4.4.7. Heterojunction Diode Current

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 photocurrents.

4.4.6.1.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:

$$n_p(x = x_p) = n_n \exp(-\frac{f_i - V_a}{V_t}) = \frac{n_{i,p}^2}{N_a} \exp\frac{V_a}{V_t} \tag{4.4.57}$$

$$p_n(x = -x_n) = p_p \exp(-\frac{f_i - V_a}{V_t}) = \frac{n_{i,n}^2}{N_d} \exp\frac{V_a}{V_t} \tag{4.4.58}$$

Where $n_{i,n}$ and $n_{i,p}$ 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:

$$n_p(x) = n_{p0} + n_{p0}(\exp\frac{V_a}{V_t} - 1)\exp\frac{x + x_p}{L_n} \quad \text{for } x < -x_p \tag{4.4.59}$$

$$p_n(x) = p_{n0} + p_{n0}(\exp\frac{V_a}{V_t} - 1)\exp(-\frac{x - x_n}{L_p}) \quad \text{for } x_n < x \tag{4.4.60}$$

$$J_n(x) = qD_n\frac{dn}{dx} = q\frac{D_n n_{p0}}{L_n}(\exp\frac{V_a}{V_t} - 1)\exp\frac{x + x_p}{L_n} \quad \text{for } x < -x_p \tag{4.4.61}$$

$$J_p(x) = qD_p\frac{dp}{dx} = q\frac{D_p p_{n0}}{L_p}(\exp\frac{V_a}{V_t} - 1)\exp(-\frac{x - x_n}{L_n}) \quad \text{for } x_n < x \tag{4.4.62}$$

Where L_p and L_n are the hole respectively the electron diffusion lengths in the n-type and p-type material, respectively 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}:

$$J_{ideal} = J_n(x = x_p) + J_p(x = -x_n) = q(\frac{D_n n_{p0}}{L_n} + \frac{D_p p_{n0}}{L_p})(\exp\frac{V_a}{V_t} - 1) \quad (4.4.63)$$

$$J_{ideal} = q(\frac{D_n n_{i,p}^2}{L_n N_a} + \frac{D_p n_{i,n}^2}{L_p N_d})(\exp\frac{V_a}{V_t} - 1) \quad (4.4.64)$$

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*-type and i-type material can cause a significant difference between the electron and hole current and that independent of the doping concentrations.

4.4.6.2.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.

4.4.6.2.1. Band-to-band recombination

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

$$U_{b-b} = b(np - n_i^2) \quad (4.4.65)$$

where b is the bimolecular recombination rate. For bulk GaAs this value is 1.1 x 10^{-10} cm^3s^{-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:

$$U_{b-b} = bn_i^2(\exp\frac{V_a}{V_t} - 1) \quad (4.4.66)$$

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

$$J_{b-b} = q\int_{x_n}^{x_p} U_{b-b}\,dx \quad (4.4.67)$$

For uniform material (homojunction) this integration yielded:

$$J_{b-b} = qbn_i^2 (\exp \frac{V_a}{V_t} - 1) x_d \tag{4.4.68}$$

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

$$J_{b-b} qb(n_{i,n}^2 x_n + n_{i,p}^2 x_p)(\exp \frac{V_a}{V_t} - 1) \tag{4.4.69}$$

4.4.6.2.2. Schockley-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 cross-section s is given by

$$U_{SHR} = \frac{np - n_i^2}{n + p + 2n_i \cosh \frac{E_i - E_t}{kT}} N_t s \ v_{th} \tag{4.4.70}$$

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 $t_0 = \frac{1}{N_t s \ v_{th}}$ this expression simplifies to:

$$U_{SHR} = \frac{np - n_i^2}{n + p + 2n_i \cosh \frac{E_i - E_t}{kT}} \frac{1}{t_0} \tag{4.4.71}$$

