta E_{\ell p}$  given by:

$$\Delta E_{\ell n} = \Delta E_c - q\phi_n - kT \ln \frac{N_{cn}}{N_d} - E_{\ell n} \quad [4.4.26]$$

$$\Delta E_{\ell p} = \Delta E_v - q\phi_p - kT \ln \frac{N_{vp}}{N_a} - E_{\ell p} \quad [4.4.27]$$

where  $E_{\ell n}$  and  $E_{\ell p}$  are the  $\ell$ th energies of the electrons respectively holes relative to the conduction respectively valence band edge. These nine equations can be used to solve for the nine unknowns by applying numerical methods. A quick solution can be obtained for a symmetric diode, for which all the parameters (including material parameters) of the n and p region are the same. For this diode  $N$  equals  $P$  because of the symmetry. Also  $x_n$  equals  $x_p$  and  $\phi_n$  equals  $\phi_p$ . Assuming that only one energy level namely the  $\ell=1$  level is populated in the quantum well one finds:

$$N = P = N_{cqw} \ln[1 + \exp((qV_a/2 - E_{1n} - E_g/2)/kT)] \quad [4.4.28]$$

where  $E_g$  is the bandgap of the quantum well material.

Numeric simulation for the general case reveal that, especially under large forward bias conditions, the electron and hole density in the quantum well are the same to within a few percent. An energy band diagram calculated using the above equations is shown in the figure below:

