

ABSTRACT

LI, XIANGMING. Modeling and Measurement of the Differential Resistance and Ideality Factors in Heterostructure Light Emitting Diodes and Laser Diodes. (Under the direction of Dr. Robert M. Kolbas.)

In this work, experimental measurements and modeling have been conducted to investigate the nonlinear behavior of the differential resistance and ideality factors in semiconductor heterostructure light emitting diodes (LEDs) and laser diodes (LDs). The modeling consists of both analytical models that experimentalist can easily apply, and numerical models to account for physical mechanisms that can not be solved in closed form. Good agreement is found between the experimental results and the modeling. The limitation of using simple diode equations with constant series/shunt resistance and ideality factors are outlined, and a methodology for including the majority carrier injection and the minority carrier leakage in the model leads to relatively straightforward explanations for complex phenomena such as the reversal of the kink polarity in the differential resistance at laser threshold observed in some laser diodes.

Variable derivative ideality factors which can be measured from different orders of derivatives from the current-voltage characteristics are defined and proposed as important parameters to indicate dominant recombination path(s) and bias level in the active region of LEDs and LDs. The ideality factor associated with a single recombination pathway with power-law dependency of current on the carrier concentration in an intrinsic and quasi-neutral active region is found to have a fixed value inversely proportional to the power factor at low bias conditions. The ideality factor is no longer a constant at high injection levels due

to carrier degeneracy. When multiple recombination mechanisms exist at the same time in the same active region, changes in the ideality factors can be observed when the additional recombination paths become significant.

The process of majority carrier injection from the device terminals to the active region creates additional nonlinearity in the differential resistance and the ideality factors. A semi-analytical model, in which the interaction between the confining layer and the active region is implied in the thermionic emission boundary conditions at heterointerfaces, is proposed to investigate the effects from majority carrier injection. Instead of being the sum of values directly from the active region and from the heterointerfaces, analysis shows that the differential resistance and ideality factors at the device terminals are partially from the active region and the remainder from the heterointerface. The model was extended to a simple laser model with the inclusion of junction quasi-Fermi level splitting saturation in the active region upon threshold. The model predicts: 1) reduced or even zero kink height in both the differential resistance and the ideality factors at threshold, and; 2) decreasing differential resistance and increasing ideality factor after threshold at the device terminals due to majority carrier injection.

The effects from minority carrier overflow on laser diode differential resistance are investigated through a simplified one dimensional self-consistent numerical model. Simulations showed: 1) that the majority carrier injection could be responsible for the decrease and the disappearance of the differential resistance and the ideality factor kinks at threshold (due to less interaction between the active region and the confining layers as in the

semi-analytical model), and; 2) the minority carrier overflow could create kinks with reverse polarity.

Measurements on various LEDs and LDs at different temperatures showed good agreement with the proposed models. The analytical and numerical models correlated many experimentally observed features with specific physical mechanisms. This work has made possible the modeling of semiconductor optoelectronic devices with relatively simple parameters and methods, and experimentalists can use this approach to understand and characterize complex device phenomena.

Modeling and Measurement of the Differential Resistance and Ideality Factors in Heterostructure Light Emitting Diodes and Laser Diodes

by
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DEDICATION

To my family

BIOGRAPHY

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LIST OF SYMBOLS

$\Delta E_C, \Delta E_V$	conduction band and valance band discontinuity
A	monomolecular recombination coefficient
a	differential gain
A_j	active region area
B	bimolecular recombination coefficient
C	Auger recombination coefficient
D_n, D_p	electron and hole diffusion coefficient
E_C, E_V	conduction band and valance band edge
E_{F0}	Fermi level at thermal equilibrium
E_{Fn}, E_{Fp}	electron and hole quasi-Fermi levels
E_g	bandgap of active material
f_j	fraction associated with junction
I	current
J	current density
J_S	saturation current density
k_B	Boltzmann's constant
L	light intensity
L_j	active layer thickness
m	diode ideality factor
m_e^*	electron effective mass
m_h^*	hole effective mass
m_0	electron mass
m_1	diode ideality factor measured from the first derivatives

m_2	diode ideality factor measured from the second derivatives
m_{ext}	external diode ideality factor as measured at terminals
n, p	electron and hole concentrations
N_A	acceptor concentration
N_C	conduction band effective density of states
N_D	donor concentration
n_s	saturation density
n_{tr}	transparency concentration
N_V	valance band effective density of states
n_V	voltage number defined as $(V_j - E_g/q)/V_T$
q	electron charge
R_d	differential resistance
R_S	series resistance
T	lattice temperature
V	voltage
$V_C(x)$	conduction band profile as function of x
V_{cf}	difference between the electron quasi-Fermi level and the conduction band edge
$V_{cladding}$	difference between the terminal and the junction voltages
V_{ext}	voltage at the device terminals
V_{fv}	difference between the hole quasi-Fermi level and the valance band edge
V_j	junction voltage
V_T	thermal voltage, $k_B T/q$
W_d	depletion region width
β_{sp}	spontaneous emission factor

ε	permittivity
κ	power factor in recombination current as $I \propto n^\kappa$
μ_n, μ_p	electron and hole mobility
ξ	band-filling factor introduced by the difference between the Boltzmann distribution and the Fermi-Dirac distribution
v_n	electron thermal velocity

Chapter 1

Introduction

1.1 Research Context: Modeling and Measurement of the Differential Resistance and Ideality Factors in Heterostructure Light Emitting Diodes and Laser Diodes

Heterostructures, particularly double heterostructure (DH) light emitting diodes (LEDs) and laser diodes (LDs), are widely used in our everyday life and they are important subjects of semiconductor physics research and photonic devices [1]. There are many applications for these optoelectronic devices in fields such as scientific instrumentation, machining, telecommunication, consumer electronics (e.g. CD/DVD players), and solid-state lighting.

Light-current-voltage ($L/I/V$) measurements are the basic testing methodology for light emitting diodes and laser diodes. Their derivatives, typically the derivatives with respect to current such as dL/dI , dV/dI , d^2L/dI^2 , d^2V/dI^2 , and the derivatives with respect to voltage such as dL/dV , dI/dV , d^2L/dV^2 , d^2I/dV^2 , are rich with information but relatively under utilized. These derivative measurements are capable of directly finding the slopes and therefore the fine structure in the $L/I/V$ characteristics. Among these derivative measurements, differential resistance/conductance spectroscopy is the one that is most widely used. It has been demonstrated that derivative measurements are a powerful tool in extracting diode parameters such as the ideality factor and series resistance [2-8]. Nevertheless, previous studies were mainly carried out on devices that have “kinks” in the electrical or optical derivative characteristics such as laser diodes [9-12] and resonant tunneling diodes [13, 14].

Several techniques can be used to obtain the derivatives of $L/I/V$. Numerical differentiation between data points from the $L/I/V$ measurements are relative simple but this approach is susceptible to measurement noise and error. The most widely used method is the ac technique, in which a small amount of sinusoidal signal is superimposed on the dc bias current (or voltage), and the derivatives can be inferred from the corresponding ac amplitudes in the voltage (or current) and light. With technologies such as phase-sensitive detection (lock-in amplifiers) and frequency mixing, the derivatives of $L/I/V$ can be obtained in a more accurate and fast way. In this thesis, experiment data were taken with a custom-made derivative machine using the ac technique [15, 16, 17].

It has been reported that the stimulated emission/recombination in semiconductor laser diodes changed the device I - V characteristics [18]. The abrupt drop of differential resistance

at self-sustained oscillation threshold was observed by Eliseev *et al.* in homostructure GaAs laser diodes [9], and later in heterostructure lasers [4, 11] including quantum well lasers [19]. It was assumed that the sudden drop of laser diode differential resistance was a result of junction voltage saturation upon lasing threshold. A theoretical model was developed by Paoli for the electrical derivatives in the vicinity of threshold by including the coupling between the electrical and the optical fields from the classical phenomenological photon-electron rate equations [20], and by Joyce and Dixon who also included the nonradiative recombination in the model [21]. Similar treatments were used for models that considered Auger recombination and carrier leakage from the active region [22, 23]. In these “recombination models”, the nonlinear resistance of a device is considered to originate mainly from the active region, which is modeled as an ideal *pn* junction diode with a constant ideality factor. The “junction voltage” of a laser diode is expected to saturate upon lasing threshold and the terminal voltage V_{ext} is assumed to be related to the “junction voltage” V_j through $V_j = V_{ext} - IR_S$, where I is the device current and R_S is the series resistance from the other layers and the Ohmic contacts.

1.2 Purpose of This Work

In this dissertation, studies are focused on the differential resistance and ideality factors of heterostructure light emitting diodes (LEDs) and laser diodes (LDs) as they are related to various derivative measurements (e.g. dV/dI , d^2V/dI^2). The nonlinearity in the differential resistance is considered as a result of both the carrier transport across heterojunction

interfaces (majority carrier injection and minority carrier leakage) and the recombination mechanisms in the active region. The “recombination model” of the active region previously described is extended to general power-law carrier concentration dependent recombination currents, especially the widely used *ABC* model for semiconductor optoelectronic devices with and without laser action. The relation between the differential resistance/conductance and the ideality factor from recombination mechanisms in the active region are investigated. Instead of using a constant ideality factor as a key parameter as in most textbook models, non-constant local ideality factors measurable from derivative measurements are introduced and the changes in these ideality factors associated with the active region quality and bias condition are studied. In addition to recombination in the active region, carrier transport across heterojunctions contributes to the nonlinearity in the differential resistance. A semi-analytical model and a numerical model are proposed and both include thermionic emission boundary conditions at the heterojunction interface to study the effects of the majority carrier injection and the minority carrier overflow on device differential resistance and ideality factors.

1.3 Dissertation Outline

The definition and the extraction techniques of the constant ideality factors are briefly introduced in Chapter 2, Section 2.1 and 2.2. The relation between the non-constant ideality factors and the derivative measurements is derived in Section 2.3 and the concept of “derivative ideality factors” is introduced. In Section 2.4, the ideality factors associated with

a single recombination current pathway with power-law dependency on the carrier concentration are derived. The model is further extended for LEDs and LDs where several recombination mechanisms exist at the same time with the *ABC* model in Section 2.5. Ideality factors measured from some commercial LEDs and LDs are presented in Section 2.6. In this section, the model and the experimental measurements are compared and methods for parameter extraction and device quality evaluation are presented.

In addition to the recombination in the active region of a LED or LD, the differential resistance and ideality factors are also affected by the process of majority carrier injection from device terminals to the active region. In Chapter 3, a semi-analytical model is proposed to investigate the effects of majority carrier injection. The device is based on the active region described in Chapter 2 with cladding layers added next to the active region. The model is briefly introduced in Section 3.1, and the assumptions for the semi-analytical model are stated in Section 3.2. Derivations of the current-voltage equation with the “*Thermionic Emission-Diffusion*” model and the “*Thermionic Emission*” model are presented in Section 3.3, followed by a discussion of the relation between the internal and the external electrical characteristics arising from the majority carrier injection across heterojunction boundaries in Section 3.4. In Section 3.5, the differential resistance and ideality factors associated with quasi-Fermi level splitting saturation effects in the active region are addressed. Low temperature experimental data are shown in Section 3.6 and conclusions are presented in Section 3.7.

In Chapter 4, the effects from minority carrier overflow are considered in addition to the majority carrier injection effects from the previous chapter. No analytical model can be found

and a simplified one dimensional (1-D) self-consistent numerical model is proposed and implemented. Following the introduction in Section 4.1, the details of the numerical model are described in Section 4.2. Sample simulation results with a simplified heterostructure laser diode are shown and compared with the semi-analytical model in Section 4.3. Important parameters that affect the laser diode over-barrier leakage currents are discussed. Simulations of the effects of minority carrier leakage on laser terminal differential resistance are demonstrated and compared with experiment data, followed by a summary in Section 4.4.

Important conclusions of this work are summarized in Chapter 5 and some proposals for future work are also given in this chapter.

Chapter 2

Electrical Derivative Measurements and Ideality Factors

2.1 Introduction

Derivative spectroscopy is an excellent tool for finding details in the electrical and optical characteristics of diodes as it is possible to directly measure the slopes in the light-current-voltage ($L/I/V$) measurements. Previous work has been done on devices such as laser diodes and tunneling diodes, and investigations were mainly focused on the “kinks” in the derivatives when a resonant phenomenon occurs [9-14].

In this chapter, derivative measurements are further extended and generalized for devices such as light emitting diodes, and laser diodes before lasing threshold. The ideality factor of a

diode is found to be closely related to electrical derivatives and the use of ideality factors for device parameter extraction are explored.

The organization of this chapter is as follows: in Section 2.2, the definition of ideality factor and its extraction methods are briefly reviewed. The non-constant ideality factor and its link to different orders of the electrical derivatives are described in Section 2.3. A new “derivative ideality factor” is introduced in this section. The theoretical constant and non-constant ideality factor associated with power-law currents are investigated in Section 2.4. These ideality factors are related to the power factor of the recombination currents as well as the device bias level. In Section 2.5, the theory is extended for device active region with multiple recombination mechanisms. The model with ABC recombination coefficients indicates that the changes in the ideality factor are associated with additional recombination paths being turned on. In Section 2.6, examples using this theory for parameter extraction are presented, followed by a summary in Section 2.7.

2.2 The Constant Ideality Factor

2.2.1 The origin and the definition of ideality factor

The “traditional” ideality factor m (sometimes denoted with other symbols such as n or η), or the so called non-ideality factor, quality factor, m -factor, curve shape factor, is a constant used to describe the simple exponential dependency in the current-voltage characteristics of a semiconductor junction as

$$J = J_S \cdot \left[\exp\left(\frac{V_j}{m \cdot V_T}\right) - 1 \right] \quad (2.1)$$

where V_j is the junction voltage, V_T is the thermal voltage $k_B T/q$, and J_S is the saturation current density when the diode is reverse biased. When m equals to 1.0, it is the “ideal” junction because it follows the well-known Shockley diode equation.

The ideality factor is a useful parameter as it can be used to account for the main recombination pathway inside the device around a certain bias level, and it can be used to identify the material and the device quality. For example, in a simple p - n junction diode, the diffusion current in the quasi-neutral region has an ideality of 1.0 [24], while the generation-recombination current through single mid-gap trap level in the depletion region has an ideality factor of 2.0 from the renowned Sah-Noyce-Shockley (SNS) model [25, 26]. The actual Shockley-Read-Hall (SRH) recombination current is bias dependent [30] and typically the value of m is between 1.0 and 2.0 [27-29].

2.2.2 The ideality factor measurement techniques

First, the ideality factor can be obtained from the slope of the current from the semi-logarithmic plot of the forward current as a function of voltage, i.e. the $\ln(I)$ - V plot as by definition [31]:

$$m = \frac{1}{V_T} \cdot \frac{dV_j}{d \ln(I)} \quad (2.2)$$

As $d \ln(I) = (1/I) dI$,

$$\frac{1}{V_T} \cdot \frac{dV_j}{d \ln(I)} = \frac{I}{V_T} \cdot \frac{dV_j}{dI} \quad (2.3)$$

we can see that this method of fitting the slope is equivalent to the method using the first derivative as will be shown.

Equation (2.1) is oversimplified for real diodes. For example, there can be more than one recombination/shunt current pathway for a single diode so that the lumped circuit model for the diode will be complicated, and elaborated techniques are required to extract the multiple ideality factors. Nevertheless, a linear or nonlinear series/shunt resistance has to be considered even without taking into account of multiple current paths and ideality factors. Due to the multiple/non-constant ideality factors and shunt/series resistance of a device, the linear portion in the $\ln(I)$ - V plot is reduced or it may no longer exist.

We consider the most typical diode model consisting of a “junction” in series with a linear series resistor as in Figure 2.1. The “junction voltage” V_j needs to be calculated using the series resistance from the equation

$$V_j = V_{ext} - I \cdot R_S \quad (2.4)$$

where R_S is the equivalent series resistance of the device, V_{ext} is the voltage applied or measured from device terminals. It is worth mentioning that the concept of “junction voltage” V_j is actually vague, and the resistances can be nonlinear due to various mechanisms. These additional complexities will be addressed in the subsequent chapters.

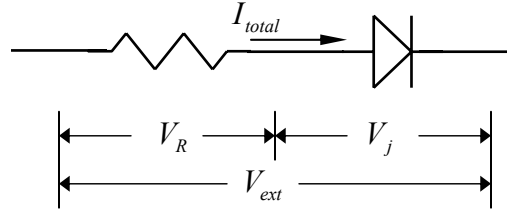


Figure 2.1: Simplified model for a diode: an ideal junction with a series resistance.

With equation (2.4), (2.1) becomes

$$J = J_S \cdot \left[\exp\left(\frac{V_{ext} - I \cdot R_S}{m \cdot V_T}\right) - 1 \right] \quad (2.5)$$

In order to apply (2.2) to obtain the ideality factor by finding the slope in current-voltage semi-logarithmic drawing, the condition

$$m \cdot V_T \ll V_{ext} \ll I \cdot R_S \quad (2.6)$$

needs to be met. The existence of R_S reduces the available linear interval in the $\ln(I)$ - V plot and raises the difficulties in extracting the ideality factor. To overcome this problem, various techniques were developed and they can be divided in to several main categories:

- Direct fitting with numerical optimization [32-35].
- Construct Norde [36] and Norde-like [37-40] special function and find the minimum/maximum in the curves.
- Use the integral [41-50] or the derivatives [4-8] of the I - V measurements.

Among the above methods, the ones using the differential resistance/conductance are one of the most reliable and cost-effective methods. In the following derivations, a device with an equivalent circuit as shown in Figure 2.1 is used as an example to illustrate how the ideality factor can be extracted with the first and the second current derivative of voltages.