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

$$np = n_i^2 (\exp \frac{V_a}{2V_t} - 1) \tag{4.4.72}$$

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

$$U_{SHR,\max} = \frac{n_i}{2t_0} (\exp \frac{V_a}{2V_t} - 1) \tag{4.4.73}$$

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

$$\Delta J_n = -\Delta J_p = q\int_{-x_p}^{x_n} U_{SHR}\, dx \qquad (4.4.74)$$

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

$$\Delta J_n = qU_{SHR,\max} x' = q\frac{x' n_i}{2t_0}(\exp\frac{V_a}{2V_t} - 1) \qquad (4.4.75)$$

where

$$x' = \frac{\int_{-x_p}^{x_n} U_{SHR}\, dx}{U_{SHR,\max}} \qquad (4.4.76)$$

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:

$$n = N_c \exp\frac{E_{F,n} - E_c}{kT} \qquad (4.4.77)$$

$$p = N_v \exp\frac{E_v - E_{F,p}}{kT} \qquad (4.4.78)$$

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

4.4.6.3.Recombination/generation in a quantum well

4.4.6.3.1. Band-to-band recombination

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

$$U_{b-b,qw} = B_1(N_1P_1 - N_{i,1}^2) + B_2(N_2P_2 - N_{i,2}^2) + ... \qquad (4.4.79)$$

with

$$N_{i,n}^2 = N_{c,qw} N_{v,qw} \exp(-\frac{E_{g,qw,n}}{kT}) \qquad (4.4.80)$$

and

$$E_{g,qw,n} = E_g + E_{n,e} + E_{n,h} \quad (4.4.81)$$

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

$$N_1 = N_{c,qw} \ln(1 + \exp\frac{E_{F,n} - E_c - E_{1,e}}{kT}) \quad (4.4.82)$$

$$P_1 = N_{v,qw} \ln(1 + \exp\frac{E_v - E_{F,p} - E_{1,h}}{kT}) \quad (4.4.83)$$

both expressions can be combined yielding

$$V_a = \frac{E_{F,n} - E_{F,p}}{q} = V_t \ln[(e^{N_1 / N_{c,qw}} - 1)(e^{P_1 / N_{v,qw}} - 1)] + \frac{E_{g,qw,1}}{q} \quad (4.4.84)$$

4.4.6.3.1.1. Low voltage approximation (non-degenerate carrier concentration)

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

$$V_a = V_t \ln(\frac{N_1 P_1}{N_{c,qw} N_{v,qw}}) + \frac{E_{g,qw,1}}{q} \quad (4.4.85)$$

and the current becomes

$$J_{b-b,qw} = qU_{b-b,qw} = qB_1 N_{i,1}^2 (\exp\frac{V_a}{V_t} - 1) \quad (4.4.86)$$

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

4.4.6.3.1.2. 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:

$$V_a = \frac{E_{g,qw,1}}{q} + V_t (\frac{N_1}{N_{c,qw}} + \frac{P_1}{N_{v,qw}}) \quad (4.4.87)$$

If in addition one assumes that $N_1 = P_1$ and $N_{c,qw} << N_{v,qw}$ this yields:

$$N_1 = N_{c,qw} \frac{qV_a - E_{g,qw}}{kT} \tag{4.4.88}$$

and the current becomes:

$$J_{b-b,qw} = qU_{b-b,qw} = qB_1 N_{c,qw}^2 \left(\frac{qV_a - E_{g,qw}}{kT}\right)^2 \tag{4.4.89}$$

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

4.4.6.3.2. SHR recombination

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

$$U_{SHR,qw} = \frac{NP - N_i^2}{N + P + 2N_i} \frac{1}{t_0} \tag{4.4.90}$$

and the recombination current equals:

$$\Delta J_n = -\Delta J_p = qU_{SHR,qw} = q \frac{NP - N_i^2}{N + P + 2N_i} \frac{1}{t_0} \tag{4.4.91}$$

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

4.4.6.4. 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 $L_n = \sqrt{D_n t_n}$ and $L_p = \sqrt{D_p t_p}$, 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 lifetime is obtained by summing the recombination rates and therefore summing the inverse of the life times.

$$t_{n,p} = \frac{1}{\frac{1}{t_{SHR}} + \frac{1}{t_{b-b}}} \tag{4.4.92}$$

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

$$U_{SHR} = \frac{p_n - p_{n0}}{t_{SHR}} = \frac{p_n - p_{n0}}{t_0} \text{ or } t_{SHR} = t_0 \tag{4.4.93}$$

$$U_{b-b} = b(N_d p_n - n_i^2) = \frac{p_n - p_{n0}}{t_{b-b}} \text{ or } t_{b-b} = \frac{1}{bN_d} \tag{4.4.94}$$

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

$$t_p = \frac{1}{\frac{1}{t_0} + bN_d} \tag{4.4.95}$$

4.4.6.5. The total diode current

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

$$J_{total} = J_{b-b} + J_{SHR} + J_{ideal} \tag{4.4.96}$$

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.