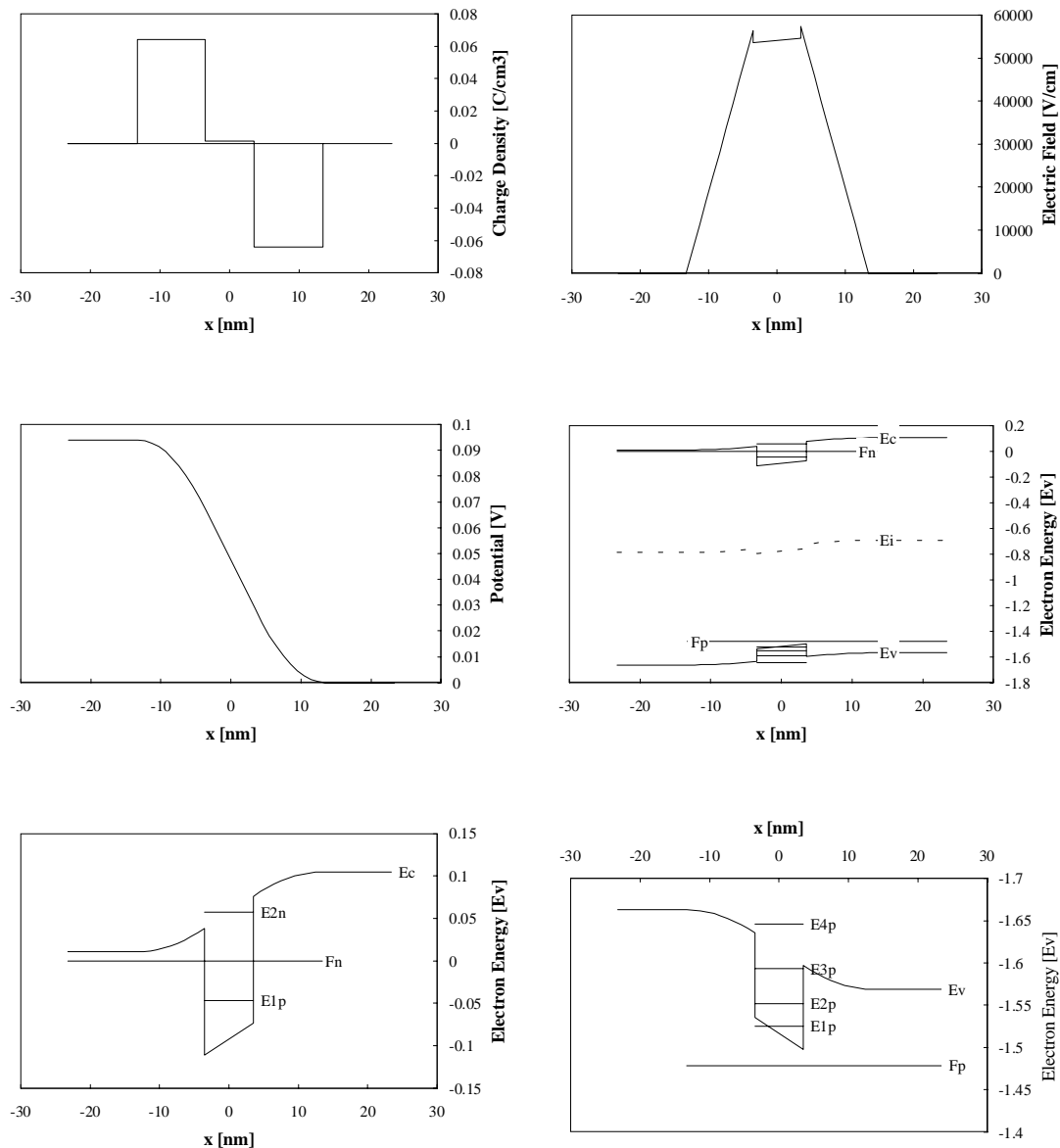


Fig.4.5 Energy band diagram of a GaAs/AlGaAs p-n junction with a quantum well in between. The aluminum concentration is 40% for both the p and n region, and zero in the well. The doping concentrations  $N_a$  and  $N_d$  are  $4 \times 10^{17} \text{ cm}^{-3}$  and  $V_a=1.4 \text{ V}$ .

From the numeric simulation of a GaAs n-qw-p structure we find that typically only one electron level is filled with electrons, while several hole levels are filled with holes or

$$N = N_1 \cong P = P_1 + P_2 + P_3 + \dots \quad [4.4.29]$$

If all the quantized hole levels are more than  $3kT$  below the hole quasi-Fermi level one can rewrite the hole density as:

$$P = P_1 \sum_{\ell} \exp\left(\frac{E_{1p} - E_{\ell p}}{kT}\right) \quad [4.4.30]$$

and the applied voltage is given by:

$$V_a = \frac{E_{gqw1}}{q} + V_t \ln(e^{N/N_{c1}})(e^{N/N_{v1}^*} - 1) \quad [4.4.31]$$

with

$$\begin{aligned} N_{v1}^* &= N_v \sum_{\ell} \exp\left(\frac{E_{1p} - E_{\ell p}}{kT}\right) \\ &= N_v (1 + \exp^{-3E_{1p}/kT} + \exp^{-8E_{1p}/kT} + \exp^{-15E_{1p}/kT} + \dots) \end{aligned} \quad [4.4.32]$$

## 4.5 Currents across a p-n heterojunction

This section is very similar to the one discussing currents across a homojunction. Just as for the homojunction we find that current in a p-n junction can only exist if there is recombination or generation of electron and holes somewhere throughout the structure. The ideal diode equation is a result of the recombination and generation in the quasi-neutral regions (including recombination at the contacts) whereas recombination and generation in the depletion region yield enhanced leakage or photo currents.

### 4.5.1 Ideal diode equation

For the derivation of the ideal diode equation we will again assume that the quasi-Fermi levels are constant throughout the depletion region so that the minority carrier densities at the edges of the depletion region and assuming "low" injection are still given by:

$$n_p(x = x_p) = n_n e^{-(\phi_i - V_a)/V_t} = \frac{n_{ip}^2}{N_a} e^{V_a/V_t} \quad [4.5.1]$$

$$p_n(x = -x_n) = p_p e^{-(\phi_i - V_a)/V_t} = \frac{n_{in}^2}{N_d} e^{V_a/V_t} \quad [4.5.2]$$