The first and second current derivatives of the junction voltage can be calculated from (2.1) when $V_j \gg m \cdot V_T$ as

$$\frac{dV_j}{dI} = m \cdot V_T \cdot \frac{1}{I} \quad (2.7)$$

$$\frac{d^2V_j}{dI^2} = -m \cdot V_T \cdot \frac{1}{I^2} \quad (2.8)$$

Therefore the ideality factor can be calculated with either the first derivative or the second derivative as

$$m = \frac{1}{V_T} \cdot \left(I \cdot \frac{dV_j}{dI} \right) \quad (2.9)$$

or

$$m = \frac{1}{V_T} \cdot \left(-I^2 \cdot \frac{d^2V_j}{dI^2} \right) \quad (2.10)$$

The series resistance can be taken into account as in (2.4). Differentiate the equation and with (2.7), (2.8),

$$\frac{dV_{ext}}{dI} = R_s + m \cdot V_T \cdot \frac{1}{I} \quad (2.11)$$

$$\frac{d^2V_{ext}}{dI^2} = -m \cdot V_T \cdot \frac{1}{I^2} \quad (2.12)$$

Then

$$I \cdot \frac{dV_{ext}}{dI} = I \cdot R_s + m \cdot V_T \quad (2.13)$$

$$I^2 \cdot \frac{d^2V_{ext}}{dI^2} = -m \cdot V_T \quad (2.14)$$

With the first derivative measurement, the ideality factor of a diode with linear series resistance can be obtained from the intercept of the $I \cdot \frac{dV_{ext}}{dI}$ versus I curve at $I=0$ as from

(2.13):

$$m = \frac{1}{V_T} \left(I \cdot \frac{dV_{ext}}{dI} - I \cdot R_s \right) \quad (2.15)$$

With the second derivative measurement, (2.14) indicates that the ideality factor can be directly plotted without the effects from series resistance as

$$m = \frac{1}{V_T} \cdot \left(-I^2 \cdot \frac{d^2V_{ext}}{dI^2} \right) \quad (2.16)$$

As the derivatives can be measured directly through analog measurements instead of through differentiating the I - V measurement data, the derivative measurements offer a potentially more direct and accurate way to obtain the ideality factors. Note that the $I \cdot \frac{dV}{dI}$

and $I^2 \cdot \frac{d^2V}{dI^2}$ plots are in general more convenient to use than the $\frac{dV}{dI}$ and $\frac{d^2V}{dI^2}$ themselves

as they provide excellent presentations for parameter extraction (relate more directly to ideality factors), and their ranges of data are much smaller than the derivatives themselves so that some important features in the plots can be more easily seen.

The above measurement of ideality factors with electrical derivatives was first proposed by Paoli [2] and Dixon [3, 4]. Werner [5] later proposed three different plots to extract ideality factor and series resistance from differential resistance and conductance.

Table 2.1: Werner's methods of extracting ideality factor and series resistance with differential resistance/conductance.

	Equation	Plot	Parameter extraction method
A	$\frac{1}{I} \cdot \frac{dI}{dV_{ext}} = \frac{1}{m \cdot V_T} \cdot \left(1 - \frac{dI}{dV_{ext}} \cdot R_S \right)$	$\frac{1}{I} \cdot \frac{dI}{dV_{ext}}$ vs. $\frac{dI}{dV_{ext}}$	y-axis intercept: $1/m \cdot V_T$ x-axis intercept: $1/R_S$ slope: $R_S / m \cdot V_T$
B	$\frac{dV_{ext}}{dI} = \frac{m \cdot V_T}{I} + R_S$	$\frac{dV_{ext}}{dI}$ vs. $\frac{1}{I}$	y-axis intercept: R_S slope: $m \cdot V_T$ x-axis intercept: $-R_S / m \cdot V_T$
C	$I \cdot \frac{dV_{ext}}{dI} = I \cdot R_S + m \cdot V_T$	$I \cdot \frac{dV_{ext}}{dI}$ vs. I	y-axis intercept: $m \cdot V_T$ slope: R_S x-axis intercept: $-m \cdot V_T / R_S$

2.3 The Local Ideality Factor and the Electrical Derivatives

The above derivations are based on the assumption that the ideality factor m is a constant independent of injection current levels within the region of interest. However, the ideality factor can no longer be fitted as a constant in various cases such as:

- The current-voltage relationships are inherently not exponential. For example, the inclusion of image-force barrier lowering or the distribution of interface states in Schottky diodes. Non-exponential dependence also exists in a diode in high injection levels where carrier degeneracy is significant, or if certain conduction mechanism such as tunneling takes place in a device.
- During the transition between different dominant recombination mechanisms, the ideality factor is expected to change from one value to another for devices with multiple current paths.

We define a “local” ideality factor $m(I)$ for those situations where the ideality factor is not a constant so that it fits into the diode equation as

$$I = I_s \cdot \exp\left(\frac{V_j}{m(I) \cdot V_T}\right) \quad (2.17)$$

Despite the fact that the “constant” becomes dependent on the injection current level, we keep the term “ideality factor”. The variable ideality factor indeed ruins the beauty of simplicity in the original motivation of defining this parameter, it however relates to the inner working of a diode and helps us understand the physical processes in the diode.

When the ideality factor is not a constant, the previous extraction techniques may not be valid in extracting the current dependent $m(I)$. When the ideality factor is a constant, from (2.9) the first derivative results,

$$I \cdot \frac{dV_j}{dI} = m \cdot V_T \quad (2.18)$$

However, if the dm/dI term is no longer zero, differentiating (2.17) results in

$$dI = \frac{I}{m \cdot V_T} \cdot dV_j + I \cdot \frac{V_j}{V_T} \cdot \left(-\frac{1}{m^2} \right) \cdot dm \quad (2.19)$$

$$\frac{dV_j}{dI} = m \cdot V_T \cdot \frac{1}{I} + V_j \cdot \frac{1}{m} \cdot \frac{dm}{dI} \quad (2.20)$$

Then

$$\begin{aligned} I \cdot \frac{dV_j}{dI} &= m \cdot V_T + V_j \cdot \frac{I}{m} \cdot \frac{dm}{dI} \\ &= \left(m + \frac{V_j}{V_T} \cdot \frac{I}{m} \cdot \frac{dm}{dI} \right) \cdot V_T \end{aligned} \quad (2.21)$$

which is different from the value from (2.18). If we directly calculate m from the $I \cdot \frac{dV_j}{dI}$ curve, we actually get a slightly different value instead of getting the real local ideality factor m . We define this generalized ideality factor as the “first derivative ideality factor” m_1 as

$$m_1 = m + \frac{V_j}{V_T} \cdot \frac{I}{m} \cdot \frac{dm}{dI} \quad (2.22)$$

Following a similar procedure, for the second derivative,

$$\frac{d^2V_j}{dI^2} = -m \cdot V_T \cdot \frac{1}{I^2} + \left(\frac{V_T}{I} + \frac{dV_j}{dI} \cdot \frac{1}{m} \right) \cdot \frac{dm}{dI} - V_j \cdot \frac{1}{m^2} \cdot \left(\frac{dm}{dI} \right)^2 + V_j \cdot \frac{1}{m} \cdot \left(\frac{d^2m}{dI^2} \right) \quad (2.23)$$

$$\begin{aligned} & -I^2 \cdot \frac{d^2V_j}{dI^2} \\ & = m \cdot V_T - \left(I \cdot V_T + I^2 \cdot \frac{dV_j}{dI} \cdot \frac{1}{m} \right) \cdot \frac{dm}{dI} + I^2 \cdot V_j \cdot \frac{1}{m^2} \cdot \left(\frac{dm}{dI} \right)^2 - I^2 \cdot V_j \cdot \frac{1}{m} \cdot \left(\frac{d^2m}{dI^2} \right) \end{aligned} \quad (2.24)$$

A “second derivative ideality factor” m_2 can be obtained from the $I \cdot \frac{d^2V}{dI^2}$ plot as

$$m_2 = m - \left(I + \frac{I^2}{V_T} \cdot \frac{dV_j}{dI} \cdot \frac{1}{m} \right) \cdot \frac{dm}{dI} + \frac{I^2}{V_T} \cdot V_j \cdot \frac{1}{m^2} \cdot \left(\frac{dm}{dI} \right)^2 - \frac{I^2}{V_T} \cdot V_j \cdot \frac{1}{m} \cdot \left(\frac{d^2m}{dI^2} \right) \quad (2.25)$$

Note that both m_1 and m_2 are different from the actual $m(I)$ unless m is independent of current level. It is possible to calculate m from m_1 and m_2 , with (2.22) and (2.25) if d^2m/dI^2 can be neglected.

To summarize, when the ideality factor is dependent on current level, the values extracted from the derivative measurements are close to but not equal to the local ideality factor $m(I)$.

A first and a second derivative ideality factor m_1 and m_2 are defined through the first and the

second order derivative measurements as $\frac{I}{V_T} \cdot \frac{dV}{dI}$ and $\frac{I^2}{V_T} \cdot \frac{d^2V}{dI^2}$ respectively. With this

definition, m_1 and m_2 will be equal to the same constant m when dm/dI is zero (i.e. the ideality factors is current independent). In this thesis, unless mentioned otherwise, the word “ideality factor” will refer to “first derivative ideality factor (m_1)”.

2.4 Ideality Factors with Power-Law Recombination Current

As mentioned before, one of the most important reasons to find the ideality factor of a diode is to identify the corresponding recombination pathway, including the mechanism and the place where it happens. It will be shown in this section that the derivative ideality factors are useful in investigating the power-law dependency currents with $I \propto n^\kappa$ in a diode, where κ is the power factor and n is the excess carrier concentration. A single current pathway is assumed for the derivation in this section.

2.4.1 The current derivatives of junction voltage

The first derivative of the junction voltage with respect to current without assuming exponential dependency in the I - V_j can be written as

$$\frac{dV_j}{dI} = \frac{dV_j}{dn} \cdot \frac{dn}{dI} \quad (2.26)$$

The second derivative is far more complicated as will be shown in (2.27).

$$\begin{aligned}
\frac{d^2 V_j}{dI^2} &= \frac{d}{dI} \left(\frac{dV_j}{dI} \right) \\
&= \frac{d}{dn} \left(\frac{dV_j}{dI} \right) \cdot \left(\frac{dn}{dI} \right) \\
&= \frac{d}{dn} \left(\frac{dV_j}{dn} \cdot \frac{dn}{dI} \right) \cdot \left(\frac{dn}{dI} \right) \\
&= \left[\left(\frac{d}{dn} \frac{dV_j}{dn} \right) \cdot \frac{dn}{dI} + \frac{dV_j}{dn} \cdot \left(\frac{d}{dn} \frac{dn}{dI} \right) \right] \cdot \left(\frac{dn}{dI} \right) \\
&= \left[\frac{d^2 V_j}{dn^2} \cdot \frac{dn}{dI} - \frac{dV_j}{dn} \cdot \left(\frac{dn}{dI} \right)^2 \cdot \left(\frac{d^2 I}{dn^2} \right) \right] \cdot \left(\frac{dn}{dI} \right) \\
&= \frac{d^2 V_j}{dn^2} \cdot \left(\frac{dn}{dI} \right)^2 - \frac{dV_j}{dn} \cdot \left(\frac{dn}{dI} \right)^3 \cdot \left(\frac{d^2 I}{dn^2} \right)
\end{aligned} \tag{2.27}$$

However, it is still possible to separate the expressions into components related to the two parts:

1. The $\frac{d^2 V_j}{dn^2}$ and $\frac{dV_j}{dn}$ terms depend only on the carrier concentration dependency on quasi-Fermi levels (Boltzmann or Fermi-Dirac statistics may apply; use 3-D or 2-D density of states for bulk or quantum-well active region).
2. The $\frac{dn}{dI}$ and $\frac{d^2 I}{dn^2}$ terms relate to the recombination mechanism.

Therefore, the current derivatives of the junction voltage can be traced to the multiplication of the V_j - n and the I - n relations. They will be discussed in more details below.

2.4.2 The V_j - n relation in a homogeneous intrinsic quasi-neutral bulk active region

The $\frac{d^2 V_j}{dn^2}$ and $\frac{dV_j}{dn}$ terms in (2.26) and (2.27) indicate how fast the carrier concentration can be increased by increasing the quasi-Fermi level splitting. We assume that most of the recombination happens in a homogeneous, neutral and intrinsic active region. For bulk semiconductor with simple parabolic band structure, they are related through Fermi-Dirac integral as

$$\begin{cases} n = N_C \cdot \mathcal{F}_{1/2} \left(-\frac{V_{cf}}{V_T} \right) \\ p = N_V \cdot \mathcal{F}_{1/2} \left(-\frac{V_{fv}}{V_T} \right) \\ V_j = (E_{Fn} - E_{Fp}) / q = (E_g / q) - V_{cf} - V_{fv} \end{cases} \quad (2.28)$$

where $\mathcal{F}_{1/2}$ is the Fermi integral of order 1/2 defined as

$$\mathcal{F}_{1/2}(\zeta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}}{1 + \exp(x - \zeta)} dx \quad (2.29)$$

where $V_T = k_B \cdot T / q$ is the “thermal voltage” with T being the lattice temperature and k_B being the Boltzmann’s constant. The energy levels are shown in Figure 2.2. E_{F0} is the carrier Fermi energy at thermal equilibrium. E_g is the bandgap of active material. N_C , N_V are the conduction band and the valence band effective density of states. E_{Fn} and E_{Fp} are electron and hole quasi-Fermi level respectively. V_{cf} is the difference between the conduction band edge and the

electron quasi-Fermi level, V_{fv} is the difference between the hole quasi-Fermi level and the valance band edge.

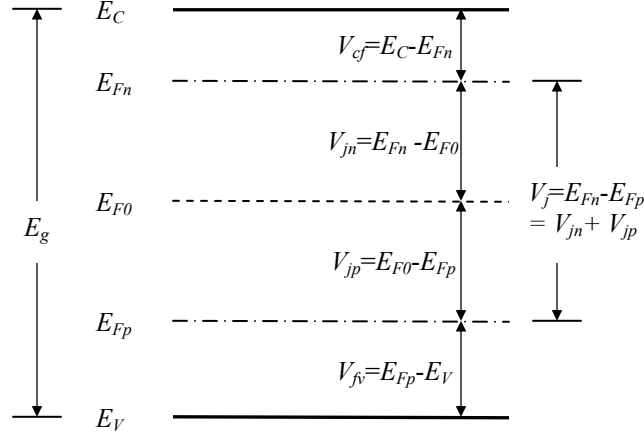


Figure 2.2: Nomenclatures for the energy levels in the active layer material.

In general, the V_{j-n} is expected to be complicated in a real device. However, if the material is intrinsic, charge neutrality is valid and the region of interest is homogeneous, some greatly simplified results can be found. For heterostructure LEDs and LDs under moderate biased levels, these assumptions might be valid. The simplification is shown as follows.

When these conditions are met, the Fermi-Dirac distribution can be approximated by Maxwell-Boltzmann distribution as

$$\begin{cases} n = N_C \cdot \exp\left(-\frac{V_{cf}}{V_T}\right) \\ p = N_V \cdot \exp\left(-\frac{V_{fv}}{V_T}\right) \\ n = p \end{cases} \quad (2.30)$$

Multiplying n and p results in

$$n^2 = N_C \cdot N_V \cdot \exp\left(-\frac{V_{cf} + V_{fv}}{V_T}\right) = N_C \cdot N_V \cdot \exp\left(\frac{V_j - E_g}{V_T}\right) \quad (2.31)$$

then the carrier concentration can be expressed in terms of junction voltage as

$$n = n_0 \cdot \exp\left(\frac{V_j}{2 \cdot V_T}\right) \quad (2.32)$$

with

$$n_0 = N_C \cdot N_V \cdot \exp\left(-\frac{E_g}{2 \cdot V_T}\right) \quad (2.33)$$

Therefore, in this simplest case

$$\frac{dV_j}{dn} = \frac{V_T}{n} \cdot 2 \quad (2.34)$$

Note that at a very low bias level, the band-bending in a device active region may be strong so that charge neutrality will not be met.

When the Boltzmann distribution is no longer valid, carrier densities have to be calculated numerically with the Fermi-Dirac integral as:

$$n^2 = N_C \cdot N_V \cdot \left[\mathcal{F}_{1/2} \left(-\frac{V_{cf}}{V_T} \right) \right] \cdot \left[\mathcal{F}_{1/2} \left(-\frac{V_{fv}}{V_T} \right) \right] \quad (2.35)$$

with

$$V_j = (E_{Fn} - E_{Fp}) / q = (E_g / q) - V_{cf} - V_{fv} \quad (2.36)$$

Obviously the result will approach (2.32) when both the electron quasi-Fermi level and the hole quasi-Fermi level are far away from the corresponding band edge. In this case, the splitting of the quasi-Fermi levels is symmetric, i.e. the difference in N_C , N_V cannot be “felt” by carriers so that the total V_j will be divided into equal halves for electrons and holes, resulting in a factor of 2 in (2.34).

The above derivation is for intrinsic material. For moderately doped material, there will be “majority carriers” and “minority carriers”. Following the same procedure, it can be found that this factor will be 1.0.

When V_j is approaching E_g , due to the different effective density of states, the splitting is expected to be asymmetric and should be affected by

1. The N_C/N_V ratio, i.e. the curvature difference in the parabolic E - k diagram between the conduction and valence bands. The corresponding quasi-Fermi level is expected to move faster with a smaller density of states in order to achieve the same carrier concentration to maintain charge neutrality.
2. The distribution function, or how close to the band edges the quasi-Fermi levels are. This is reflected in the $(V_j - E_g/q)$ value.

