4.3.8. The hetero p-n junction

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.[1].

4.3.8.1. 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 ΔE_c to be positive if $E_{c,n} > E_{c,p}$ and ΔE_v to be positive if $E_{v,n} < E_{v,p}$.

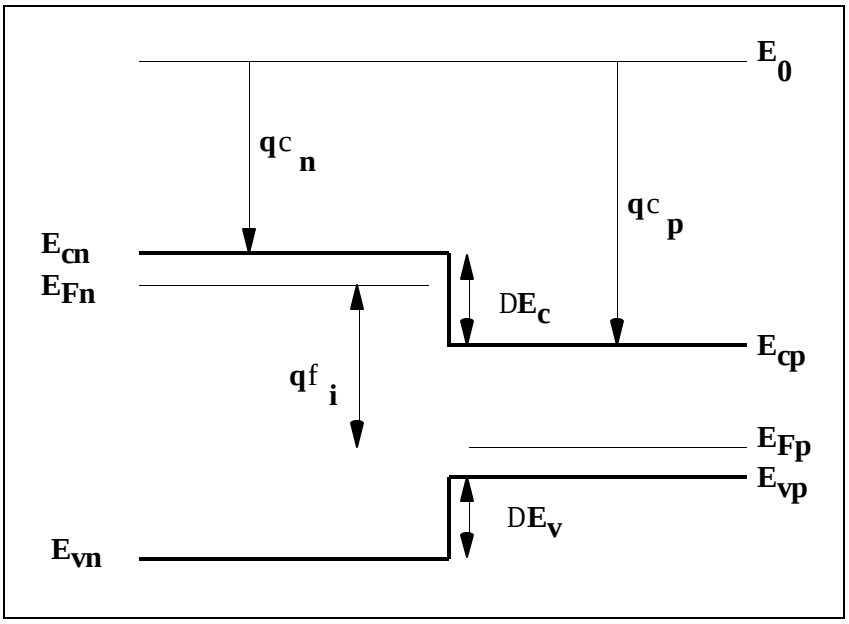

Figure 4.3.5 Flat-band energy band diagram of a p-n heterojunction

4.3.8.2. 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:

$$qf_i = E_{F,n} - E_{F,p} = E_{F,n} - E_{c,n} + E_{c,n} + E_{c,p} - E_{F,p} \qquad (4.3.52)$$

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

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[1] Wolfe, C. Holonyak, N. Stillman, G. Physical properties of semiconductors, Prentice Hall, Chapter 9.

$$qf_i = \Delta E_c + kT \ln \frac{n_{n0} N_{c,p}}{n_{p0} N_{c,n}} \tag{4.3.53}$$

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

$$qf_i = -\Delta E_v + kT \ln \frac{p_{p0} N_{v,n}}{p_{n0} N_{v,p}} \tag{4.3.54}$$

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

$$qf_i = \frac{\Delta E_c - \Delta E_v}{2} + kT \ln \frac{N_d N_a}{n_{i,n} n_{i,p}} + \frac{kT}{2} \ln \frac{N_{v,n} N_{c,p}}{N_{c,n} N_{v,p}} \tag{4.3.55}$$

where n_{in} and n_{ip} are the intrinsic carrier concentrations of the n and p-type region, respectively. ΔE_c and ΔE_v are positive quantities if the bandgap of the n-type region is smaller than that of the *p*-type region and the sum of both equals the bandgap difference. 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:

$$qf_i = \frac{\Delta E_c - \Delta E_v}{2} + kT \ln \frac{N_d N_a}{n_{i,n} n_{i,p}} \tag{4.3.56}$$

4.3.8.3.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.

$$f_n + f_p = f_i - V_a \tag{4.3.57}$$

$$f_n = \frac{qN_d x_n^2}{2e_{s,n}} \text{ and } f_p = \frac{qN_a x_n^2}{2e_{s,p}} \tag{4.3.58}$$

$$qN_a x_p = qN_d x_n \tag{4.3.59}$$

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 $N_a \frac{e_{s,p}}{e_s}$, N_d by $N_d \frac{e_{s,n}}{e_s}$, x_p by $x_p \frac{e_s}{e_{s,p}}$, and x_n by $x_n \frac{e_s}{e_{s,n}}$. Adding x_n and x_p yields the total depletion layer width x_d:

$$x_d = x_n + x_p = \sqrt{\frac{2e_{s,n}e_{s,p}}{q}\frac{(N_a + N_d)^2(f_i - V_a)}{N_a N_d (N_a e_{s,p} + N_d e_{s,n})}} \tag{4.3.60}$$