Where  $n_{in}$  and  $n_{ip}$  refer to the intrinsic concentrations of the n and p region. Solving the diffusion equations with these minority carrier densities as boundary condition and assuming a "long" diode we obtain the same expressions for the carrier and current distributions:

$$n_p(x) = n_{p0} + n_{p0} (e^{V_a/V_t} - 1) e^{(x+x_p)/L_n}, \quad x < -x_p \quad [4.5.3]$$

$$p_n(x) = p_{n0} + p_{n0} (e^{V_a/V_t} - 1) e^{-(x-x_n)/L_p}, \quad x > x_n \quad [4.5.4]$$

$$J_n(x) = q D_n \frac{dn}{dx} = q \frac{D_n n_{p0}}{L_n} (e^{V_a/V_t} - 1) e^{(x+x_p)/L_n}, \quad x < -x_p \quad [4.5.5]$$

$$J_p(x) = -q D_p \frac{dp}{dx} = q \frac{D_p p_{n0}}{L_p} (e^{V_a/V_t} - 1) e^{-(x-x_n)/L_p}, \quad x > x_n \quad [4.5.6]$$

Where  $L_p$  and  $L_n$  are the hole respectively the electron diffusion lengths in the n-type respectively p-type material. The difference compared to the homojunction case is contained in the difference of the material parameters, the thermal equilibrium carrier densities and the width of the depletion layers. Ignoring recombination of carriers in the base yields the total ideal diode current density  $J_{ideal}$ :

$$\begin{aligned}
J_{\text{ideal}} &= J_n(x=x_p) + J_p(x=-x_n) = q \left( \frac{D_n n_{p0}}{L_n} + \frac{D_p p_{n0}}{L_p} \right) (e^{V_a/V_t} - 1) \\
&= q \left( \frac{D_n n_i^2}{L_n N_a} + \frac{D_p n_i^2}{L_p N_d} \right) (e^{V_a/V_t} - 1)
\end{aligned} \tag{4.5.6}$$

This expression is valid only for a p-n diode with infinitely long quasi-neutral regions. For diodes with a quasi-neutral region shorter than the diffusion length, and assuming an infinite recombination velocity at the contacts, the diffusion length can simply be replaced by the width of the quasi-neutral region. For more general boundary conditions, we refer to section 4.2.1.c

Since the intrinsic concentrations depend exponentially on the energy bandgap, a small difference in bandgap between the n and p-type material can cause a significant difference between the electron and hole current and that independent of the doping concentrations.

#### 4.5.2 Recombination/generation in the depletion region

Recombination/generation currents in a heterojunction can be much more important than in a homojunction because most recombination/generation mechanisms depend on the intrinsic carrier concentration which depends strongly on the energy bandgap. We will consider only two major mechanisms: band-to-band recombination and Shockley-Hall-Read recombination.

##### a) Band-to-band recombination

The recombination/generation rate due to band-to-band transitions is given by:

$$U_{\text{bb}} = b(np - n_i^2) \tag{4.5.7}$$

where  $b$  is the bimolecular recombination rate. For bulk GaAs this value is  $1.1 \cdot 10^{-10} \text{ cm}^3\text{s}^{-1}$ . For  $np > n_i^2$  (or under forward bias conditions) recombination dominates, whereas for  $np < n_i^2$  (under reverse bias conditions) thermal generation of electron-hole pairs occurs. Assuming constant quasi-Fermi levels in the depletion region this rate can be expressed as a function of the applied voltage by using the "modified" mass-action law  $np = n_i^2 e^{V_a/V_t}$ , yielding:

$$U_{\text{bb}} = b n_i^2 (e^{V_a/V_t} - 1) \tag{4.5.8}$$

The current is then obtained by integrating the recombination rate throughout the depletion region:

$$J_{bb} = q \int_{-x_n}^{x_p} U_{bb} dx \quad [4.5.9]$$

For uniform material (homojunction) this integration yielded:

$$J_{bb} = q b n_i^2 (e^{V_a/V_t} - 1) x_d \quad [4.5.10]$$

Whereas for a p-n heterojunction consisting of two uniformly doped regions with different bandgap, the integral becomes:

$$J_{bb} = q b (n_i^2 x_n + n_{ip}^2 x_p) (e^{V_a/V_t} - 1) \quad [4.5.11]$$

#### b) Shockley-Hall-Read recombination

Provided bias conditions are "close" to thermal equilibrium the recombination rate due to a density  $N_t$  of traps with energy  $E_t$  and a recombination/generation crosssection  $\sigma$  is given by

$$U_{SHR} = \frac{np - n_i^2}{n + p + 2n_i \cosh\left(\frac{E_i - E_t}{kT}\right)} N_t \sigma v_{th} \quad [4.5.12]$$