Compared with (2.34), we define a band-filling factor ξ_1 associated with the first derivative so that

$$\frac{dV_j}{dn} = \frac{V_T}{n} \cdot \xi_1 \quad (2.37)$$

$$\xi_1 = \frac{dV_j}{dn} \cdot \frac{n}{V_T} = \frac{dV_j}{d(\ln n)} \cdot \frac{1}{V_T} \quad (2.38)$$

$\xi_1=1$ means the carrier density will double if quasi-Fermi level splitting is increased by an amount equal to thermal voltage. Similarly, a ξ_2 associated with the second derivative is defined as

$$\xi_2 = -\frac{d^2V_j}{dn^2} \cdot \frac{n^2}{V_T} \quad (2.39)$$

It will be shown later that ξ_1 is directly related to ideality factor while ξ_2 is not. Note that the total quasi-Fermi level splitting V_j can be divided into n - part and p - part with

$$V_j = V_{jn} + V_{jp} \quad (2.40)$$

as shown in Figure 2.2. The ξ values can also be divided into the two parts. For example,

$$\xi_1^{(n)} = \frac{dV_{jn}}{d(\ln n)} \cdot \frac{1}{V_T} = \frac{\mathcal{F}_{1/2}(V_{cf}/V_T)}{\mathcal{F}_{-1/2}(V_{cf}/V_T)} \quad (2.41)$$

$$\xi_1^{(p)} = \frac{dV_{jp}}{d(\ln p)} \cdot \frac{1}{V_T} = \frac{\mathcal{F}_{1/2}(V_{fv}/V_T)}{\mathcal{F}_{-1/2}(V_{fv}/V_T)} \quad (2.42)$$

where $\mathcal{F}_{\pm 1/2}$ is the Fermi integral of order $\pm \frac{1}{2}$. Due to the difference between the conduction band and the valance band density of states, V_{cf} and V_{fv} are different with the same V_j except at low bias level, and therefore the corresponding band-filling factors are different.

If the material is known, the N_C/N_V ratio is known, then ξ can be described solely as a function of $(V_j - E_g/q)$. We define a “voltage number” n_V indicating how many multiples of the thermal voltage the quasi-Fermi level splitting is above the bandgap by normalizing the junction voltage to thermal voltage as:

$$n_V = \frac{V_j - E_g / q}{V_T} \quad (2.43)$$

Numerical examples of the band-filling factor ξ as function of n_V are shown in the Figure 2.3. Parameters for the calculation are listed in Table 2.2. ξ_1 and ξ_2 are identical at low bias level ($n_V < -10$). At high bias level, ξ_1 and ξ_2 both increase with junction voltage while they are different between each other. In Figure 2.4, the electron and the hole contributions to the band-filling factors ξ_1 are plotted as function of normalized junction quasi-Fermi level splitting. It can be seen that due to the large density of states, the hole quasi-Fermi level barely moves even at high bias level, resulting in only a small variation for the entire bias region. In other words, the band-filling factors are mainly from the contribution of electrons.

Table 2.2: Parameters for the calculations used in the example.

Parameter	Symbol	Value/Unit
Bandgap	E_g	1.42 eV
Electron effective mass	m_e^*	0.067 m_0
Hole effective mass	m_h^*	0.48 m_0
Conduction band effective density of states	N_C	$4.42 \times 10^{17} \text{ cm}^{-3}$
Valance band effective density of states	N_V	$8.47 \times 10^{18} \text{ cm}^{-3}$
Acceptor concentration	N_A	0
Donor concentration	N_D	0

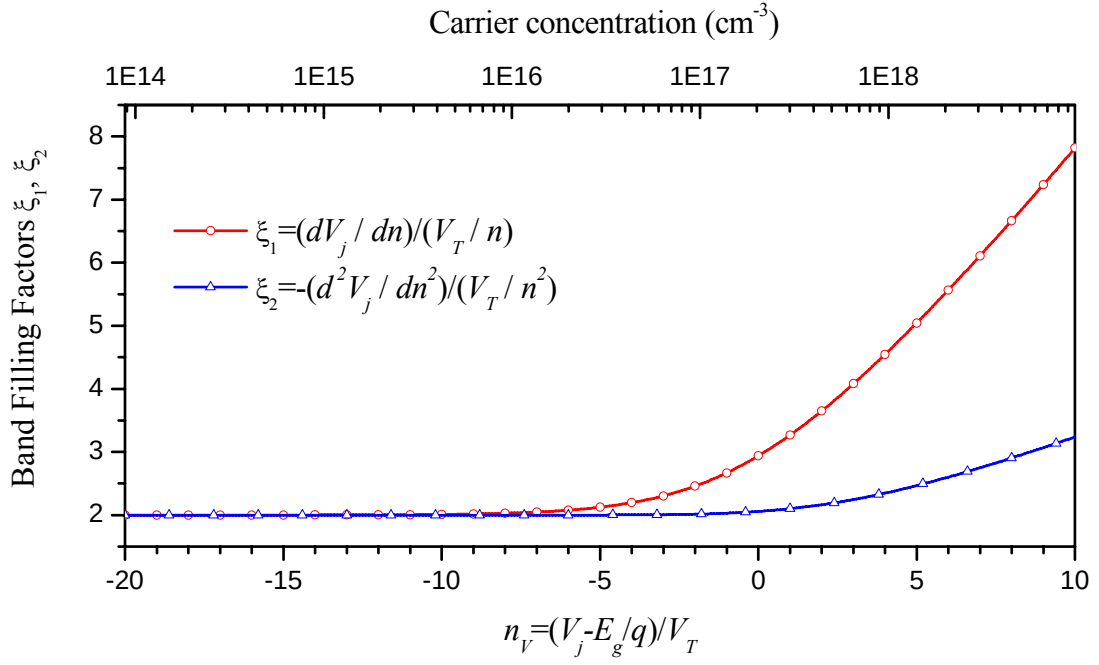


Figure 2.3: Numerical values of band-filling factors ξ_1 and ξ_2 as function of normalized junction quasi-Fermi level splitting. Corresponding carrier concentration is indicated on the top axis.

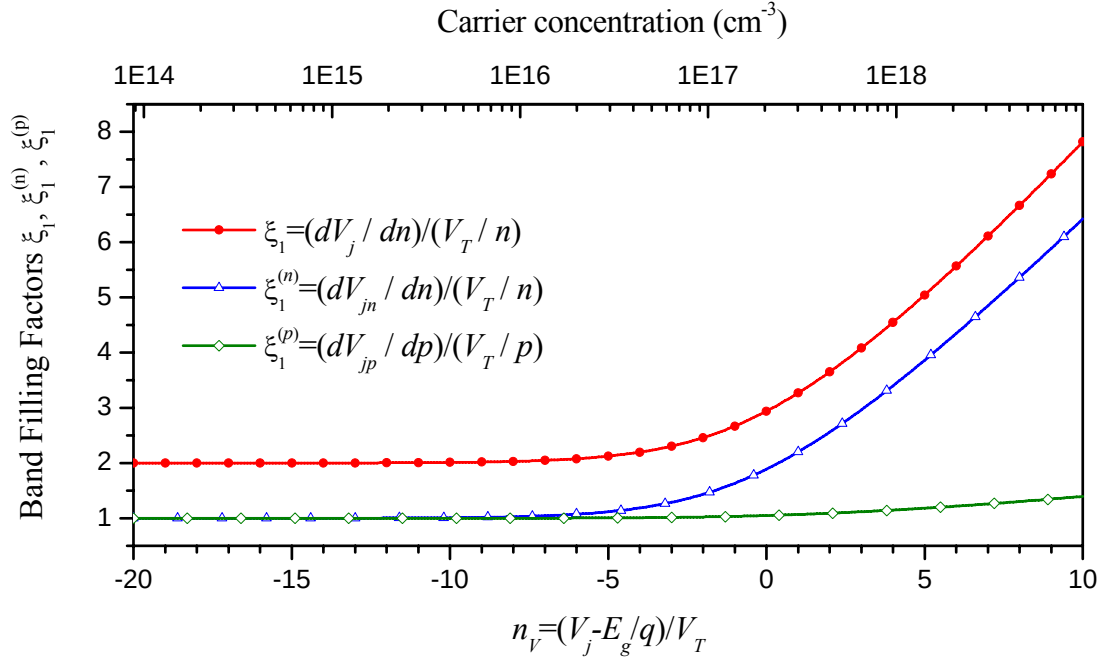


Figure 2.4: The electron and the hole contribution to the band-filling factors ξ_1 as function of normalized junction quasi-Fermi level splitting. Corresponding carrier concentration is indicated on the top axis.

In conclusion, the defined band-filling factors ξ_1 and ξ_2 :

- Arise from the carrier distribution function. They are constant and equal when the junction is biased at a low voltage level.
 - Deviation from the low biased level constant values ($\xi_{1,2} > \xi_0 = 2$) and from each other ($\xi_1 \neq \xi_2$) are negligible until the number $n_V > -10$, i.e. the quasi-Fermi level splitting is close to bandgap.
 - ξ is mainly a function of the N_C/N_V ratio (determined by material) and the n_V number (determined by bias level). With a given material, both ξ_1 and ξ_2 reflect the difference between the Boltzmann distribution and the Fermi-Dirac distribution.
 - ξ can be divided into the contribution from electrons and the contribution from holes.
- Due to the large different density of states between the two kinds of carries, normally the contribution from electrons is much higher than that from holes.

2.4.3 Ideality factors with power-law recombination currents in a neutral region

The $\frac{dn}{dI}$ and $\frac{d^2I}{dn^2}$ terms in the derivatives (2.26) and (2.27) tell us how the currents are related to carrier concentrations. Unlike drift or tunneling processes, if the current is from recombination, i.e. the annihilation of electrons and holes accompanied by the generation of heat or light, very often there are explicit relationships between the recombination currents and the carrier densities such as the power-law dependency:

$$I \propto n^\kappa \quad (2.44)$$

where κ is the power factor determined by the recombination mechanism.

With the power-law I - n relationship, the first derivative can be expressed with

$$\frac{dn}{dI} = \frac{n}{I} \cdot \frac{1}{\kappa} \quad (2.45)$$

and the second derivatives can be written in forms such as

$$\frac{d^2I}{dn^2} = \frac{I}{n^2} \cdot \kappa \cdot (\kappa - 1) \quad (2.46)$$

Therefore, for recombination currents with power-law carrier density dependencies, there are simple analytical expressions for the derivatives.

The first and the second derivative ideality factors are previously defined as

$$\begin{cases} m_1 = \frac{I}{V_T} \cdot \frac{dV_j}{dI} \\ m_2 = -\frac{I^2}{V_T} \cdot \frac{d^2V_j}{dI^2} \end{cases} \quad (2.47)$$

With the derivatives from the V_j - n and I - n relationship, for recombination currents with

$I \propto n^\kappa$, the junction differential resistance will be

$$\begin{aligned} \frac{dV_j}{dI} &= \left(\frac{dV_j}{dn} \right) \cdot \left(\frac{dn}{dI} \right) \\ &= \left(\frac{V_T}{n} \cdot \xi_1 \right) \cdot \left(\frac{n}{I} \cdot \frac{1}{\kappa} \right) \\ &= \frac{V_T}{I} \cdot \frac{\xi_1}{\kappa} \end{aligned} \quad (2.48)$$

Therefore the associated first derivative ideality factor is

$$m_1 = \frac{I}{V_T} \cdot \frac{dV_j}{dI} = \frac{\xi_1}{\kappa} \quad (2.49)$$

The second derivative from (2.27) becomes

$$\begin{aligned} \frac{d^2V_j}{dI^2} &= \frac{d^2V_j}{dn^2} \cdot \left(\frac{dn}{dI} \right)^2 - \frac{dV_j}{dn} \cdot \left(\frac{dn}{dI} \right)^3 \cdot \left(\frac{d^2I}{dn^2} \right) \\ &= \frac{d^2V_j}{dn^2} \cdot \left(\frac{n}{I} \cdot \frac{1}{\kappa} \right)^2 - \frac{dV_j}{dn} \cdot \left(\frac{n}{I} \cdot \frac{1}{\kappa} \right)^3 \cdot \left(\frac{I}{n^2} \cdot \kappa \cdot (\kappa - 1) \right) \\ &= \frac{d^2V_j}{dn^2} \cdot \left(\frac{n}{I} \cdot \frac{1}{\kappa} \right)^2 - \frac{dV_j}{dn} \cdot \left(\frac{n}{I^2} \cdot \frac{1}{\kappa^2} \cdot (\kappa - 1) \right) \\ &= \left(-\frac{V_T}{n^2} \cdot \xi_2 \right) \cdot \left(\frac{n}{I} \cdot \frac{1}{\kappa} \right)^2 - \left(\frac{V_T}{n} \cdot \xi_1 \right) \cdot \left(\frac{n}{I^2} \cdot \frac{1}{\kappa^2} \cdot (\kappa - 1) \right) \\ &= -\left(\frac{V_T}{I^2} \right) \cdot \frac{\xi_2}{\kappa^2} - \left(\frac{V_T}{I^2} \right) \cdot \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1) \\ &= -\left(\frac{V_T}{I^2} \right) \cdot \left[\frac{\xi_2}{\kappa^2} + \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1) \right] \end{aligned} \quad (2.50)$$

The second derivative ideality factor can be simplified as

$$m_2 = -\frac{I^2}{V_T} \cdot \frac{d^2V_j}{dI^2} = \frac{\xi_2}{\kappa^2} + \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1) \quad (2.51)$$

At low biased level, $\xi_1 = \xi_2 = \xi_0 = 2$, the ideality factors can be reduced to:

$$\begin{cases} m_1 = \frac{\xi_1}{\kappa} = \frac{2}{\kappa} \\ m_2 = \frac{\xi_2}{\kappa^2} + \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1) = \frac{2}{\kappa^2} + \frac{2}{\kappa^2} \cdot (\kappa - 1) = \frac{2}{\kappa} \end{cases} \quad (2.52)$$

It can be seen that m_1 and m_2 are the same so that a single constant ideality factor $m = \frac{2}{\kappa}$ can be used for this situation.

When the bias level is close to the voltage corresponding to bandgap energy, both ideality factors are dependent on ξ , i.e. they change with injection level following the ξ - n_V trends as previously discussed.

2.4.4 Summary of the derivative ideality factors

The derived relationship between the ideality factors and the electrical derivatives with the power-law dependency currents are summarized in Table 2.2. It can be seen that

- Each of the power law dependency currents obeys the ideal diode equation and it is possible to fit a constant ideality factor under the low junction voltage condition. The first and the second derivative ideality factors are the same for this condition.
- Ideality factors will increase from the low bias level constant values and will be different between m_1 and m_2 due to the difference in the band filling factor ξ_1 and ξ_2 when the number $n_V > -10$, i.e. the quasi-Fermi level splitting is close to or higher than bandgap.

Under this high injection condition, the derivative ideality factors with power law currents are functions of bias level as well as the effective density of states of each band.

Table 2.2: Summary of the first and the second electrical derivatives parameters with power-law recombination currents.

	First derivative	Second derivative
General V_j - I	$\frac{dV_j}{dI} = \frac{dV_j}{dn} \cdot \frac{dn}{dI}$	$\frac{d^2V_j}{dI^2} = \frac{d^2V_j}{dn^2} \cdot \left(\frac{dn}{dI}\right)^2 - \frac{dV_j}{dn} \cdot \left(\frac{dn}{dI}\right)^3 \cdot \left(\frac{d^2I}{dn^2}\right)$
V_j - n with charge neutrality	$\frac{dV_j}{dn} = \frac{V_T}{n} \cdot \xi_1$ $\xi_1=2$ for $q \cdot V_j \ll E_g$	$\frac{d^2V_j}{dn^2} = -\frac{V_T}{n^2} \cdot \xi_2$ $\xi_2=2$ for $q \cdot V_j \ll E_g$
n - I with $I \propto n^\kappa$	$\frac{dn}{dI} = \frac{n}{I} \cdot \frac{1}{\kappa}$	$\frac{d^2I}{dn^2} = \frac{I}{n^2} \cdot \kappa \cdot (\kappa - 1)$
V_j - I with charge neutrality and $I \propto n^\kappa$	$\frac{dV_j}{dI} = \frac{V_T}{I} \cdot \frac{\xi_1}{\kappa}$	$\frac{d^2V_j}{dI^2} = -\left(\frac{V_T}{I^2}\right) \cdot \left[\frac{\xi_2}{\kappa^2} + \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1)\right]$
Ideality factor m with charge neutrality and $I \propto n^\kappa$	$m_1 = \frac{I}{V_T} \cdot \frac{dV_j}{dI} = \frac{\xi_1}{\kappa}$ $m_1 = \frac{2}{\kappa}$ for $q \cdot V_j \ll E_g$	$m_2 = -\frac{I^2}{V_T} \cdot \frac{d^2V_j}{dI^2} = \frac{\xi_2}{\kappa^2} + \frac{\xi_1}{\kappa^2} \cdot (\kappa - 1)$ $m_2 = \frac{2}{\kappa}$ for $q \cdot V_j \ll E_g$

2.5 Ideality Factors with the ABC Recombinations Coefficients

The recombination currents in the active region of a device usually come from multiple mechanisms. For opto-electronic devices, very often they are described as

$$I \propto A \cdot n + B \cdot n^2 + C \cdot n^3 \quad (2.53)$$

where the constant A refers to the monomolecular recombination coefficient, B is the bimolecular recombination coefficient and C is the Auger recombination coefficient.

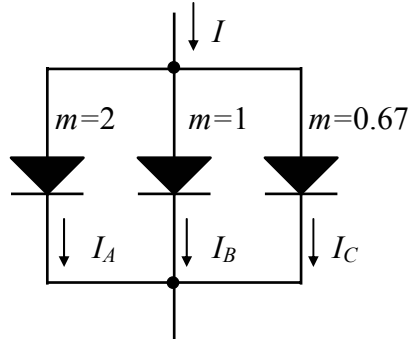


Figure 2.5: Equivalent circuit diagram for the active layer with the ABC recombination current paths.

The ideality factor associated with each of the components can be obtained from the previous derivation. At low bias level, each of them is $m = \frac{2}{\kappa}$ with κ being the power factor. Therefore the corresponding ideality factors for the individual A , B , C components are 2, 1, and 0.67 respectively.