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

$$C_j = \frac{1}{\frac{x_n}{e_{s,n}} + \frac{x_p}{e_{s,p}}} = \sqrt{\frac{qe_{s,n}e_{s,p}}{2}\frac{N_a N_d}{(N_a e_{s,p} + N_d e_{s,n})(f_i - V_a)}} \tag{4.3.61}$$

4.3.8.4.Abrupt P-i-N junction

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

$$f_n + f_p + f_u = f_i - V_a \tag{4.3.62}$$

$$f_n = \frac{qN_d x_n^2}{2e_{s,n}},\ f_p = \frac{qN_a x_p^2}{2e_{s,p}} \text{ and } f_u = \frac{qN_a x_p d}{2e_{s,u}} \tag{4.3.63}$$

$$qN_a x_p = qN_d x_n \tag{4.3.64}$$

Where f_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:

$$x_d = x_n + x_p + d \tag{4.3.65}$$

$$C_j = \frac{1}{\frac{x_n}{e_{s,n}} + \frac{x_p}{e_{s,p}} + \frac{d}{e_s}} \tag{4.3.66}$$

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

$$x_n = \frac{\sqrt{(\frac{de_{s,n}}{e_{s,u}})^2 + \frac{2e_{s,n}(f_i - V_a)}{qN_d}(1 + \frac{N_d}{N_a})} - \frac{de_{s,n}}{e_{s,u}}}{(1 + \frac{N_d}{N_a})} \tag{4.3.67}$$

A solution for x_p can be obtained from [4.2.16] by replacing N_d by N_a, N_a by N_d, $e_{s,n}$ by $e_{s,p}$, and $e_{s,p}$ by $e_{s,n}$. 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:

$$f(x) = -\frac{qN_d}{2e_{s,n}}(x + x_n)^2 \text{ for } -x_n < x < 0 \tag{4.3.68}$$

$$f(x) = -f_n - \frac{qN_d x_n}{2e_{s,n}} x \text{ for } 0 < x < d \tag{4.3.69}$$

$$f(x) = -(f_i - V_a) + \frac{qN_a}{2e_{s,p}}(x - d - x_p)^2 \text{ for } d < x < d + x_p \tag{4.3.70}$$