where  $n_i$  is the intrinsic carrier concentration,  $v_{th}$  is the thermal velocity of the carriers and  $E_i$  is the intrinsic energy level. For  $E_i = E_t$  and  $\tau_0 = \frac{1}{N_t \sigma v_{th}}$  this expression simplifies to

$$U_{SHR} = \frac{np - n_i^2}{n + p + 2n_i} \frac{1}{\tau_0} \quad [4.5.13]$$

Throughout the depletion region the product of electron and hole density is given by the "modified" mass action law:

$$np = n_i^2 e^{V_a/V_t} \quad [4.5.14]$$

This enables to find the maximum recombination rate which occurs for  $n = p = n_i e^{V_a/2V_t}$

$$U_{SHR,max} = \frac{n_i (e^{V_a/2V_t} - 1)}{2 \tau_0} \quad [4.5.15]$$



The total recombination current is obtained by integrating the recombination rate over the depletion layer width:

$$\Delta J_n = -\Delta J_p = q \int_{-x_p}^{x_n} U_{SHR} dx \quad [4.5.16]$$

which can be written as a function of the maximum recombination rate and an "effective" width  $x'$ :

$$\Delta J_n = q U_{SHR,max} x' = q \frac{x' n_i (e^{V_a/2V_t} - 1)}{2 \tau_0} \quad [4.5.17]$$

where

$$x' = \frac{\int_{-x_p}^{x_n} U_{SHR} dx}{U_{SHR,max}} \quad [4.5.18]$$

Since  $U_{SHR,max}$  is larger than or equal to  $U_{SHR}$  anywhere within the depletion layer one finds that  $x'$  has to be smaller than  $x_d = x_n + x_p$ . (Note that for a p-i-N or p-qw-N structure the width of the intrinsic/qw layer has to be included).

The calculation of  $x'$  requires a numerical integration. The carrier concentrations  $n$  and  $p$  in the depletion region are given by:

$$n = N_c e^{(E_{fn}-E_c)/kT} \quad [4.5.19]$$

$$p = N_v e^{(E_v-E_{fp})/kT} \quad [4.5.20]$$

Substituting these equations into [4.5.18] then yields  $x'$ .

### 4.5.3 Recombination/generation in a quantum well

#### a) Band-to-band recombination

Recognizing that band-to-band recombination between different states in the quantum well have a different coefficient, the total recombination including all possible transitions can be written as:

$$U_{qw} = B_1(N_1 P_1 - N_{i1}^2) + B_2(N_2 P_2 - N_{i2}^2) + \dots \quad [4.5.21]$$

with

$$N_{i\ell}^2 = N_{cq\ell} N_{vq\ell} e^{-E_{gq\ell}/kT} \quad [4.5.22]$$

and

$$E_{gq\ell} = E_g + E_{\ell n} + E_{\ell p} \quad [4.5.23]$$

where  $E_{\ell n}$  and  $E_{\ell p}$  are calculated in the absence of an electric field. To keep this derivation simple, we will only consider radiative transitions between the  $\ell = 1$  states for which:

$$N_1 = N_{cq1} \ln(1 + e^{(E_{fn} - E_c - E_{1n})/kT}) \quad [4.5.24]$$

$$P_1 = N_{vq1} \ln(1 + e^{(E_v - E_{fp} - E_{1p})/kT}) \quad [4.5.25]$$

both expressions can be combined yielding

$$V_a = \frac{E_{fn} - E_{fp}}{q} = V_t \ln[(e^{N_1/N_{cq1}} - 1)(e^{P_1/N_{vq1}} - 1)] + \frac{E_{gq1}}{q} \quad [4.5.26]$$

#### **α) Low voltage approximation (non-degenerate carrier concentration)**

For low or reversed bias conditions the carrier densities are smaller than the effective densities of states in the quantum well. Equation [4.2.55] then simplifies to:

$$V_a = V_t \ln\left(\frac{N_1 P_1}{N_{cq1} N_{vq1}}\right) + \frac{E_{gq1}}{q} \quad [4.5.27]$$

and the current becomes

$$J_{bbqw} = q U_{bbqw} = q B_1 N_{i1}^2 (e^{V_a/V_t} - 1) \quad [4.5.28]$$

This expression is similar to the band-to-band recombination current in bulk material.