4.4.6.6. The graded p-n diode

4.4.6.6.1. 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.

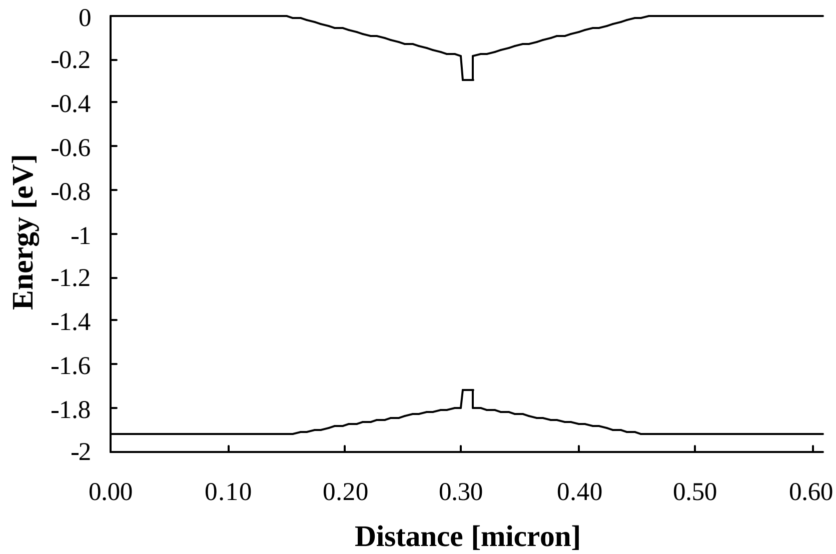

Fig. 4.6 **Flat band diagram of a graded AlGaAs p-n diode with *x* = 40 % in the cladding regions, *x* varying linearly from 40 % to 20 % in the graded regions and *x* = 0% in the quantum well.**

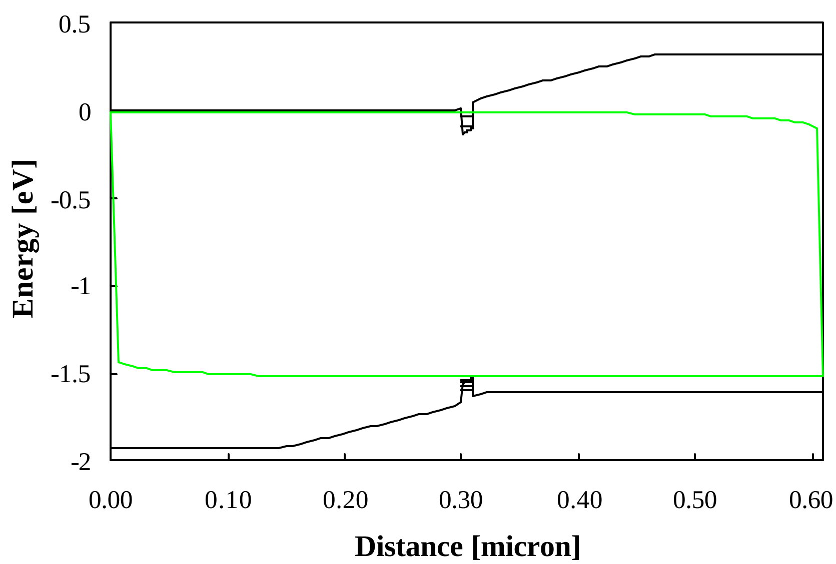

Fig. 4.7 **Energy band diagram of the graded p-n diode shown above under forward bias. V_a = 1.5 V, N_a = 4 x 10^{17} cm^{-3}, N_d = 4 x 10^{17} cm^{-3}. Shown are the conduction and valence band edges (solid lines) as well as the quasi-Fermi energies (dotted lines).**

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 energy, 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 energy 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:

$$\mathcal{E}_{gr} = -\frac{1}{q}\frac{dE_{c0}(x)}{dx} \quad \text{in the } n\text{-type graded region} \tag{4.4.97}$$

$$\mathcal{E}_{gr} = -\frac{1}{q}\frac{dE_{v0}(x)}{dx} \quad \text{in the } n\text{-type graded region} \tag{4.4.98}$$

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.