However, in a device the three components are not isolated from each other. The equivalent circuit model is shown in Figure 2.5. Note that the three diodes share the same carrier

concentration and quasi-Fermi levels. The values of A , B and C correspond to the different “base strength” I_S of each diode branch, so that a diode can actually be “turned on” only when the carrier concentration reaches a certain level. It can be imagined that the variation of ideality factors as a function of bias voltage level will be dependent on the ratios of the ABC values. With some typical ABC values for GaAs material and the parameters as in Table 2.1, the first derivative ideality factor m_1 as a function of the quasi-Fermi level splitting is shown in Figure 2.6. The differences between m_1 and m_2 are shown in Figure 2.7. In Figure 2.8, the first derivative ideality factor m_1 and its n - and p - components are plotted as a function of normalized junction voltage. It can be seen that the rapid increase of ideality factor at very high bias level is mainly a contribution from the conduction band band-filling.

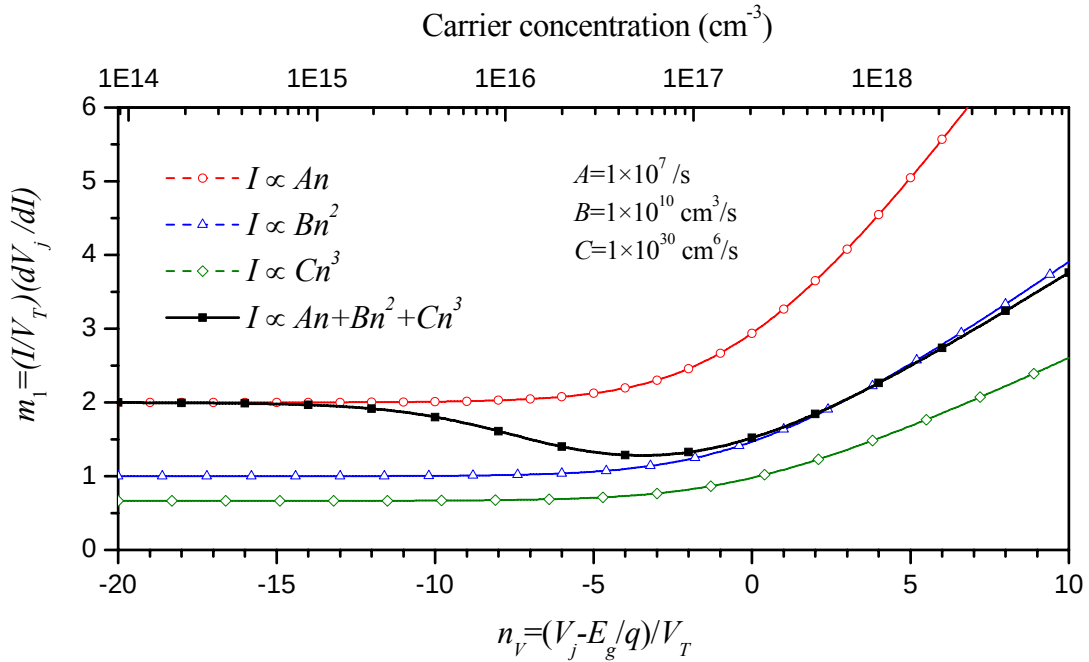


Figure 2.6: The first derivative ideality factors m_1 as function of junction voltage with the ABC model. The ideality factor has a “dip” due to the transition of dominant recombination mechanism when the bias voltage is close to bandgap.

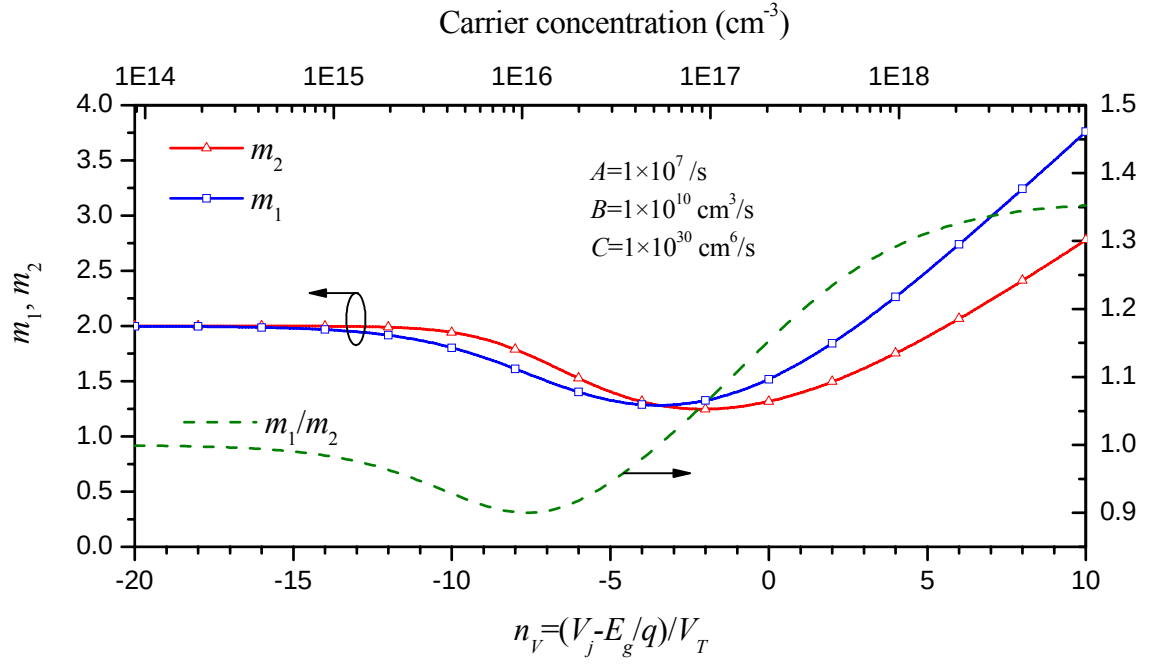


Figure 2.7: The first and the second derivative ideality factors as function of junction voltage with the *ABC* model. The ratio between the two derivative ideality factors is plotted as a dashed line.

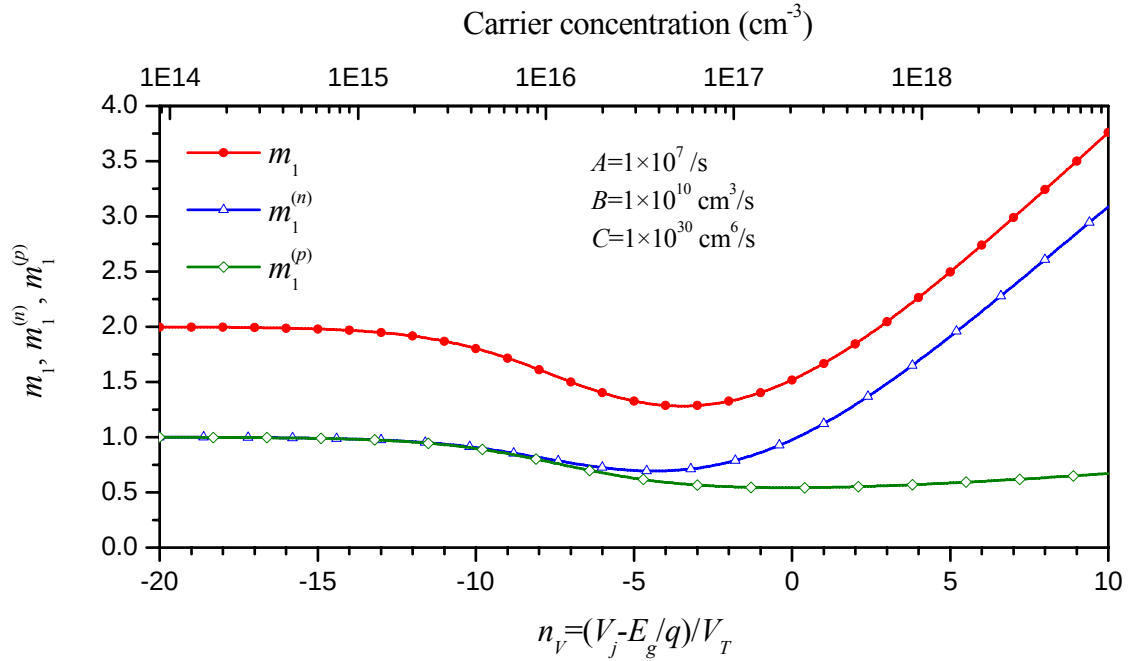


Figure 2.8: The first derivative ideality factor m_1 and its *n*- and *p*- components as a function of normalized junction voltage.

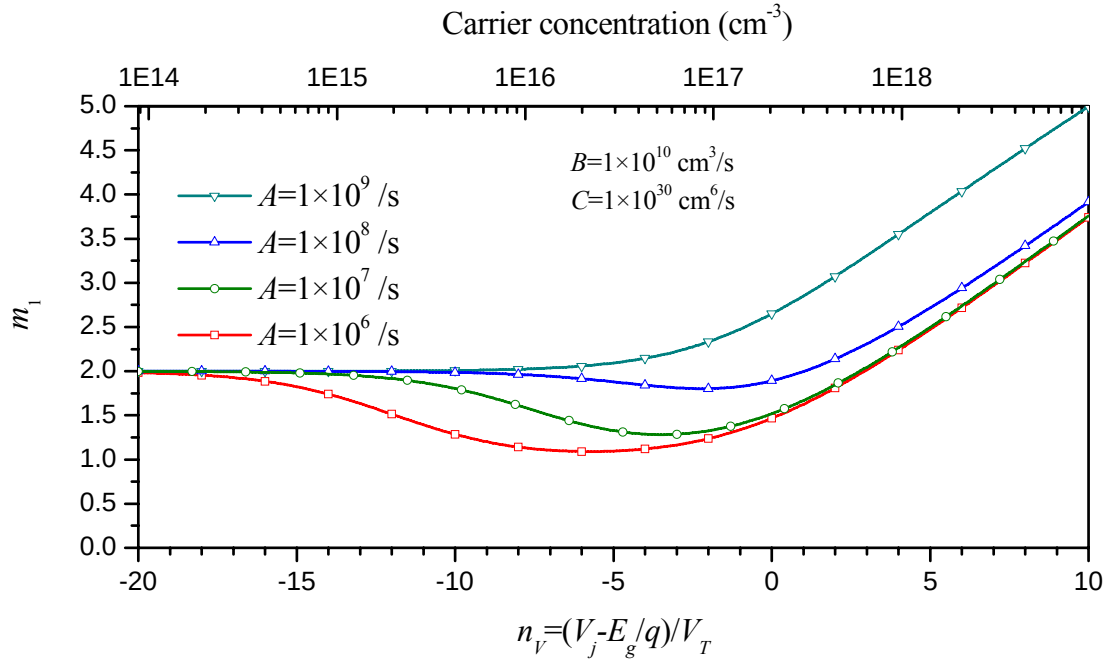


Figure 2.9: The first derivative ideality factor m_I with different monomolecular recombination coefficients as a function of normalized junction voltage.

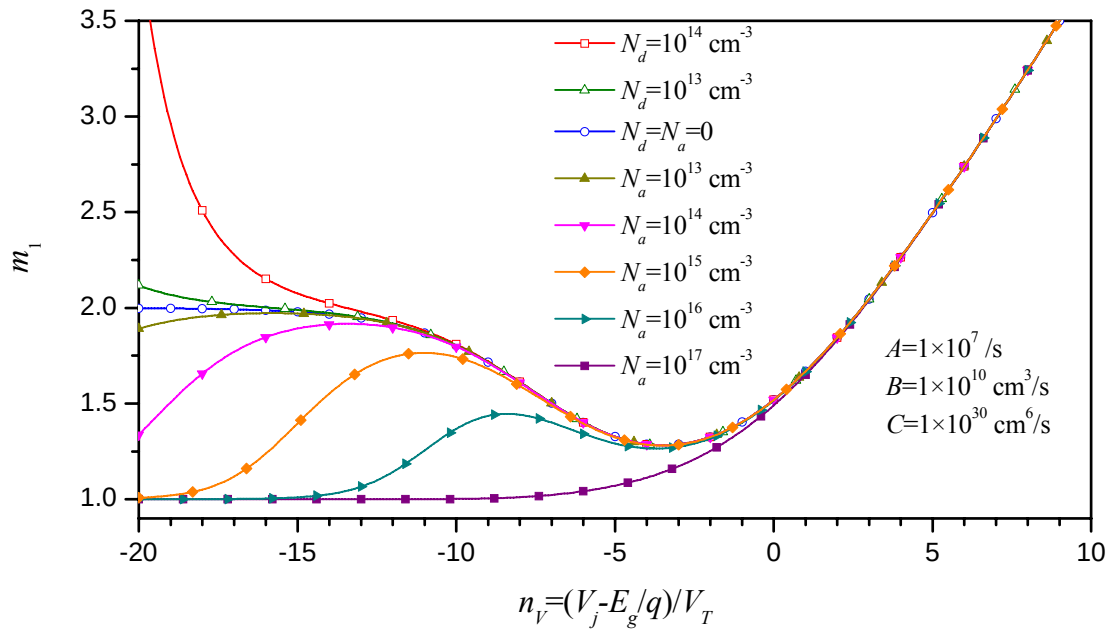


Figure 2.10: The first derivative ideality factor m_I with different doping concentrations as a function of normalized junction voltage.

In Figure 2.9, the first derivative ideality factors m_I with different monomolecular recombination coefficients are plotted as a function of normalized junction voltage. It can be seen that the transition region where a “dip” appears can disappear due to a large nonradiative recombination current. In Figure 2.10, the first derivative ideality factors m_I with different doping concentrations as a function of normalized junction voltage are shown. When the intrinsic assumption is relaxed, the ideality factor at low bias level no longer stays at 2.0 and it is affected by the doping concentration. Due to the large hole density of states, when the active region is heavily p -doped, hole quasi-Fermi level barely moves so that the total ideality factor is close to 1.0.

To conclude, the ideality factors of a homogeneous intrinsic quasi-neutral active region:

- They are a constant at very low current level, which is same as the ones with a single recombination path. They also change with bias (junction voltage) level when the quasi-Fermi level splitting is close to bandgap energy.
- With multiple recombination paths in the same active region, the ideality factors are different from the individual ones. New features such as “dips” or “kinks” may appear.
- At low internal junction voltage, if the monomolecular recombination (typically defect-related) is dominant, only the “ $2kT$ current” can be seen.
- The Auger recombination will dominate the I - V characteristics at extremely high bias level. It is normally overshadowed by other recombinations unless in situations with very high carrier concentration and small bandgap.
- For a good LED or LD where bimolecular recombination is desired to be dominant at normal injection levels, a “dip” or a kink in the ideality factor vs. junction voltage curve

is expected, as it is changing from nonradiative recombination with ideality factor of 2.0 to radiative recombination with ideality factor of 1.0. This kink is similar to those from laser threshold but the size should be much smaller. Nonetheless the kink will appear at a much smaller current value than the laser threshold.

- When the monomolecular recombination coefficient is large due to defects in the active region, the “dip” in the ideality factors may be reduced or even disappear.
- Most of the transitions in ideality factors happen when the quasi-Fermi level splitting is around the bandgap value.
- For given material, if the ABC coefficients (actually their ratio) are known, the ideality factors m_1 , m_2 and their ratio are basically determined by n_V or $(qV_j - E_g)$.
- When the intrinsic assumption is relaxed, the ideality factors from recombination in the active region at very low bias level will deviate from 2.0. As the ideality factor reflects the internal quasi-Fermi level movement, due to the different density of states of conduction band and valance band, the n - doping will normally increase the ideality factor while the p - type will decrease.

2.6 Measurements and Parameter Extraction

2.6.1 The first derivative ideality factor of light emitting diodes

The first derivative ideality factors of some commercial light-emitting diodes were tested. Their $L/I/V$ characteristics, the differential resistances (and therefore the first derivative ideality factors) and the dL/dV were measured. The details on the measurement system are described elsewhere [15, 16, 17]. The ideality factors and the dL/dV of LEDs with different materials are plotted in Figure 2.11 to Figure 2.14. These LEDs are made by Avago Technologies and the materials include AlGaAs, AlInGaP and InGaN.

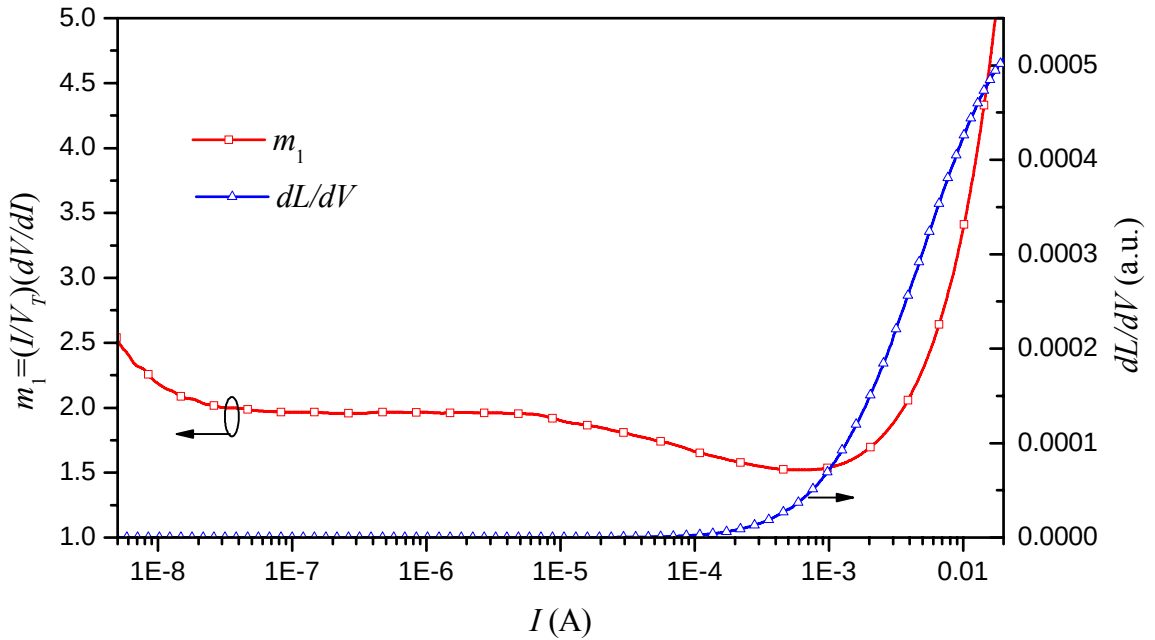


Figure 2.11: The measured first derivative ideality factor m_1 and dL/dV as a function of device current using a semi-logarithmic scale. The device is HLMP-K101 AlGaAs double heterostructure light emitting diode.