#### **β) High voltage approximation (strongly degenerate)**

For strong forward bias conditions the quasi-Fermi level moves into the conduction and valence band. Under these conditions equation [4.4.26] reduces to:

$$V_a = \frac{E_{gqw}}{q} + V_t \left( \frac{N_1}{N_{cqw}} + \frac{P_1}{N_{vqw}} \right) \quad [4.5.29]$$

If in addition one assumes that  $N_1 = P_1$  and  $N_{cqw} \ll N_{vqw}$  this yields:

$$N_1 = N_{cqw} \frac{qV_a - E_{gqw}}{kT} \quad [4.5.30]$$

and the current becomes:

$$J_{bbqw} = q U_{bbqw} = q B_1 N_{cqw}^2 \left( \frac{qV_a - E_{gqw}}{kT} \right)^2 \quad [4.5.31]$$

for GaAs/AlGaAs quantum wells,  $B_1$  has been determined experimentally to be  $5 \cdot 10^{-5} \text{ cm}^2 \text{ s}^{-1}$

#### b) SHR recombination

A straight forward extension of the expression for bulk material to two dimensions yields

$$U_{SHR \text{ qw}} = \frac{NP - N_i^2}{N + P + 2N_i} \frac{1}{\tau_0} \quad [4.5.32]$$

and the recombination current equals:

$$\Delta J_n = -\Delta J_p = q U_{SHR \text{ qw}} = q \frac{NP - N_i^2}{N + P + 2N_i} \frac{1}{\tau_0} \quad [4.5.33]$$

This expression implies that carriers from any quantum state are equally likely to recombine with a midgap trap.

#### 4.5.4 Recombination mechanisms in the quasi-neutral region

Recombination mechanisms in the quasi-neutral regions do not differ from those in the depletion region. Therefore, the diffusion length in the quasi-neutral regions, which is defined as  $L_n = \sqrt{D_n \tau_n}$  and  $L_p = \sqrt{D_p \tau_p}$ , must be calculated based on band-to-band as well as SHR recombination. Provided both recombination rates can be described by a single time constant, the carrier life time is obtained by summing the recombination rates and therefore summing the inverse of the life times.

$$\tau_{n,p} = \frac{1}{\frac{1}{\tau_{SHR}} + \frac{1}{\tau_{b-b}}} \quad [4.5.34]$$

for low injection conditions and assuming n-type material, we find:

$$U_{SHR} = \frac{p_n - p_{n0}}{\tau_{SHR}} = \frac{p_n - p_{n0}}{\tau_0} \text{ or } \tau_{SHR} = \tau_0 \quad [4.5.35]$$

$$U_{b-b} = b (N_d p_n - n_i^2) = \frac{p_n - p_{n0}}{\tau_{b-b}} \text{ or } \tau_{b-b} = \frac{1}{b N_d} \quad [4.5.36]$$

yielding the hole life time in the quasi-neutral n-type region:

$$\tau_p = \frac{1}{\frac{1}{\tau_0} + b N_d} \quad [4.5.37]$$

#### 4.5.5 The total diode current

Using the above equations we find the total diode current to be:

$$J_{total} = J_{bb} + J_{SHR} + J_{ideal} \quad [4.5.38]$$

from which the relative magnitude of each current can be calculated. This expression seems to imply that there are three different recombination mechanisms. However the ideal diode equation depends on all recombination mechanism which are present in the quasi-neutral region as well as within the depletion region, as described above.

The expression for the total current will be used to quantify performance of heterojunction devices. For instance, for a bipolar transistor it is the ideal diode current for only one carrier type which should dominate to ensure an emitter efficiency close to one. Whereas

for a light emitting diode the band-to-band recombination should dominate to obtain a high quantum efficiency.

#### 4.5.6 The graded p-n diode

##### a) General discussion of a graded region

Graded regions can often be found in heterojunction devices. Typically they are used to avoid abrupt heterostructures which limit the current flow. In addition they are used in laser diodes where they provide a graded index region which guides the lasing mode. An accurate solution for a graded region requires the solution of a set of non-linear differential equations.