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

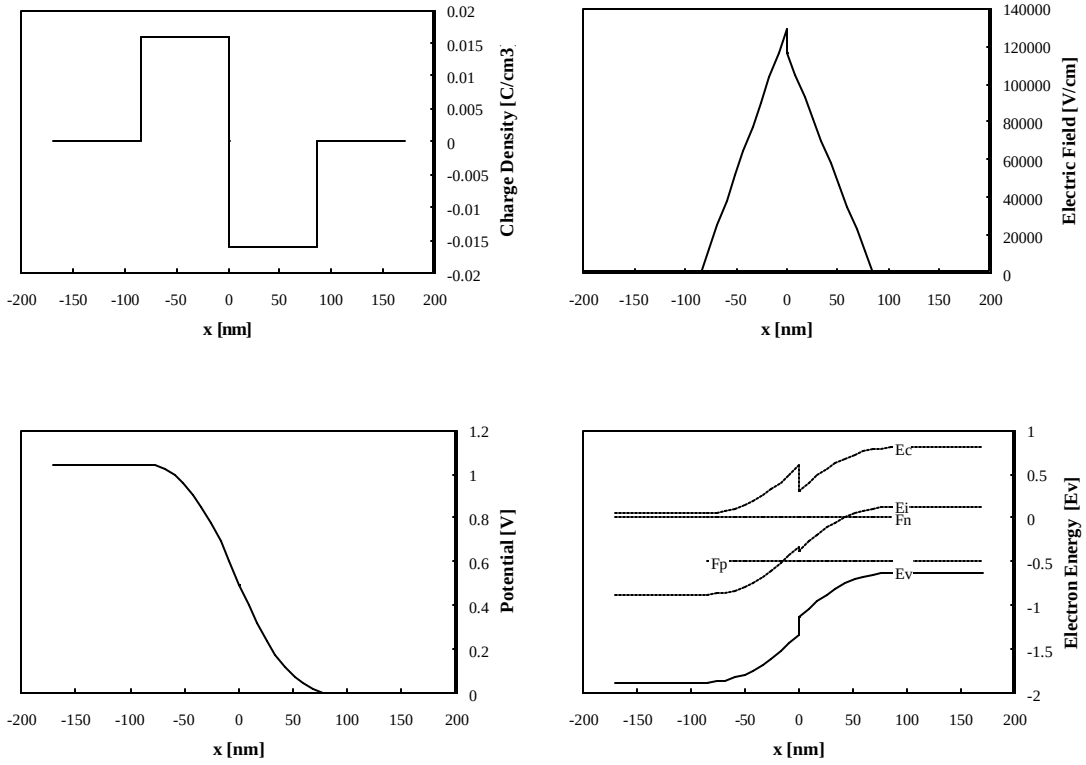

Figure 4.3.6 Charge distribution, electric field, potential and energy band diagram of an AlGaAs/GaAs p-n heterojunction with V_a = 0.5 V, x = 0.4 on the left and x = 0 on the right. $N_d = N_a = 10^{17}\text{cm}^{-3}$

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*-type 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.

4.3.8.5.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 $e_{s,m}$. 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:

$$f_n + f_p + f_m = f_i - V_a \tag{4.3.71}$$

$$f_n = \frac{qN_d x_n^2}{2e_{s,n}},\ f_p = \frac{qN_a x_p^2}{2e_{s,p}} \text{ and } f_m = (qN_a x_p + Q_1)\frac{d}{e_{s,m}} + \frac{qN_m d^2}{2e_{s,m}} \tag{4.3.72}$$

$$qN_d x_n + Q_1 + Q_2 + qN_m d = qN_a x_p \tag{4.3.73}$$

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.

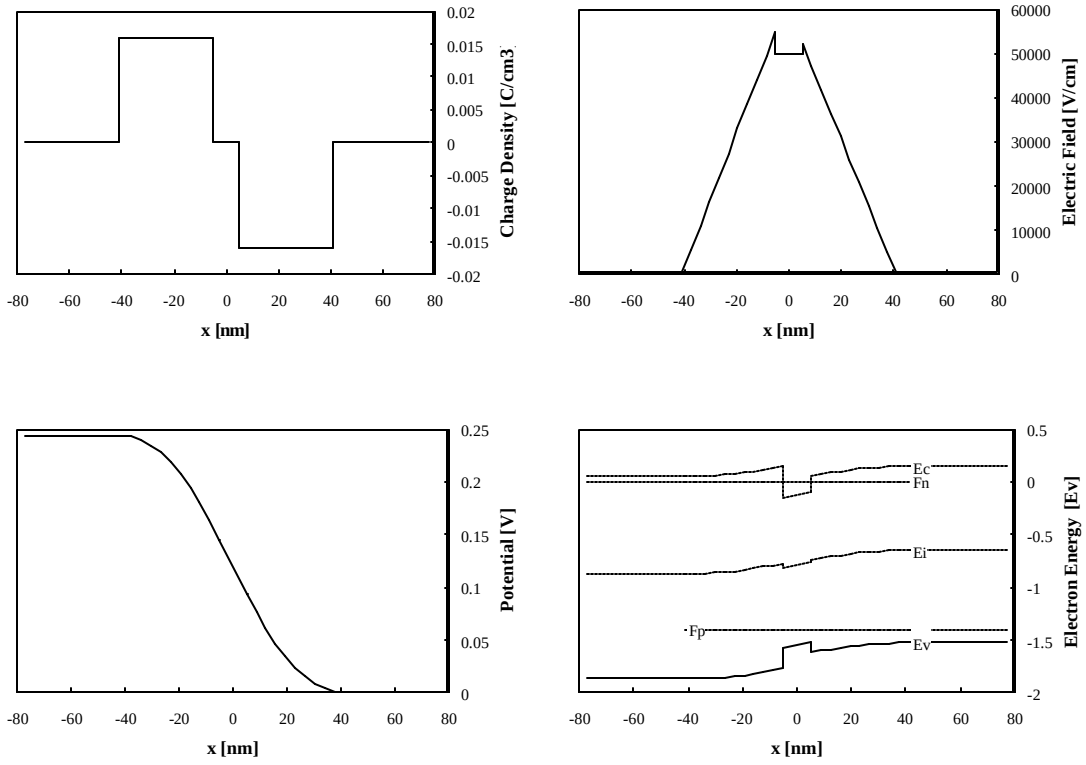

Figure 4.3.7 Charge distribution, electric field, potential and energy band diagram of an AlGaAs/GaAs p-i-n heterojunction with V_a = 1.4 V, x = 0.4 on the left, x = 0 in the middle and x = 0.2 on the right. d = 10 nm and $N_d = N_a = 10^{17}$cm^{-3}

4.3.8.6. 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.