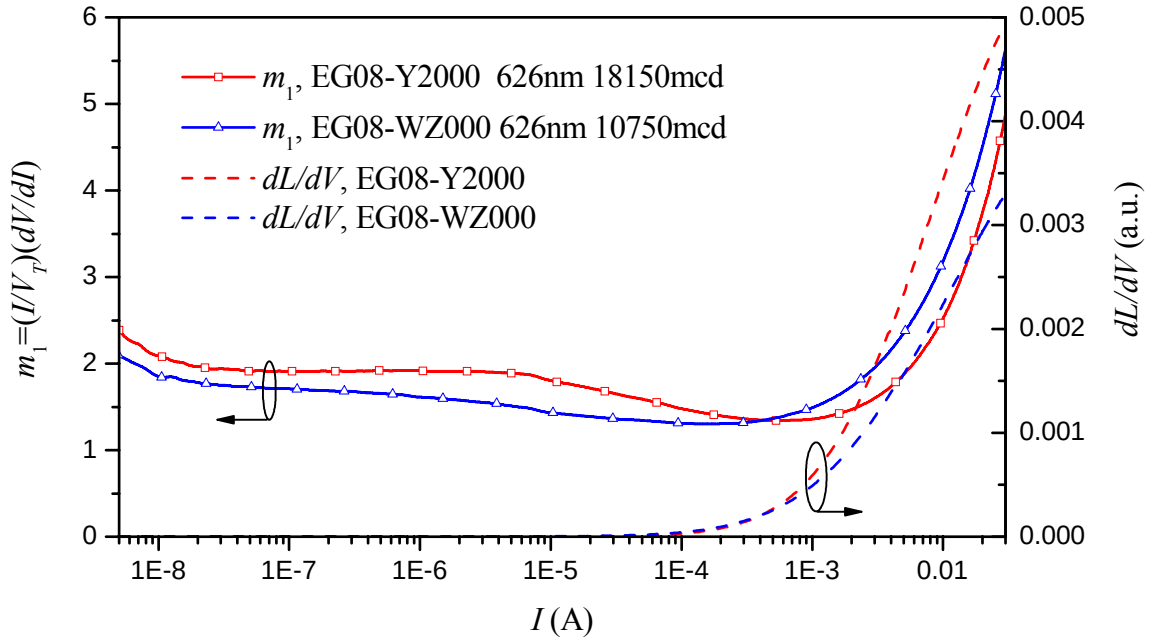


Figure 2.12: The measured first derivative ideality factor m_1 and dL/dV as a function of device current using a semi-logarithmic scale. The devices are EG08-WZ000 and EG08-Y2000 AlInGaP light emitting diodes.

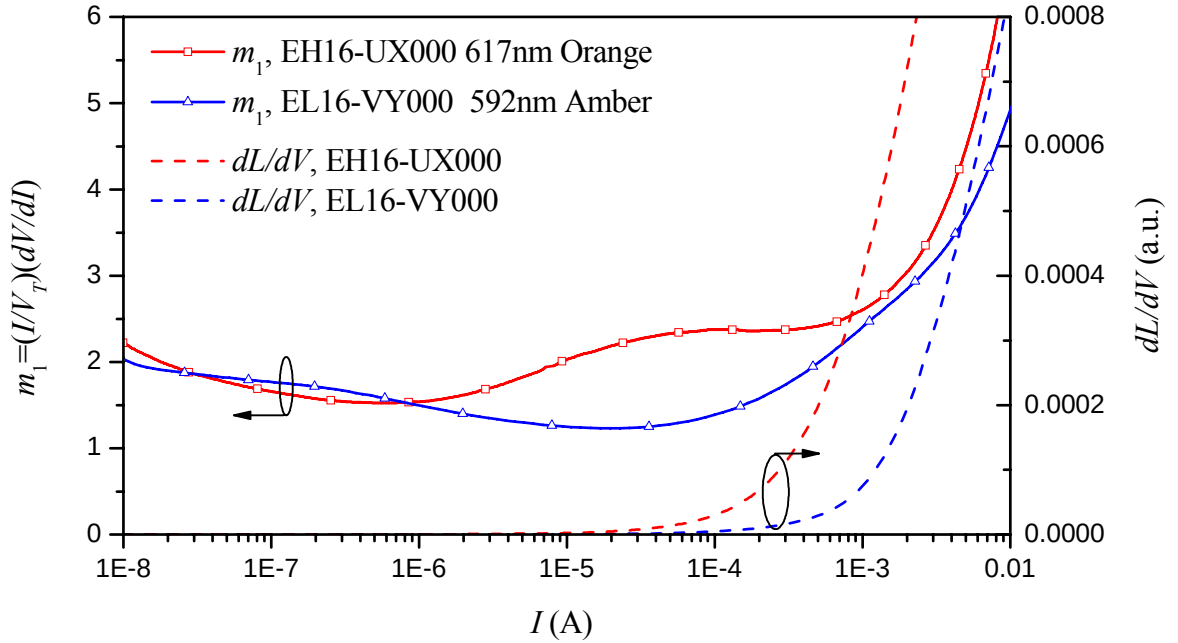


Figure 2.13: The measured first derivative ideality factor m_1 and dL/dV as a function of device current using a semi-logarithmic scale. The devices are EH16-UX000 and EL16-VY000 AlInGaP II light emitting diodes.

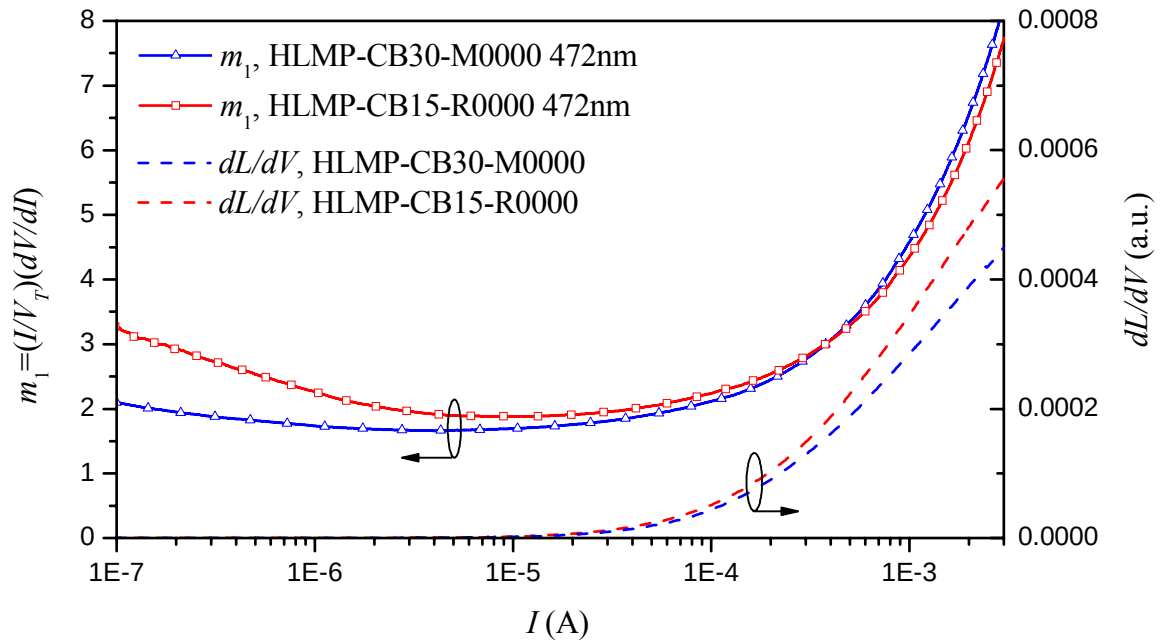


Figure 2.14: The measured first derivative ideality factor m_l and dL/dV as a function of device current using a semi-logarithmic scale. The devices are HLMP-CB15-R0000 and HLMP-CB30-M0000 InGaN blue light emitting diodes.

From Figure 2.11 to Figure 2.14, it can be seen in these LED derivative measurement data:

- The increase of spontaneous light output is accompanied by a change (normally a reduction or a “dip”) in the ideality factor.
- At low current level right before light emission is significant, the ideality factors of most LEDs are close to 2.0.
- At high current levels, all the ideality factors without extracting the series resistance increase rapidly with current.
- The AlGaAs double heterostructure LED (HLMP-K101) agrees best with the simple ABC model (ideality factor starts with almost 2.0 at low current, followed by a “dip” where light emission begins, and then increases with current.)

2.6.2 The first derivative ideality factor of laser diodes

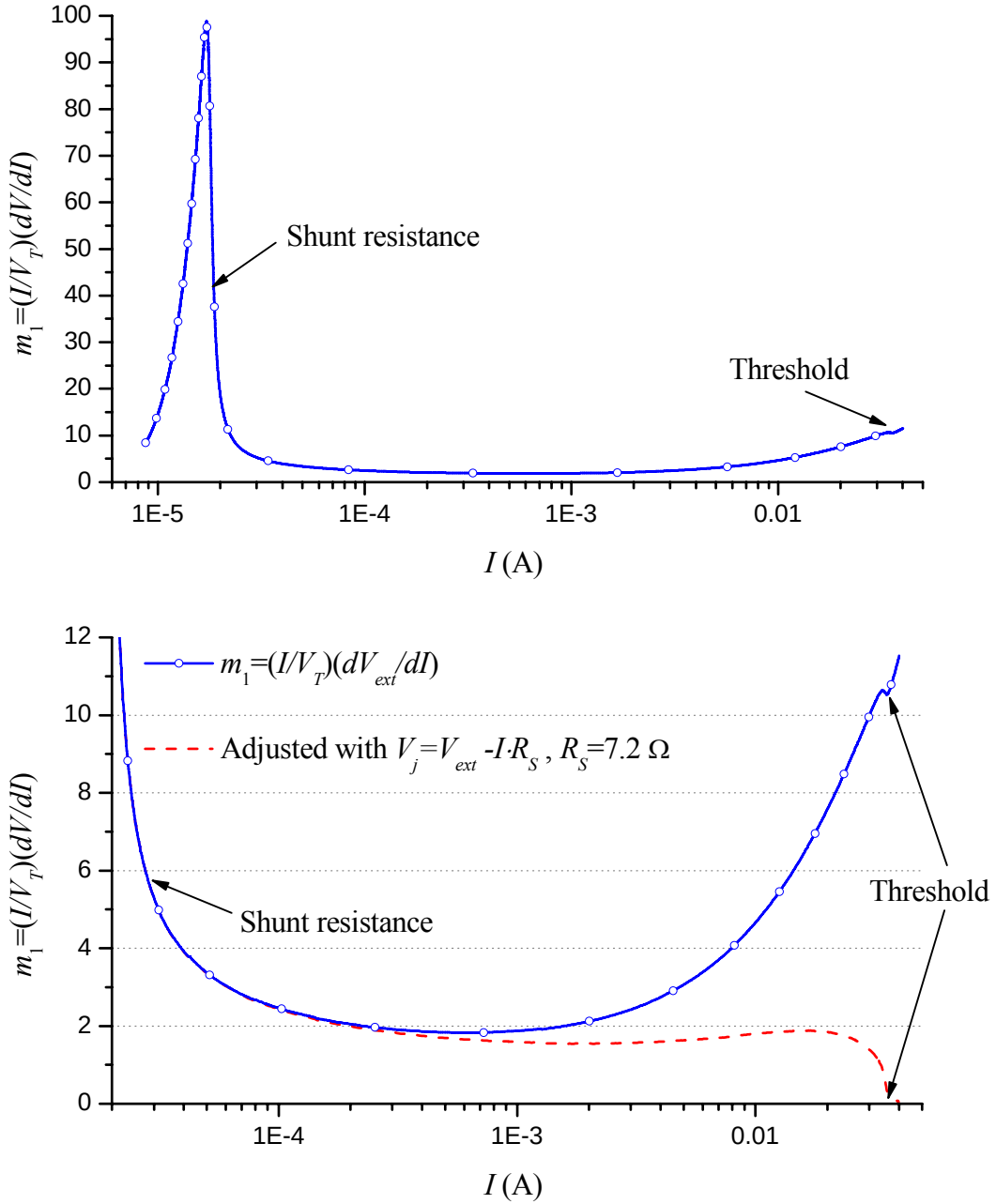


Figure 2.15: The calculated first derivative ideality factor m_1 as a function of device current using a semi-logarithmic scale. The device is a 654nm 10mW GH06510B laser diode from Sharp. The series resistance in the calculation is taken from the plateau of differential resistance after lasing threshold.

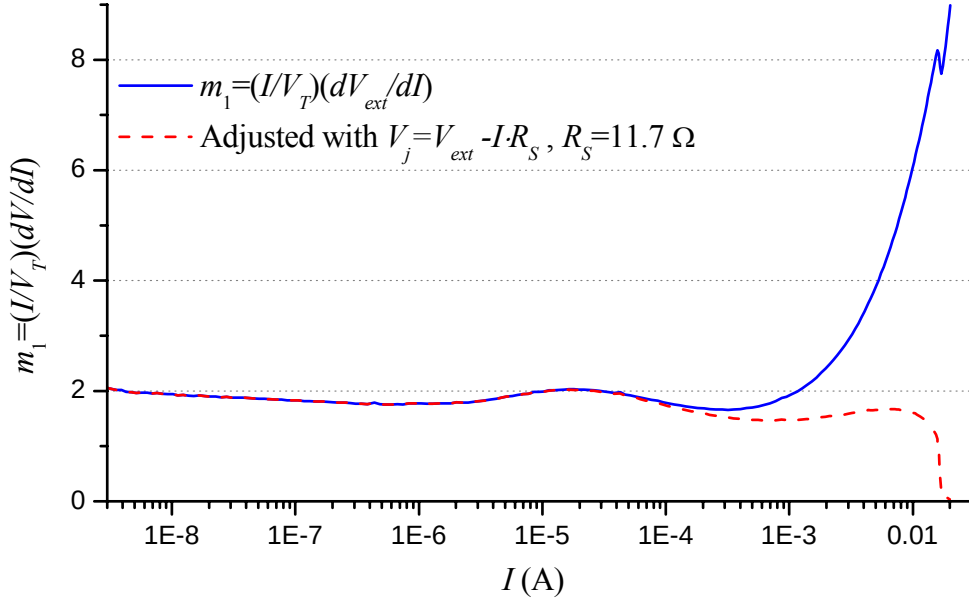


Figure 2.16: The calculated first derivative ideality factor m_1 as a function of device current using a semi-logarithmic scale. The device is a 650nm 5mW D650 laser diode from NVG. The series resistance in the calculation is taken from the plateau of differential resistance after lasing threshold.

In Figure 2.15 and Figure 2.16, the first derivative ideality factors m_1 are plotted as a function of device current in semi-logarithmic scale. The devices are 654nm 10mW GH06510B laser diode from Sharp and 650nm 5mW D650 from NVG. Unlike the LEDs, the series resistance of a laser diode can be estimated from plateau of differential resistance after lasing threshold. Similar to the LEDs, the ideality factors have a “dip” before lasing threshold where the spontaneous emission (radiative recombination) becomes significant. After threshold, the ideality factors drop to nearly zero as the internal quasi-Fermi level splitting is expected to

saturate. Note in Figure 2.15, the giant peak of ideality factor is most likely from the parallel shunt resistance as it goes to zero when the current is about zero.

2.6.3 Estimation of nonradiative recombination coefficient of a laser diode

With the model derived above, extraction of some device parameters become possible because:

- The ideality factor is a function of junction voltage, or actually “voltage number” ($qV_j - E_g)/k_B T$, which is independent of values such as device areas and absolute current densities. The curve is determined by the material and the ABC coefficients (actually $A:B:C$ ratio) only.
- The junction voltage can be inferred by $V_j = V_{ext} - I \cdot R_S$. Details about the validity of this assumption will be discussed in Chapter 3.
- For a given material, the bimolecular recombination coefficient B and the Auger recombination coefficient C are widely studied and their values are reportedly well known numbers. However, the monomolecular coefficient is dependent on many factors such as defect densities, material aging processes, which will vary from device to device.

Therefore, given a specific material and the B , C coefficients, and measurements of the derivative ideality factor measurements, it is possible to extract parameters including the A coefficient, series resistance R_S and equivalent bandgap E_g from only electric measurements. The nonradiative recombination coefficient of a laser diode is estimated in this example. The laser diode is a 650nm red laser diode with part number OED-LDP65001E from Lumex. The

detailed device structure is unknown but it is assumed that $B=1 \times 10^{10} \text{ cm}^3/\text{s}$ and $C=1 \times 10^{30} \text{ cm}^6/\text{s}$. The N_C/N_V ratio is unknown but the GaAs value of 19 is used. After measuring the differential resistance of the diode as a function of injection current, the fitting procedure is shown step by step in the following figures. The details are described in the figure captions.