Numeric simulation programs provide such solutions and can be used to gain the understanding needed to obtain approximate analytical solutions. A common misconception regarding such structures is that the flatband diagram is close to the actual energy band diagram under forward bias. Both are shown in the figure below for a single-quantum-well graded-index separate-confinement heterostructure (GRINSCH) as used in edge-emitting laser diodes which are discussed in more detail in Chapter 6.

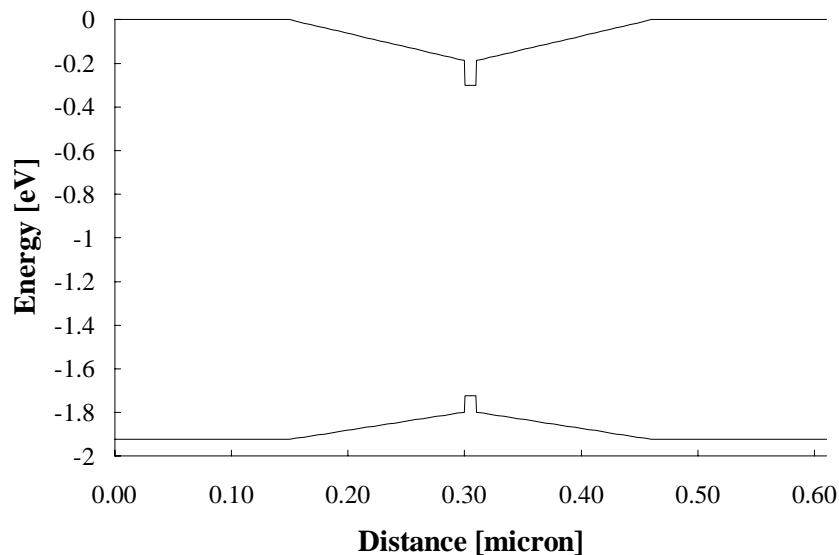


Fig. 4.6 Flat band diagram of a graded AlGaAs p-n diode with  $x = 40\%$  in the cladding regions,  $x$  varying linearly from 40% to 20% in the graded regions and  $x = 0\%$  in the quantum well.

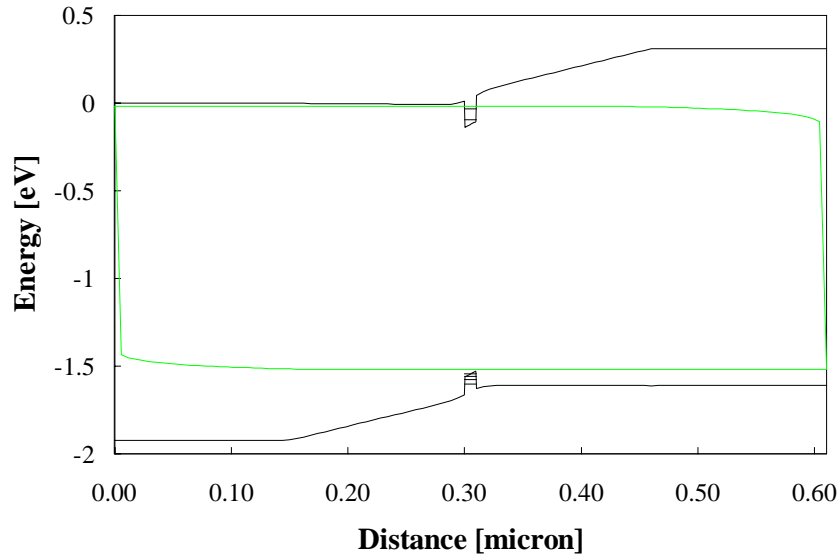


Fig. 4.7 Energy band diagram of the graded p-n diode shown above under forward bias.  $V_a = 1.5$  V,  $N_a = 4 \cdot 10^{17} \text{ cm}^{-3}$ ,  $N_d = 4 \cdot 10^{17} \text{ cm}^{-3}$ . Shown are the conduction and valence band edges (solid lines) as well as the quasi-Fermi levels (dotted lines).