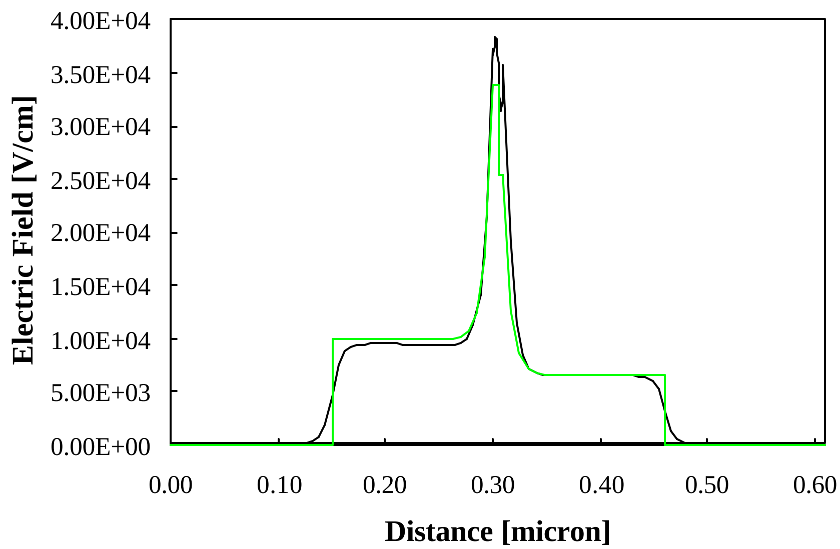

Fig. 4.8 **Electric Field within a graded p-n diode. Compared are a numeric simulation (solid line) and equation [4.5.39] (dotted line). The field in the depletion regions around the quantum well was calculated using the linearized Poisson equation as described in the text.**

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:

$$J_n = m_n n \frac{dF_n}{dx} = m_n n \frac{dE_c}{dx} + m_n n \frac{d(kT \ln \frac{n}{N_c})}{dx} \quad (4.4.99)$$

$$J_n = m_n n \frac{dF_n}{dx} = qD_n \frac{dn}{dx} - qm_n V_t \frac{n}{N_c} \frac{dN_c}{dx} \quad (4.4.100)$$

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:

$$J_n = qm_n n(E + \frac{1}{q} \frac{dE_{c0}(x)}{dx} - \frac{V_t}{N_c} \frac{dN_c}{dx}) + qD_n \frac{dn}{dx} \quad (4.4.101)$$

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 effective density of states. A similar expression can be derived for the hole current density, J_p.

4.4.6.6.2. 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

$$0 = D_n \frac{d^2 n}{dx^2} + m_n \frac{1}{q} \frac{dE_c}{dx} \frac{dn}{dx} - \frac{n}{t_n} \quad (4.4.102)$$

which can be normalized yielding:

$$0 = n'' + 2a\, n' - \frac{n}{L_n^2} \tag{4.4.103}$$

with $a = \dfrac{1}{q2V_t}\dfrac{dE_c}{dx}$, $L_n^{\,2} = D_n t_n$, $n' = \dfrac{dn}{dx}$ and $n'' = \dfrac{d^2n}{dx^2}$

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:

$$n(x) = n_{p0}(x_p)\mathrm{e}^{V_a/V_t}\ \exp[-a\,(1 + \sqrt{1 + \frac{1}{(L_n a)^2}}(x - x_p)] \tag{4.4.104}$$

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:

$$J_n = -qD_n n_{p0}(x_p)\mathrm{e}^{V_a/V_t}\, a\,(\sqrt{1 + \frac{1}{(L_n a)^2}} - 1) \tag{4.4.105}$$

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

$$J_n = \frac{qD_n n_{p0}}{L_n}\mathrm{e}^{V_a/V_t} \tag{4.4.106}$$

while for strongly graded diodes ($aL_n >> 1$) the current becomes:

$$J_n = \frac{qD_n n_{p0}(x_n)}{2a\, L_n^2}\mathrm{e}^{V_a/V_t} \tag{4.4.107}$$

For a bandgap grading given by:

$$E_g = E_{g0} + \Delta E_g \frac{x}{d} \tag{4.4.108}$$

one finds

$$a = \frac{\Delta E_g}{2kTd} \qquad (4.4.109)$$

and the current density equals:

$$J_n = J_n(a = 0)\frac{kT}{\Delta E_g}\frac{d}{L_n}\frac{n_{p0}(x_p)}{n_{p0}(0)} \qquad (4.4.110)$$

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