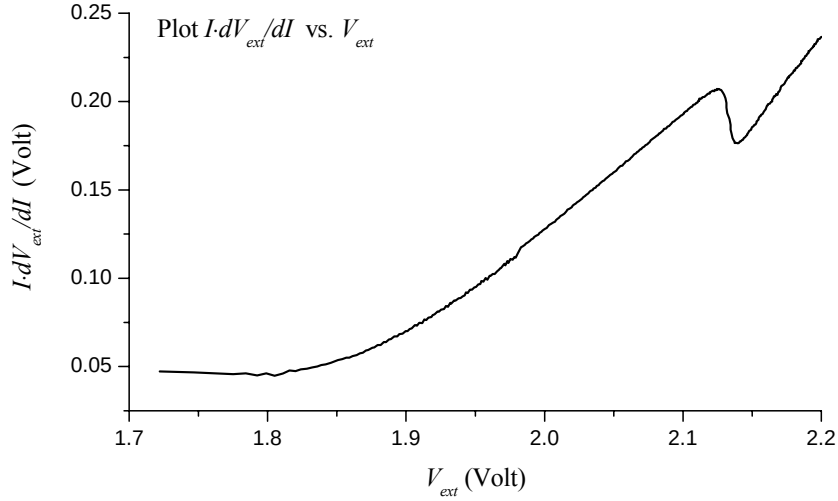


Figure 2.17: Step 1. Plot the $I \cdot dV_{ext}/dI$ vs. V_{ext} . The small kink at approximate 1.95V is a known range change in the experiment apparatus.

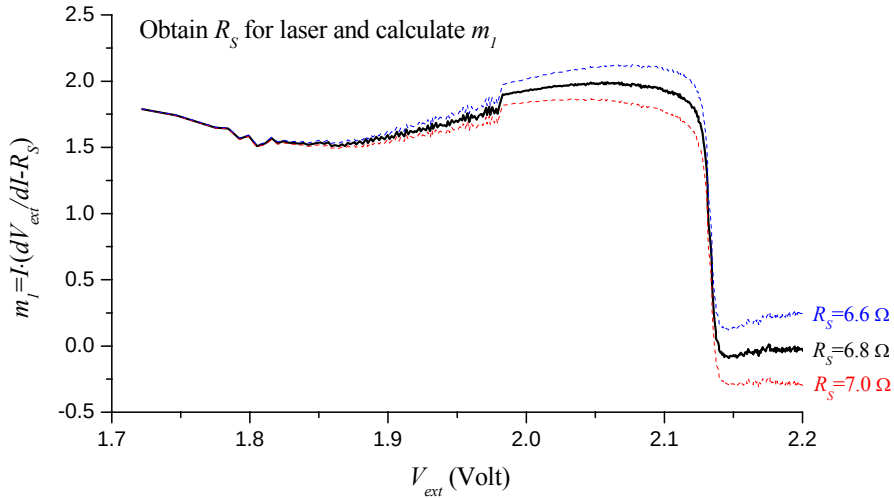


Figure 2.18: Step 2. Using the relation $m_I = I \cdot (dV_{ext}/dI - R_s)$, adjust R_s so that $m_I = 0$ after threshold. This approach assumes that quasi-Fermi level locking results in $m_I = 0$.

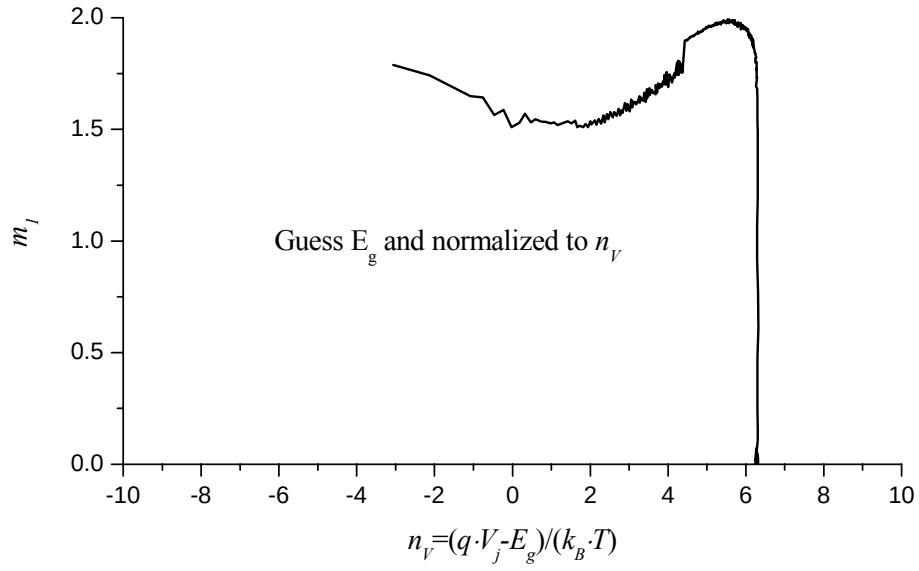


Figure 2.19: Step 3. With $n_V = (qV_j - E_g)/k_B T = (qV_{ext} - I \cdot R_S - E_g)/k_B T$, guess E_g so that qV_j is a few V_T higher than E_g at threshold. The kink at $n_V \approx 4$ is the range change that occurred at $V_{ext} \approx 1.95V$.

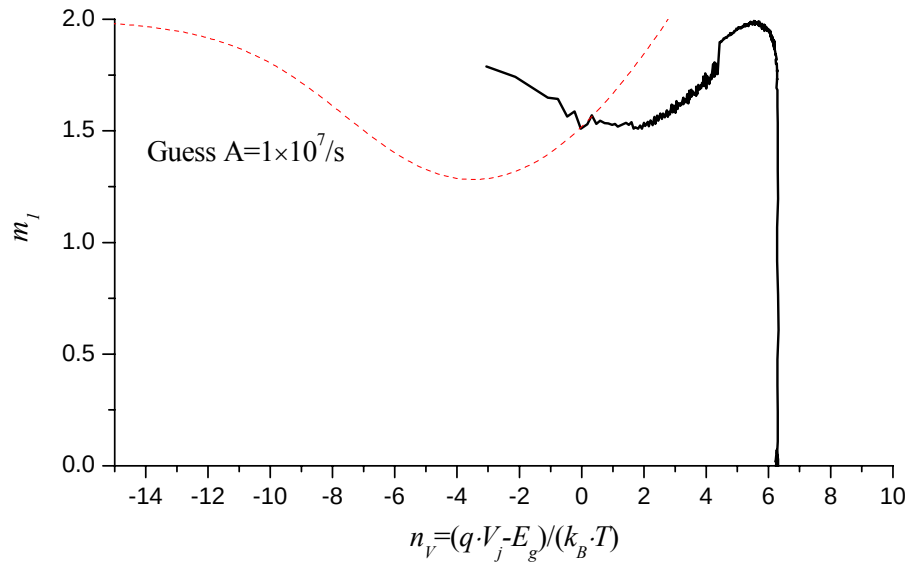


Figure 2.20: Step 4. Guess $A = 1 \times 10^7 / s$ and calculate the theoretical m_I - n_V curve.

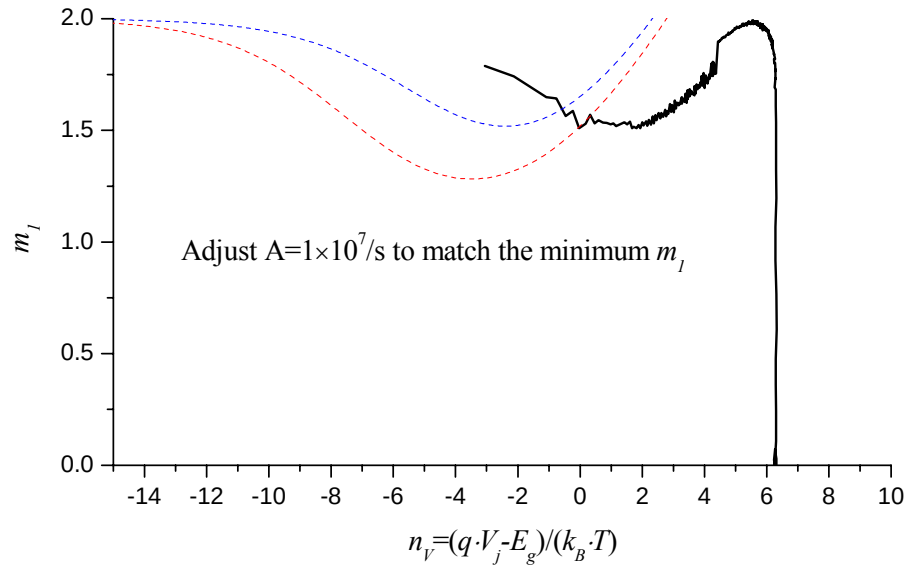


Figure 2.21: Step 5. Adjust coefficient A to $3.6 \times 10^7 / s$ to match the minimum value of m_l .

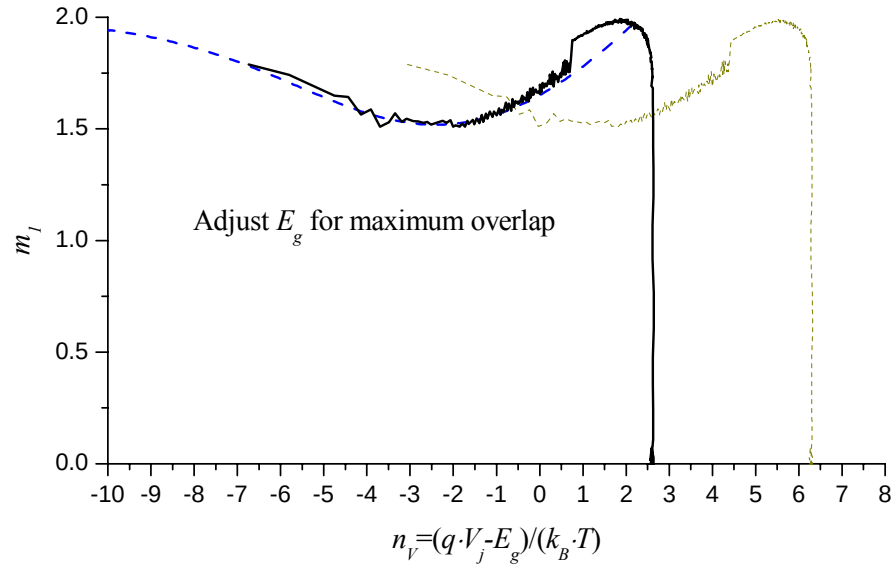


Figure 2.22: Step 6. Adjust E_g for maximum curve overlap.

The results from fitting are:

- Monomolecular coefficient $A=3.6 \times 10^7$ /s, or non-radiative lifetime $\tau_{NR}=27.8\text{ns}$.
- Series resistance $R_S=6.8\Omega$.
- Equivalent bandgap $E_g=1.895\text{eV}$, which is very close to the photon energy $h\nu=1.907\text{eV}$.
- If carrier density is $2 \times 10^{18} \text{ cm}^{-3}$ at threshold, the portion of nonradiative current at threshold consists of about 15% of the total current.

It is worth mentioning that the fitted absolute values are only estimations as the material and device structure are not known. However, the relative values can be used as indication of device quality, i.e. for those diodes whose nonradiative recombination coefficients are smaller, the “dip” will be deeper and vice versa.

2.7 Summary

In this chapter, the relation between the ideality factors and the electrical derivative measurements are investigated. The ideality factor is usually a constant measured from the slope in the semi-log scaled current-voltage graph. It can also be more directly measured from the electrical derivatives with the series resistance being extracted at the same time.

The diode ideality factor is no longer a constant at high injection level. The ideality factors measured from the electrical derivatives will vary with current, and the curves from different orders of derivative measurements on the same diode are not identical due to the current dependent local ideality factor. Non-constant “derivative ideality factor” is introduced and it

corresponds to the ideality factor calculated from the specific order of derivative measurement.

It is found that recombination currents that obey the power-law dependency on carrier densities will have fixed values of ideality factors at low bias conditions. The constant ideality factors are inversely proportional to the corresponding power factors. At a high injection level, the ideality factor with a single recombination mechanism will increase with current due to the significant difference between the Boltzmann and the Fermi-Dirac distribution function in the band filling.

With multiple recombination mechanisms in the same active region such as with the *ABC* model, changes in the derivative ideality factors can be observed when the additional recombination paths are turned on at high bias level. Examples are given on using the derivative measurement to extract the monomolecular recombination coefficient of a laser diode without any optical measurements.

Chapter 3

Semi-analytical Model for Differential Resistance and Ideality Factors of Double Heterostructure LEDs and LDs

3.1 Introduction

The ideal junction model described in Chapter 2 was based on the assumptions that the device currents are the total recombination currents in the active region (or the “junction”) of a light-emitting diode (LED) or a laser diode (LD), and the junction voltages refer to the quasi-Fermi level splitting of the active region. However, actual devices are always designed with multiple layers of materials in addition to the active layer so that carriers can be efficiently injected to this active layer and also be well confined in this region. Before carriers can reach the active layer, they have to go through multiple heterointerfaces and may

recombine in other layers, resulting in additional current recombination paths and a new voltage distribution profile. The process of carrier transport from the device terminals to the active region will inevitably alter the electrical characteristics of the diodes from pure “junction” properties to some new characteristics and it is therefore natural to investigate the effect of these processes on the electrical characteristics of the device.

The internal or the external voltages can be defined by the difference between the quasi-Fermi levels at layer boundaries. The external applied voltage is considered the quasi-Fermi level difference between the two outer-most layers, while the junction voltage is the quasi-Fermi level difference between electrons and holes within the active region, given that the active region is homogeneous. To be able to detect the characteristics of the internal active region from the device terminals, some conditions have to be met between the above two quasi-Fermi differences or the voltages. For example, the quasi-Fermi level at the device terminal could have a constant offset from the corresponding internal quasi-Fermi level, or the offset is small enough to be negligible. A more realistic and commonly used assumption is the existence of an equivalent linear series resistance for all layers other than the active layer. With this assumption, in a lumped circuit model for a diode, the two voltages (quasi-Fermi level differences) are related to each other through the device series resistance as

$$V_{ext} = I \cdot R_S + V_j \quad (3.1)$$

where V_{ext} is the terminal voltage, I is the diode current, R_S is the device series resistance including those from Ohmic contacts and from the resistance of the surrounding layers. V_j is the “junction voltage” being the quasi-Fermi level splitting in the active region.

For the series resistance R_S to be linear, we expected that drift transport is dominant outside the active layer and other recombination current paths are negligible. In practice, the series resistance R_S can be nonlinear from various components in devices such as the DBR mirrors or some Ohmic contacts. Nonlinearity of the series resistance can also arise from carrier transport through any heterojunction interface. For example, for a simplified double heterostructure diode as shown in Figure 3.1 (where the active layer is considered homogeneous and the band bending is negligible in this layer at high injection levels), the cladding layers are designed so that most carriers will be blocked from leaving the active region by the barrier created by the band discontinuity at the heterojunction interface. However, some carriers can overflow into the cladding layers to create nonlinearity in the $L/I/V$ characteristics and cause many other negative effects on the device performance.

Complicating the analysis is the possibility that the series resistance of the surrounding layer is nonlinear because of the interaction between the layers including the active region. The majority carrier transport over heterointerfaces can also be responsible for nonlinear current-voltage characteristics even in the absence of minority carrier leakage over the barrier at the interface or recombination within the cladding layer. At the interface of the heterojunction, if the thermionic emission process is important for current injection, the cladding layer and the active region can interact with each other through the forward and backward fluxes of carriers across the boundary. Nevertheless, as in Figure 3.1, there could be depletion layers in both cladding layers next to the active region. Majority carriers may have to overcome a barrier created by the depletion region band-bending before reaching the active layer [51].

The focus of this chapter is the nonlinear series resistance resulting from the majority carrier injection across heterojunction interface. The effects from the minority carrier overflow will be discussed in the next chapter. A semi-analytical model is developed for a double heterostructure device as in Figure 3.1. The device is obviously over-simplified but it is helpful to understand important factors that are related to the nonlinearity of the resistance from carrier transport over heterojunction interfaces.

The remainder of this chapter is organized as follows. The assumptions for the model are presented in Section 3.2, and the current-voltage relationship is derived with the “*thermionic emission-diffusion*” and the “*thermionic emission*” approaches in Section 3.3. The results with this current-voltage relationship are discussed in Section 3.4. The interactions between the cladding layer and the active region of double heterostructure devices are found to be significant with this model. The mechanism of the interaction and the effects on the differential resistances and ideality factors of the simple double heterostructure diode are demonstrated. The discussion is further extended to laser diodes with junction quasi-Fermi level saturation at laser threshold in Section 3.5. Finally summary and concluding remarks are presented in Section 3.6.

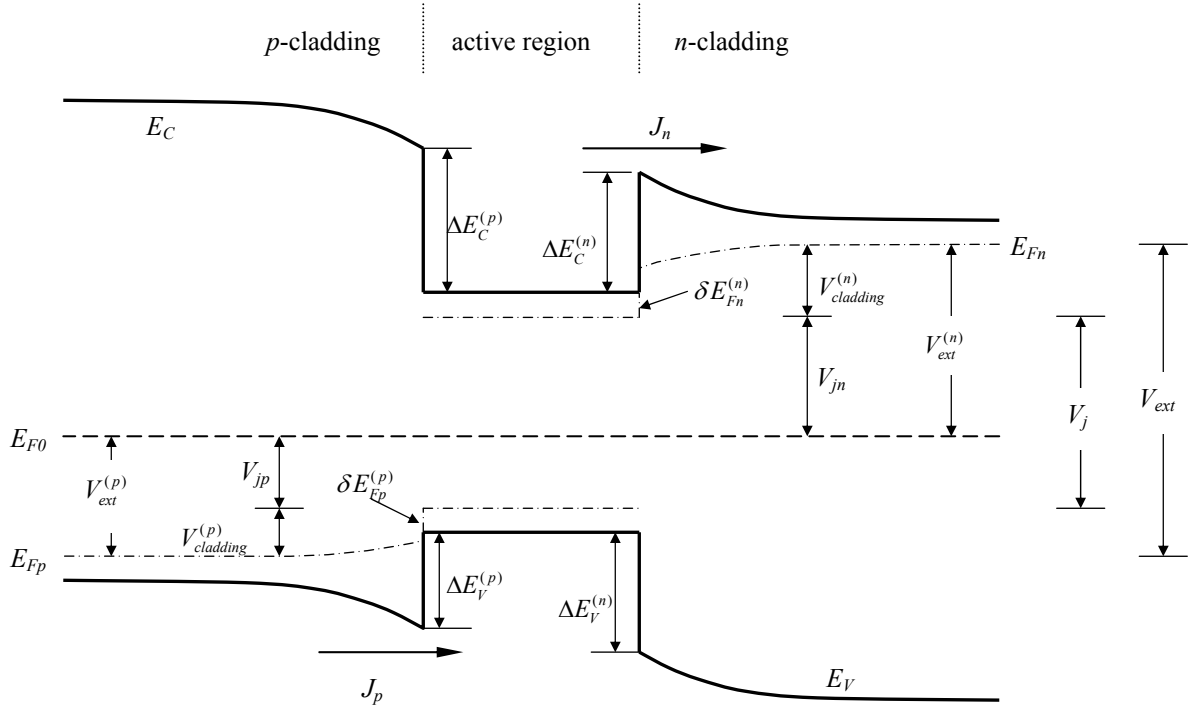


Figure 3.1: Band diagram of a simple double heterostructure diode under high injection condition. The justification of this model is presented in Section 3.2.