The first difference is that the conduction band edge in the n-type graded region as well as the valence band edge in the p-type graded region are almost constant. This assumption is correct if the majority carrier quasi-Fermi level, the majority carrier density and the effective density of states for the majority carriers don't vary within the graded region. Since the carrier recombination primarily occurs within the quantum well (as it should be in a good laser diode), the quasi-Fermi level does not change in the graded regions, while the effective density of states varies as the three half power of the effective mass, which varies only slowly within the graded region. The constant band edge for the minority carriers implies that the minority carrier band edge reflects the bandgap variation within the graded region. It also implies a constant electric field throughout the grade region which compensates for the majority carrier bandgap variation or:

$$\begin{aligned} \mathcal{E}_{\text{gr}} &= -\frac{1}{q} \frac{dE_{c0}(x)}{dx} && \text{in the n-type graded region} \\ \mathcal{E}_{\text{gr}} &= -\frac{1}{q} \frac{dE_{v0}(x)}{dx} && \text{in the p-type graded region} \end{aligned} \quad [4.5.39]$$

where  $E_{c0}(x)$  and  $E_{v0}(x)$  are the conduction and valence band edge as shown in the flatband diagram. The actual electric field is compared to this simple expression in the figure below. The existence of an electric field requires a significant charge density at each end of the graded regions caused by a depletion of carriers. This also causes a small cusp in the band diagram.

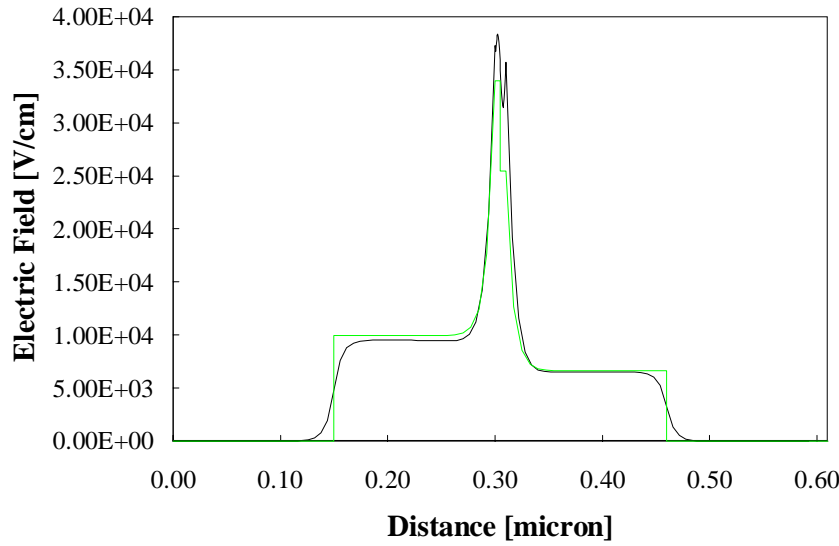


Fig. 4.8 Electric Field within a graded p-n diode. Compared are a numeric simulation (solid line) and equation [4.5.39] (dotted line). The field in the depletion regions around the quantum well was calculated using the linearized Poisson equation as described in the text.

Another important issue is that the traditional current equation with a drift and diffusion term has to be modified. We now derive the modified expression by starting from the relation between the current density and the gradient of the quasi-Fermi level:

$$\begin{aligned}
 J_n &= \mu_n n \frac{dF_n}{dx} = \mu_n n \frac{dE_c}{dx} + \mu_n n \frac{d(kT \ln n/N_c)}{dx} \\
 &= \mu_n n \frac{dE_c}{dx} + qDn \frac{dn}{dx} - q \mu_n V_t \frac{n}{N_c} \frac{dN_c}{dx}
 \end{aligned} \tag{4.5.40}$$

where it was assumed that the electron density is non-degenerate. At first sight it seems that only the last term is different from the usual expression. However the equation can be rewritten as a function of  $E_{c0}(x)$ , yielding:

$$J_n = q \mu_n n \left( \mathcal{E} + \frac{1}{q} \frac{dE_{c0}(x)}{dx} - \frac{V_t}{N_c} \frac{dN_c}{dx} \right) + q D_n \frac{dn}{dx} \quad [4.5.41]$$

This expression will be used in the next section to calculate the ideal diode current in a graded p-n diode. We will at that time ignore the gradient of the the effective density of states. A similar expression can be derived for the hole current density,  $J_p$ .