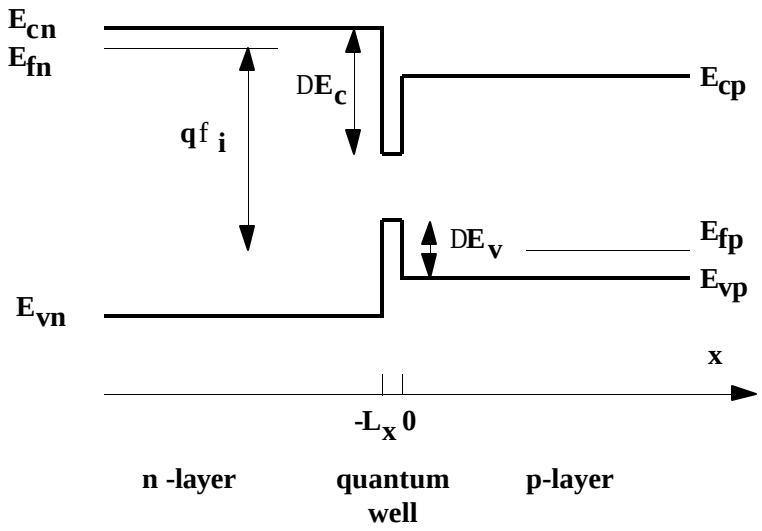

Figure 4.3.8 Flat-band energy band diagram of a p-n heterojunction with a quantum well at the interface.

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:

$$f_n + f_{qw} + f_p = f_i - V_a \tag{4.3.74}$$

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

$$f_n = \frac{qN_d x_n^2}{2e_{s,n}}, \text{ and } f_p = \frac{qN_a x_p^2}{2e_{s,p}} \tag{4.3.75}$$

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

$$f_{qw} = \frac{qN_d x_n L_x}{2e_{s,n}} + \frac{q(P-N)L_x}{2e_{s,p}} \tag{4.3.76}$$

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:

$$qN_d x_n - qN = -qP + qN_a x_p \tag{4.3.77}$$

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

$$N = N_{c,qw} \sum_{n=1}^{\infty} \ln[1 + \exp \frac{\Delta E_{n,e}}{kT}] \tag{4.3.78}$$

$$P = P_{v,qw} \sum_{n=1}^{\infty} \ln[1 + \exp \frac{\Delta E_{n,h}}{kT}] \tag{4.3.79}$$

with $\Delta E_{n,e}$ and $\Delta E_{n,h}$ given by:

$$\Delta E_{n,e} = \Delta E_c - q f_n - kT \ln \frac{N_{c,n}}{N_d} - E_{n,e} \tag{4.3.80}$$

$$\Delta E_{n,h} = \Delta E_v - q f_p - kT \ln \frac{N_{v,p}}{N_a} - E_{n,h} \tag{4.3.81}$$

where $E_{n,e}$ and $E_{n,h}$ are the n^{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 f_n equals f_p. Assuming that only one energy level namely the n = 1 level is populated in the quantum well one finds:

$$N = P = N_{c,qw} \ln[1 + \exp \frac{qV_a - 2E_{1,e} - E_g}{2kT}] \tag{4.3.82}$$

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:

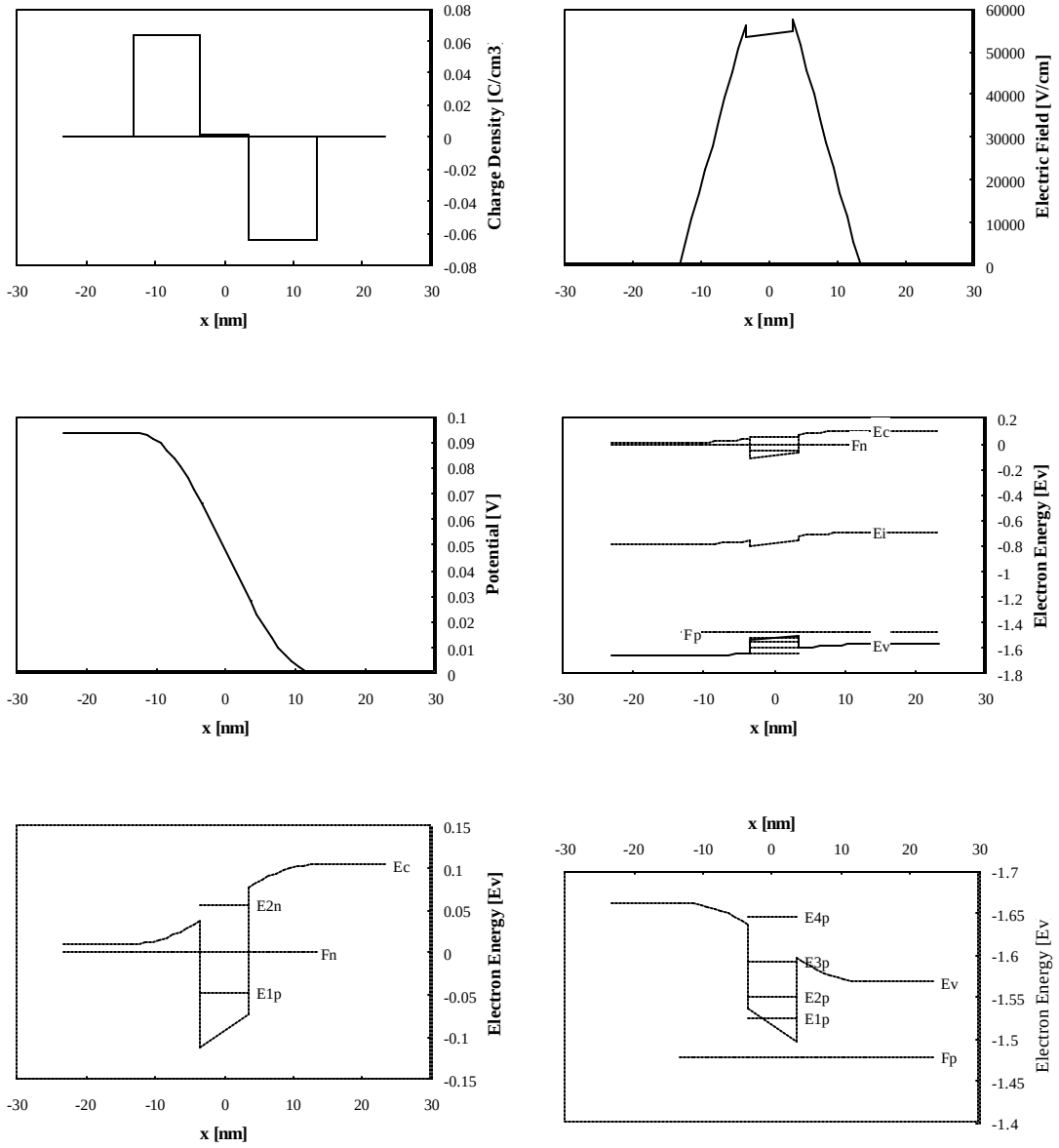

Figure 4.3.9 Energy band diagram of a GaAs/AlGaAs p-n junction with a quantum well in between. The aluminum concentration is 40 % for both the p and n region, and zero in the well. The doping concentrations N_a and N_d are 4 x 10^{17} cm^{-3} and V_a = 1.4 V.

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

$$N = N_1 \cong P = P_1 + P_2 + P_3 + ... \tag{4.3.83}$$

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

$$P = P_1 \sum_n \exp \frac{E_{1,h} - E_{n,h}}{kT} \tag{4.3.84}$$

and the applied voltage is given by:

$$V_a = \frac{E_{g,qw1}}{q} + V_t \ln(e^{N/N_c} - 1)(e^{N/N_v^*} - 1) \tag{4.3.85}$$

with

$$N_v^* = N_v \sum_n \exp \frac{E_{1,h} - E_{n,h}}{kT} \tag{4.3.86}$$

$$N_v^* = N_v (1 + \exp \frac{-3E_{1,h}}{kT} + \exp \frac{-8E_{1,h}}{kT} + \exp \frac{-15E_{1,h}}{kT} + ...) \tag{4.3.87}$$