3.2 Assumptions for the Model

The model assumes that the transport within the bulk cladding layer is governed by the classical drift-diffusion mechanism while the transport across the abrupt heterojunction with different effective masses is limited by the thermionic emission process. The current-voltage equation is derived by equating the drift-diffusion current to the thermionic emission current at the heterojunction boundary. There are some important assumptions for this model including:

- Band diagram in the homogeneous active region is flat under high injection conditions.

Justifications: when the active region quasi-Fermi level splitting is close to the band-gap

energy, or when lasing thresholds are reached for laser diodes, the active layer band-bending is negligible and the quasi-Fermi level is flat across the entire active region.

- All electrons and holes will recombine in the active layer and the injection efficiency is 100%. Justification: for well designed and processed devices using a well behaved material system, neither the over-barrier leakage current nor the parallel leakage current is significant in the device so that they are neglected in this model. All the nonlinearity comes from majority carrier transport from the cladding layer to the active layer in this simplified model.
- Classical drift-diffusion transport applies within the bulk cladding layer while recombination is neglected in this region. Justification: the cladding layer thickness is normally much longer than the mean free path of carriers so that the microscopic effects such as quantum mechanical scattering can be included in the macroscopic material parameters.
- The (full) depletion approximation for the cladding layer applies. The band-bending is in the direction which creates carrier depletion, and the bending profile is quadratic. The space charge layer or the depletion region width W_d is related to the amplitude of band-bending $V_{bending}$ as $W_d = \sqrt{2 \cdot \epsilon \cdot V_{bending} / q \cdot N_i}$, where q is the electron charge, N_i is the impurity dopant (acceptor or donor) concentration, ϵ is the permittivity of the cladding layer. The cladding layer thickness is assumed always longer than the thickness of depletion layer so that no effects from contacts need to be considered.

- For carrier transport over the abrupt heterojunction interface, Wu and Yang's derivation [52-56, 59-68] is considered as a good approximation. Although the Maxwellian distribution was assumed in their formulation, which may not be valid for high injection levels where carriers are degenerate, this formulation offers tremendous simplification in the analytical derivation and it is adapted in our model. With the heterojunction as shown in the figure below, the electron quasi-Fermi level E_{Fn} is neither continuous nor flat across the heterointerface and there is a discontinuity $\delta E_{Fn}^{(n)}$ at the heterojunction boundary. The current density across the interface is described as

$$J_n = q \cdot \left(n_1 \cdot v_{n1} - n_2 \cdot v_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{-\Delta E_C^{(n)}}{V_T}\right) \right), \quad (3.2)$$

where n_1 is the electron concentration on the n -cladding layer edge of the boundary, n_2 is the active region electron concentration. $V_T = k_B \cdot T / q$ is the thermal voltage with T being the lattice temperature and k_B being the Boltzmann's constant. $m_{n1,2}^*$ are the electron effective masses in the cladding layer and the active layer respectively. $\Delta E_C^{(n)}$ is the conduction band discontinuity at the n -cladding/active layer interface. $v_{n1,2}$ are electron thermal velocities in each material defined as $v_{n1,2} = \sqrt{2 \cdot k_B \cdot T / (\pi \cdot m_{n1,2}^*)}$. The first term in equation (3.2) corresponds to the forward injection flux from the cladding layer to the active region, and the second term corresponds to the backward flux with reverse direction.

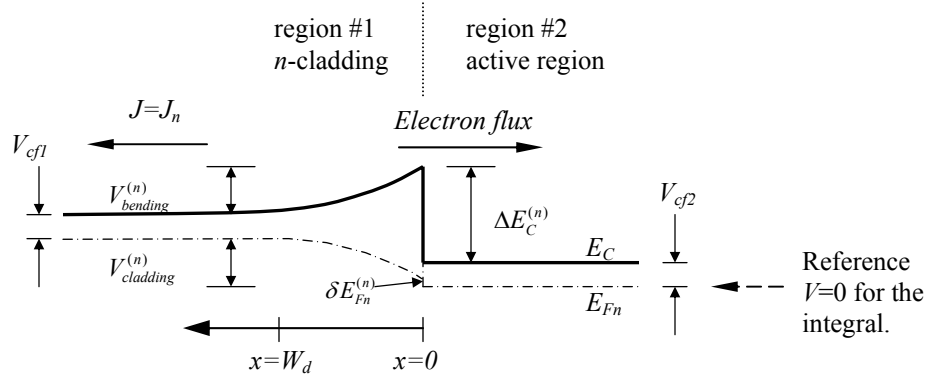


Figure 3.2: Electron (majority carrier) injection from the n -cladding layer to the active layer with the thermionic-diffusion model.

3.3 Derivation of the Current-Voltage Equations

The electron current across a cladding/active layer heterojunction interface will be derived based on the structure and nomenclatures illustrated in Figure 3.2. The derivation procedure of the current intensity formulation is similar to that for Schottky diodes found in textbooks [31] while the conclusions are unique for double heterostructure diodes.

Using this approach, once the current density J_n is known, the amount of cladding layer band-bending $V_{bending}^{(n)}$, the difference between the quasi-Fermi levels in cladding layer and in the active layer $V_{cladding}^{(n)}$, and the quasi-Fermi level discontinuity at the heterointerface $\delta E_F^{(n)}$ can be obtained with this model. In this section, the equations are first derived with the “*thermionic emission-diffusion*” model considering both the thermionic emission process across the interface and the drift-diffusion conduction in the cladding layer. Since the

interaction between the two adjacent layers actually happens through the thermionic emission process across the heterojunction interface, a derivation which is entirely based on the “*thermionic emission*” model is also presented.

3.3.1 The “*thermionic emission-diffusion*” model

This derivation is based on Crowell and Sze’s “*thermionic emission-diffusion*” formulation for Schottky diodes [57, 58]. In the cladding layer, the carrier transport can be described by the conventional drift-diffusion current equation as

$$J_n = q \cdot \mu_n \cdot n \cdot \frac{dV_C}{dx} + q \cdot D_n \cdot \frac{dn}{dx}, \quad (3.3)$$

where $V_C(x)$ is the conduction band profile, μ_n is the electron mobility and D_n is the electron diffusion coefficient. Using the depletion approximation and E_{Fn} in the active region as the reference level ($V=0$) as in shown Figure 3.2, the conduction band bending profile can be described as

$$V_C(x) = (V_{cf2} + \Delta E_C^{(n)} / q) + \frac{q \cdot N_d}{2\epsilon} \cdot (x^2 - 2 \cdot W_d \cdot x). \quad (3.4)$$

Note this is only for bending with carrier depletion. If the band bending direction is flipped so that accumulation instead of depletion is created, the profile is no longer valid as it is not quadratic.

In the active region, at given injection current density J_n , the difference between the conduction band edge and the electron quasi-Fermi level V_{cf2} can be calculated from the band structure and recombination kinetics. The V_{cf2} is normally negative (the quasi-Fermi level is

above the conduction band edge) at high injection conditions such as at lasing threshold because the conduction band effective density of states is smaller than the electron concentration at the corresponding bias level.

With $D_n = \mu_n \cdot V_T$,

$$J_n = q \cdot D_n \cdot \frac{1}{V_T} \cdot n \cdot \frac{dV_C}{dx} + q \cdot D_n \cdot \frac{dn}{dx} = q \cdot D_n \cdot \left(\frac{1}{V_T} \cdot n \cdot \frac{dV_C}{dx} + \frac{dn}{dx} \right). \quad (3.5)$$

Note it is assumed that the cladding layer is non-degenerated. The more general expressions for the diffusion coefficient and the mobility is

$$\frac{D_n}{\mu_n} = V_T \cdot \frac{\mathcal{F}_{1/2}(\xi)}{\mathcal{F}_{-1/2}(\xi)} = \frac{1}{q} \cdot \frac{dE_{Fn}}{d(\ln n)} \quad (3.6)$$

where $\mathcal{F}_{\pm 1/2}$ is the Fermi integral of order $\pm \frac{1}{2}$ and $\xi = \frac{E_{Fn} - E_C}{q \cdot V_T}$.

Multiply $\exp(\frac{V_C(x)}{V_T})$ on both sides,

$$J_n \cdot \exp(\frac{V_C(x)}{V_T}) = q \cdot D_n \cdot \left(\frac{1}{V_T} \cdot \exp(\frac{V_C(x)}{V_T}) \cdot \frac{dV_C}{dx} \cdot n(x) + \exp(\frac{V_C(x)}{V_T}) \cdot \frac{dn(x)}{dx} \right), \quad (3.7)$$

$$J_n \cdot \exp(\frac{V_C(x)}{V_T}) = q \cdot D_n \cdot \frac{d}{dx} \left(n(x) \cdot \exp(\frac{V_C(x)}{V_T}) \right). \quad (3.8)$$

Assume J_n is constant across the depletion region (given the depletion region is small and the recombination there is negligible), and integrate over the depletion layer width W_d ,

$$J_n \cdot \int_0^{W_d} \exp(\frac{V_C(x)}{V_T}) dx = q \cdot D_n \cdot \left\{ n(x) \cdot \exp(\frac{V_C(x)}{V_T}) \right\} \Big|_0^{W_d}. \quad (3.9)$$

The left-hand-side (LHS) integral is

$$\int_0^{W_d} \exp\left(\frac{V_C(x)}{V_T}\right) dx = \int_0^{W_d} \exp\left(\frac{(V_{cf2} + \Delta E_C^{(n)} / q) + \frac{q \cdot N_d}{2\epsilon} \cdot (x^2 - 2 \cdot W_d \cdot x)}{V_T}\right) dx. \quad (3.10)$$

When the contribution of the band-bending to the current mainly occurs at the height of the barrier where the electric field reaches maximum, the x^2 term is negligible in the above equation [58], the integral can be reduced to

$$\exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \cdot \int_0^{W_d} \exp\left(\frac{-\frac{q \cdot N_d}{\epsilon} W_d \cdot x}{V_T}\right) dx. \quad (3.11)$$

Then

$$LHS = J_n \cdot \left(\frac{1}{V_T} \cdot E_{\max}^{(n)} \cdot \exp\left(-\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right)^{-1} \cdot \left[1 - \exp\left(\frac{-2 \cdot V_{bending}^{(n)}}{V_T}\right) \right]. \quad (3.12)$$

If $V_{bending}^{(n)} \gg V_T$ is satisfied, it is further simplified to

$$LHS \approx J_n \cdot \left(\frac{1}{V_T} \cdot E_{\max}^{(n)} \cdot \exp\left(-\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right)^{-1} \quad (3.13)$$

where $E_{\max}^{(n)} = \sqrt{2 \cdot q \cdot N_d \cdot V_{bending}^{(n)} / \epsilon}$ can be obtained from the depletion approximation.

The right-hand-side of the integrated drift-diffusion equation is

$$\begin{aligned} & q \cdot D_n \cdot \left\{ n(x) \cdot \exp\left(\frac{V_C(x)}{V_T}\right) \right\} \Big|_0^{W_d} \\ &= q \cdot D_n \cdot \left[n(W_d) \cdot \exp\left(\frac{V_C(W_d)}{V_T}\right) - n_1 \cdot \exp\left(\frac{V_C(0)}{V_T}\right) \right] \end{aligned} \quad (3.14)$$

or

$$RHS = q \cdot D_n \cdot \left[N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - n_1 \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right], \quad (3.15)$$

where N_{C1} is effective density of states of conduction band in the n -cladding layer. n_1 is unknown and will be solved by equating the drift-diffusion current to the thermionic emission current at the heterojunction interface.

Given that the thermionic emission current density across the heterojunction interface is

$$J_n = q \cdot \left(n_1 \cdot \nu_{n1} - n_2 \cdot \nu_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{-\Delta E_C^{(n)} / q}{V_T}\right) \right), \quad (3.16)$$

then

$$\begin{aligned} RHS &= q \cdot D_n \cdot N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) \\ &- q \cdot D_n \cdot \left(\frac{J_n}{q \cdot \nu_{n1}} + n_2 \cdot \left(\frac{\nu_{n2}}{\nu_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{-\Delta E_C^{(n)} / q}{V_T}\right) \right) \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \end{aligned} \quad (3.17)$$

or

$$\begin{aligned} RHS &= q \cdot D_n \cdot \left[N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) \right] \\ &- q \cdot D_n \cdot \left[n_2 \cdot \left(\frac{\nu_{n2}}{\nu_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{V_{cf2}}{V_T}\right) \right] \\ &- q \cdot D_n \cdot \left[\frac{J_n}{q \cdot \nu_{n1}} \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right] \end{aligned} \quad (3.18)$$

With $n_2 = N_{C2} \cdot \exp(-V_{cf2}/V_T)$, where N_{C2} is the conduction band effective density of states in the active layer, V_{cf2} is the difference between the conduction band edge and the electron quasi-Fermi level in the active region, the second term can be simplified as

$$n_2 \cdot \frac{v_{n2}}{v_{n1}} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{V_{cf2}}{V_T}\right) = N_{C2} \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \quad (3.19)$$

Then

$$RHS = q \cdot D_n \cdot \left[N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - N_{C2} \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) - \frac{J_n}{q \cdot v_{n1}} \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right] \quad (3.20)$$

Combine both sides and we obtain

$$\begin{aligned} & J_n \cdot \left(\frac{1}{V_T} \cdot E_{\max}^{(n)} \cdot \exp\left(-\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right)^{-1} \\ &= q \cdot D_n \cdot \left[N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) \right] \\ & - q \cdot D_n \cdot \left[N_{C2} \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) - \frac{J_n}{q \cdot v_{n1}} \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \right] \end{aligned} \quad (3.21)$$

By defining a “diffusion velocity” $v_D^{(n)} = \mu_n \cdot E_{\max}^{(n)}$, the above equation can be simplified as

$$\begin{aligned} & J_n \cdot \left(\frac{1}{q \cdot v_D^{(n)}} + \frac{1}{q \cdot v_{n1}} \right) \cdot \exp\left(\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \\ &= N_{C1} \cdot \exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - N_{C2} \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \\ &= N_{C1} \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - \left(\frac{N_{C2}}{N_{C1}} \right) \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \right] \end{aligned} \quad (3.22)$$

With $v_{n1,2} = \sqrt{2 \cdot k_B \cdot T / (\pi \cdot m_{n1,2}^*)}$, $N_{C1,2} = 2 \left(2\pi \cdot m_{n1,2}^* \cdot k_B \cdot T / h^2 \right)^{3/2}$,

$$\left(\frac{N_{C2}}{N_{C1}} \right) \cdot \left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) = 1, \quad (3.23)$$

then

$$J_n = q \cdot \left(\frac{1}{1/\nu_D^{(n)} + 1/\nu_{n1}} \right) \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q + V_{cf2}}{V_T}\right) \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right]. \quad (3.24)$$

By defining

$$\frac{1}{\nu_n} = \frac{1}{\nu_D^{(n)}} + \frac{1}{\nu_{n1}}, \quad (3.25)$$

$$J_S^{(n)} = q \cdot \nu_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q + V_{cf2}}{V_T}\right) \quad (3.26)$$

the equation can be written as

$$J_n = J_S^{(n)} \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right] \quad (3.27)$$

A similar result can be obtained for hole current. The derived current-voltage relationship is similar to Shockley's equation for ideal diodes [31] except:

1. The applied external voltage V_{app} in the Schottky diode is replaced by $V_{cladding}$. For electrons or holes, the equation can be written as

$$J = J_S \cdot \left[\exp\left(\frac{V_{cladding}}{V_T}\right) - 1 \right], \quad (3.28)$$

where the $V_{cladding}$ and the J_S apply for only either n - or p - side (the structure with one type of the cladding layers next to the same active region) of a device. The value of $V_{cladding}$ has to be positive in order to inject majority carriers, i.e. the terminal voltage is always larger than the internal junction voltage with an amount of $V_{cladding}$ for any level of

injection. However, it is possible that the $V_{cladding}$ can be increasing or decreasing with current level.

2. For an n -type semiconductor, the barrier height Φ_{Bn} for a Schottky diode is now replaced by $(\Delta E_C^{(n)} + q \cdot V_{cf2})$, which varies with injection current because of the V_{cf2} in the active region. Therefore the $J_S^{(n)}$ is not only a function of band-bending in the cladding layer, it is also a function of factors such as recombination mechanisms in the active region.

3.3.2 The “*thermionic emission*” model

At room temperature, the “diffusion velocity” of carriers in most semiconductor materials is much higher than the “thermionic emission velocity” [31], and the thermionic emission across the heterojunction boundary is indeed the rate-limiting process. The velocity be simplified as

$$\frac{1}{v} = \frac{1}{v_{TE}} + \frac{1}{v_{DD}} \approx \frac{1}{v_{TE}} \quad (3.29)$$

In this section, it will be shown that similar result can be obtained with the “*thermionic emission*” model while the deriving procedure is greatly simplified. The device structure is illustrated in Figure 3.3. In the “*thermionic emission*” model, it is assumed that quasi-Fermi level is flat across the cladding layer, and all the electrons with higher thermal energies than the barrier height are free to flow across the heterojunction.