#### b) Ideal diode current

Calculation of the ideal diode current in a graded p-n diode poses a special problem since a gradient of the bandedge exists within the quasi-neutral region. The derivation below can be applied to a p-n diode with a graded doping concentration as well as one with a graded bandgap provided that the gradient is constant. For a diode with a graded doping concentration this implies an exponential doping profile as can be found in an ion-implanted base of a silicon bipolar junction transistor. For a diode with a graded bandgap the bandedge gradient is constant if the bandgap is linearly graded provided the majority carrier quasi-Fermi level is parallel to the majority carrier band edge.

Focusing on a diode with a graded bandgap we first assume that the gradient is indeed constant in the quasi-neutral region and that the doping concentration is constant. Using the full depletion approximation one can then solve for the depletion layer width. This requires solving a transcendental equation since the dielectric constant changes with material composition (and therefore also with bandgap energy). A first order approximation can be obtained by choosing an average dielectric constant within the depletion region and using previously derived expressions for the depletion layer width. Under forward bias conditions one finds that the potential across the depletion regions becomes comparable to the thermal voltage. One can then use the linearized Poisson equation or solve Poisson's equation exactly (section 4.1.2) This approach was taken to obtain the electric field in Fig.4.8.

The next step requires solving the diffusion equation in the quasi-neutral region with the correct boundary condition and including the minority carrier bandedge gradient. For electrons in a p-type quasi-neutral region we have to solve the following modified diffusion equation

$$0 = D_n \frac{d^2 n}{dx^2} + \mu_p \frac{1}{q} \frac{dE_c}{dx} \frac{dn}{dx} - \frac{n}{\tau_n} \quad [4.5.42]$$



which can be normalized yielding:

$$0 = n'' + 2\alpha n' - \frac{n}{L_n^2} \quad [4.5.43]$$

$$\text{with } \alpha = \frac{1}{q} \frac{dE_c}{2V_t dx}, \quad L_n^2 = D_n \tau_n, \quad n' = \frac{dn}{dx} \text{ and } n'' = \frac{d^2n}{dx^2}$$

If the junction interface is at  $x = 0$  and the p-type material is on the right hand side, extending up to infinity, the carrier concentrations equals:

$$n(x) = n_{p0}(x_p) e^{V_a/V_t} \exp[-\alpha(1 + \sqrt{1 + \frac{1}{(L_n\alpha)^2}})(x - x_p)] \quad [4.5.44]$$

where we ignored the minority carrier concentration under thermal equilibrium which limits this solution to forward bias voltages. Note that the minority carrier concentration  $n_{p0}(x_p)$  at the edge of the depletion region (at  $x = x_p$ ) is strongly voltage dependent since it is exponentially dependent on the actual bandgap at  $x = x_p$ .

The electron current at  $x = x_p$  is calculated using the above carrier concentration but including the drift current since the bandedge gradient is not zero, yielding:

$$J_n = -q D_n n_{p0}(x_p) e^{V_a/V_t} \alpha \left( \sqrt{1 + \frac{1}{(L_n\alpha)^2}} - 1 \right) \quad [4.5.45]$$

The minus sign occurs since the electrons move from left to right for a positive applied voltage. For  $\alpha = 0$  the current equals the ideal diode current in a non-graded junction:

$$J_n = -\frac{q D_n n_{p0}}{L_n} e^{V_a/V_t} \quad [4.5.46]$$

while for strongly graded diodes ( $\alpha L_n \gg 1$ ) the current becomes:

$$J_n = -\frac{q D_n n_{p0}(x_n)}{2\alpha L_n^2} e^{V_a/V_t} \quad [4.5.47]$$

For a bandgap grading given by:

$$E_g = E_{g0} + \Delta E_g \frac{x}{d} \quad [4.5.48]$$

one finds

$$\alpha = \frac{\Delta E_g}{2 k T d} \quad [4.5.49]$$

and the current density equals:

$$J_n = J_n(\alpha = 0) \frac{kT}{\Delta E_g} \frac{d}{L_n} \frac{n_{p0}(x_p)}{n_{p0}(0)} \quad [4.5.50]$$

where  $J_n(\alpha = 0)$  is the current density in the absence of any bandgap grading.