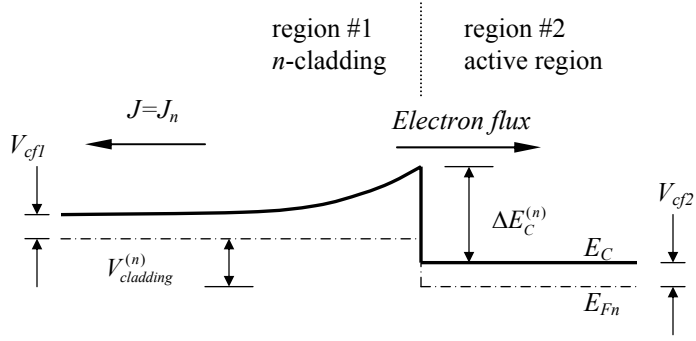


Figure 3.3: Electron (majority carrier) injection from the n -cladding layer to the active layer with the thermionic emission model. Note the quasi-Fermi level is flat across the cladding layer in this model.

For the electron current from region 2 to 1 (or the electron particle flux from region 1 to 2) in Figure 3.3, the current density is

$$J_n = q \cdot \left(n_1 \cdot v_{n1} - n_2 \cdot v_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{-\Delta E_C^{(n)} / q}{V_T}\right) \right) \quad (3.30)$$

where the n_1 is unknown and the relationship between the $V_{cladding}$ and J needs to be derived.

If the Boltzmann distribution function applies, the carrier densities next to the boundary can be described as

$$\begin{cases} n_1 = N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q + V_{cf2} - V_{cladding}^{(n)}}{V_T}\right) \\ n_2 = N_{C2} \cdot \exp\left(-\frac{V_{cf2}}{V_T}\right) \end{cases} \quad (3.31)$$

so that

$$n_1 = n_2 \cdot \frac{N_{C1}}{N_{C2}} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q - V_{cladding}^{(n)}}{V_T}\right). \quad (3.32)$$

Therefore (3.30) can be expressed as

$$\begin{aligned}
J_n &= q \cdot \left(n_2 \cdot \frac{N_{C1}}{N_{C2}} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q - V_{cladding}^{(n)}}{V_T}\right) \cdot v_{n1} - n_2 \cdot v_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*}\right) \cdot \exp\left(\frac{-\Delta E_C^{(n)} / q}{V_T}\right) \right) \\
&= q \cdot n_2 \cdot \frac{N_{C1}}{N_{C2}} \cdot v_{n1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q}{V_T}\right) \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - \left(\frac{v_{n2}}{v_{n1}}\right) \cdot \left(\frac{N_{C2}}{N_{C1}}\right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*}\right) \right]
\end{aligned} \tag{3.33}$$

As $v_{n1,2} = \sqrt{2 \cdot k_B \cdot T / (\pi \cdot m_{n1,2}^*)}$, $N_{C1,2} = 2 \left(2\pi \cdot m_{n1,2}^* \cdot k_B \cdot T / h^2 \right)^{3/2}$, in (3.33)

$$\left(\frac{v_{n2}}{v_{n1}} \right) \cdot \left(\frac{N_{C2}}{N_{C1}} \right) \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) = 1 \tag{3.34}$$

Equation (3.33) can be further simplified to

$$\begin{aligned}
J_n &= q \cdot N_{C1} \cdot v_{n1} \cdot \exp\left(-\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right) \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right] \\
&= J_S^{(n)} \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right]
\end{aligned} \tag{3.35}$$

with

$$J_S^{(n)} = q \cdot N_{C1} \cdot v_{n1} \cdot \exp\left(-\frac{V_{cf2} + \Delta E_C^{(n)} / q}{V_T}\right). \tag{3.36}$$

The “*thermionic emission*” approach produces the same result as obtained in (3.26) when the “thermionic emission velocity” at the heterojunction boundary is much smaller than the “diffusion velocity” in the adjacent confinement layer.

3.3.3 The equations for a full device

Across the full device, the terminal current-voltage can be obtain through

$$\begin{cases} J = J_p = J_n \\ V_{ext} = V_j + V_{cladding}^{(p)} + V_{cladding}^{(n)} \end{cases} \quad (3.37)$$

The electron and hole components with this model are

$$\begin{cases} J_p = J_S^{(p)} \cdot \left[\exp\left(\frac{V_{cladding}^{(p)}}{V_T}\right) - 1 \right] \\ J_S^{(p)} = q \cdot v_p \cdot N_{V1} \cdot \exp\left(-\frac{\Delta E_V^{(p)} / q + V_{fv2}}{V_T}\right) \end{cases}, \quad (3.38)$$

and

$$\begin{cases} J_n = J_S^{(n)} \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right] \\ J_S^{(n)} = q \cdot v_p \cdot N_{V1} \cdot \exp\left(-\frac{\Delta E_V^{(n)} / q + V_{cf2}}{V_T}\right) \end{cases}. \quad (3.39)$$

As in Figure 3.1, if the Fermi level of the active region at thermal equilibrium is set as a reference voltage, the junction voltages and the terminal voltages can also be denoted as

$$\begin{cases} V_j = V_j^{(n)} + V_j^{(p)} \\ V_{ext}^{(n)} = V_j^{(n)} + V_{cladding}^{(n)}, \quad V_{ext}^{(p)} = V_j^{(p)} + V_{cladding}^{(p)} \\ V_{ext} = V_{ext}^{(n)} + V_{ext}^{(p)} \end{cases} \quad (3.40)$$

The J - V_{ext} relation can be then calculated numerically with current density J as the independent variable. First, the active region J - V_j can be obtained from the recombination model, then the $V_{cladding}^{(n)}$ and the $V_{cladding}^{(p)}$ can be evaluated from the above transport model, finally the V_{ext} can be summed up from the three components. Following this procedure, they are virtually decoupled from each other in the calculation. However, all the components in

this model are nonlinear so that a numerical calculation has to be employed for each of them. Nevertheless, in the next section, it will be shown that the cladding layer voltages are actually strongly coupled with the active region junction voltages due to the interaction between the two layers. The final results are more complicated than simply adding up three diodes.

3.4 Interaction between the Active Layer and the Cladding Layer

3.4.1 Introduction

The derived current-voltage equation for the n - or p - side of the device is similar to the Shockley equation as

$$J = J_S \cdot \left[\exp\left(\frac{V_{cladding}}{V_T}\right) - 1 \right] \quad (3.41)$$

Usually the symbol J_S is used to denote a constant “saturation” current density when a diode is reverse biased. In this model the symbol is kept while it does not have the same physical meaning. Instead of being a constant, the J_S in this model is strongly dependent on the bias level and it is different for the n - and the p - side of the device. It will be shown that this variable J_S actually provides important information about the interactions between the active layer and the confining layer at each side of the heterojunction.

As in (3.2), the electron thermionic emission current across the boundary is given as

$$J_n^{TE} = q \cdot \left(n_1 \cdot v_{n1} - n_2 \cdot v_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot \exp\left(\frac{-\Delta E_C^{(n)} / q}{V_T}\right) \right), \quad (3.42)$$

and similarly the hole thermionic emission current is

$$J_p^{TE} = q \cdot \left(p_1 \cdot v_{p1} - p_2 \cdot v_{p2} \cdot \left(\frac{m_{p1}^*}{m_{p2}^*} \right) \cdot \exp\left(-\frac{\Delta E_V^{(p)} / q}{V_T}\right) \right). \quad (3.43)$$

For both carriers the second terms in the above equations represent the backward flux from the thermionic emission. If the band discontinuity $\Delta E_C^{(n)}$ for electrons or $\Delta E_V^{(p)}$ for holes is high or the temperature (and therefore the V_T) is low, the backward thermionic emission flux

is greatly reduced and the interaction between the two layers is expected to be weak. On the other hand, when the strength of interaction is strong, the “thermal flux” $(q \cdot n \cdot v)$ or $(q \cdot p \cdot v)$ of electrons or holes with concentration of $10^{18}/\text{cm}^3$ in both layers at room temperature can be in the orders of 10^4 to 10^5 A/cm^2 for materials such as $\text{Al}_x\text{Ga}_{1-x}\text{As}$. If the device current of a LED or LD is about 10^3 A/cm^2 , the net current is only a small portion of either side of the flux. In other words, the device current can be a result of small difference between two large currents. In this situation, the changes in the junction characteristic can possibly be reflected at the terminals.

In this section, it will be shown that the interaction through the thermionic emission process across the heterojunction boundary can be explained with the injection level dependent J_S . The effects of the interactions on the differential resistance and the ideality factor of a heterostructure device are studied. A simple device with parameters given in Table 3.1 is used as an example.

Table 3.1: Parameters for the active region used in the example device structures. Note they are typical parameters for GaAs.

Parameter	Symbol	Value/Unit
Bandgap	E_g	1.42 eV
Electron effective mass	m_e^*	$0.067m_0$
Hole effective mass	m_h^*	$0.48 m_0$
Conduction band effective density of states	N_C	$4.42 \times 10^{17} \text{ cm}^{-3}$
Valance band effective density of states	N_V	$8.47 \times 10^{18} \text{ cm}^{-3}$
Acceptor concentration	N_A	0
Donor concentration	N_D	0
Nonradiative recombination coefficient	A	$1 \times 10^7 \text{ s}^{-1}$
Bimolecular recombination coefficient	B	$1 \times 10^{10} \text{ cm}^3/\text{s}$
Auger recombination coefficient	C	$1 \times 10^{-30} \text{ cm}^6/\text{s}$
Active region thickness	L_j	150 nm

3.4.2 The J/J_S ratio

As mentioned before, unlike in the ideal pn -junction or Schottky diode, the J_S in this model is indeed highly dependent on active region junction voltage. In the n - type structure,

$$J_S^{(n)} = q \cdot \nu_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q + V_{cf2}}{V_T}\right) \quad (3.44)$$

which varies exponentially as a function of the V_{cf2} in the active region. The dependency on the active region bias condition provides the interaction between the two layers. The cladding layer voltage drop of the n - or p - structure is given by

$$V_{cladding} = V_T \cdot \ln\left(\frac{J}{J_S} + 1\right), \quad (3.45)$$

and we see that the (J/J_S) ratio is a key parameter.

In Chapter 2, it was shown that the quasi-Fermi levels (and therefore V_{cf2} and V_{fv2}) in the active region can be related to the corresponding ideality factor m_j . If the effective density of states for electrons and holes are known and the recombination mechanisms are the typical power-law dependency currents, e.g. with $A/B/C$ coefficients, then $m_j^{(n)}$ and the $m_j^{(p)}$ can be directly inferred from the junction voltage V_j . It will be shown below, with n -cladding as an example, that the (J/J_S) ratio can also be related to V_j as well as the ideality factor of the active junction.

Assume that the recombination current in the active region can be expressed as

$$J = J_0 \cdot \exp\left(\frac{V_j^{(n)}}{m_j^{(n)} \cdot V_T}\right) \quad (3.46)$$

where J_0 is a constant, $V_j^{(n)}$ is the n - part of the junction quasi-Fermi level splitting, i.e. the difference between the electron quasi-Fermi level at biased condition and the Fermi level at thermal equilibrium. $m_j^{(n)}$ is the corresponding ideality factor related to electron quasi-Fermi level splitting and the V_T is the thermal voltage. Using

$$\begin{cases} J_s^{(n)} = q \cdot v_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)} / q + V_{cf2}}{V_T}\right) \\ V_{cf2} = V_{cf0}^{(n)} - V_j^{(n)} \end{cases} \quad (3.47)$$

where the $V_{cf0}^{(n)}$ is the voltage corresponding to the difference between the conduction band edge and the electron Fermi level at thermal equilibrium in the active region. Then $J_s^{(n)}$ can then be written as

$$\begin{aligned} J_s^{(n)} &= q \cdot v_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)}}{q \cdot V_T}\right) \cdot \exp\left(-\frac{V_{cf2}}{V_T}\right) \\ &= q \cdot v_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)}}{q \cdot V_T}\right) \cdot \exp\left(-\frac{V_{cf0}^{(n)}}{V_T}\right) \cdot \exp\left(\frac{V_j^{(n)}}{V_T}\right) \\ &= q \cdot v_n \cdot N_{C1} \cdot \exp\left(-\frac{\Delta E_C^{(n)}}{q \cdot V_T}\right) \cdot \exp\left(-\frac{V_{cf0}^{(n)}}{V_T}\right) \cdot \left[\exp\left(\frac{V_j^{(n)}}{m_j^{(n)} \cdot V_T}\right)\right]^{m_j^{(n)}} \\ &= \frac{q \cdot v_n \cdot N_{C1}}{\exp\left(-\frac{\Delta E_C^{(n)}}{q \cdot V_T}\right) \cdot \exp\left(-\frac{V_{cf0}^{(n)}}{V_T}\right) \cdot (J_0)^{m_j^{(n)}}} \cdot J^{m_j^{(n)}}. \end{aligned} \quad (3.48)$$

Therefore, the (J/J_s) ratio can be expressed as

$$\frac{J}{J_s^{(n)}} = \left[\frac{(J_0)^{m_j^{(n)}} \cdot \exp\left(\frac{\Delta E_C^{(n)}}{q \cdot V_T}\right) \cdot \exp\left(\frac{V_{cf0}^{(n)}}{V_T}\right)}{q \cdot v_n \cdot N_{C1}} \right] \cdot J^{(1-m_j^{(n)})} \quad (3.49)$$

where the first term is J independent, and the second term indicates that the ratio is related to the absolute current density J through ideality factor as

$$\frac{J}{J_s^{(n)}} \propto J^{(1-m_j^{(n)})} \quad (3.50)$$

From the above equations with an n - type structure, it can be seen that the (J/J_s) ratio is affected by various parameters such as:

- Band gaps and band alignment between the two layers. Through the thermionic process across the heterojunction interface, a larger band discontinuity $\Delta E_C^{(n)}$ will reduce the interaction between the two layer, which also results in a bigger value of the (J/J_s) ratio through $\exp(\frac{\Delta E_C^{(n)}}{q \cdot V_T})$ as in equation (3.49). The same dependency applies with the parameter $V_{cf0}^{(n)}$, which is related to the band gap and the doping of the active material.
- Effective Richardson constant of cladding layer material. It is reflected in the $q \cdot v_n \cdot N_{C1}$ term in (3.49). A higher $A^* T^2$ current results in a smaller (J/J_s) ratio.
- Temperature. It not only affects the $A^* T^2$ current, but also changes the $\exp(\frac{\Delta E_C^{(n)}}{q \cdot V_T})$ and the $\exp(\frac{V_{cf0}^{(n)}}{V_T})$ terms exponentially. At low temperatures, if the band discontinuity $\Delta E_C^{(n)}$

and the $V_{cf0}^{(n)}$ do not change a lot, the smaller thermal voltage V_T will dramatically increase the (J/J_S) ratio, resulting in a much smaller interaction between the layers.

- Absolute current density. The second term $J^{(1-m_j^{(n)})}$ in (3.49) indicates that the (J/J_S) ratio is a function of J .
- Active region ideality factor m_j . The ideality factor affects the current independent part as well as the current dependent term in (3.49). With the neutral active region model and the typical $A/B/C$ recombination coefficients as in Chapter 2, the ideality factor of the n - or p - part is expected to decrease from 1.0 to a value between 0.5 and 1.0, and then increase with bias level. As $(J/J_S^{(n)}) \propto J^{(1-m_j^{(n)})}$, the (J/J_S) ratio is then expected to increase when $1-m_j^{(n)} > 0$ and then decrease when $1-m_j^{(n)} < 0$. Therefore the bias levels where $m=1$ are special points for the ratio. At a low bias level, the ideality factor from n - or p - part is about 1.0, and the (J/J_S) ratio is independent of J . At other bias levels, when the m is smaller than 1.0, the (J/J_S) ratio increases with current, while when the m is greater than 1.0, the ratio decrease with current.
- Nonradiative recombination strength in the active region. When the junction quasi-Fermi levels are not close to the band edges, the ideality factors associated with the n - or p - side is about 1.0. Under this low bias condition, the J_0 in (3.49) is mainly determined by the monomolecular recombination coefficient. A higher nonradiative recombination rate in the active region will correspond to a larger J_0 and a corresponding larger (J/J_S) ratio.

The (J/J_S) ratio with the device parameters given in Table 3.1 are calculated with this model. The (J/J_S) ratios with band discontinuities of $5V_T$ and $10V_T$ for n - and p - type structures are plotted as function of junction voltage normalized to the bandgap energy in Figure 3.4. The corresponding junction ideality factors are also plotted. The (J/J_S) ratios as function of junction voltage can be categorized in to three regions. First, at low bias voltage, it starts out with a nearly constant value until the corresponding ideality factor begins to change. As discussed above, the constant value reflects the strength of interaction between the two layers. The ratio is determined by parameters such as band alignment, device temperature, effective masses in the cladding layer, nonradiative recombination lifetime in the active layer and etc. It can be seen in Figure 3.4 that larger band discontinuities corresponds to higher values of the (J/J_S) ratio or less interaction between the layers. Second, if there is a transition region in the ideality factor, i.e. the m_j falls between 0.5 and 1.0 for electrons or holes, there is a corresponding transition region for the (J/J_S) ratio in which the ratio keeps increasing until the ideality factor increases to 1.0 again. Third, for the region where the corresponding the ideality factor greater than 1.0, the (J/J_S) ratio drops with junction voltage and it approaches zero at high bias level.

The same data is also plotted as function of current density in Figure 3.5. Note that for a current density below $5000\text{A}/\text{cm}^2$, most of the corresponding junction voltages are within only a few thermal voltages below and above the bandgap. With the given parameters, the (J/J_S) ratio is decreasing for electrons while it is increasing for holes with current densities between $500\text{A}/\text{cm}^2$ and $5000\text{A}/\text{cm}^2$.

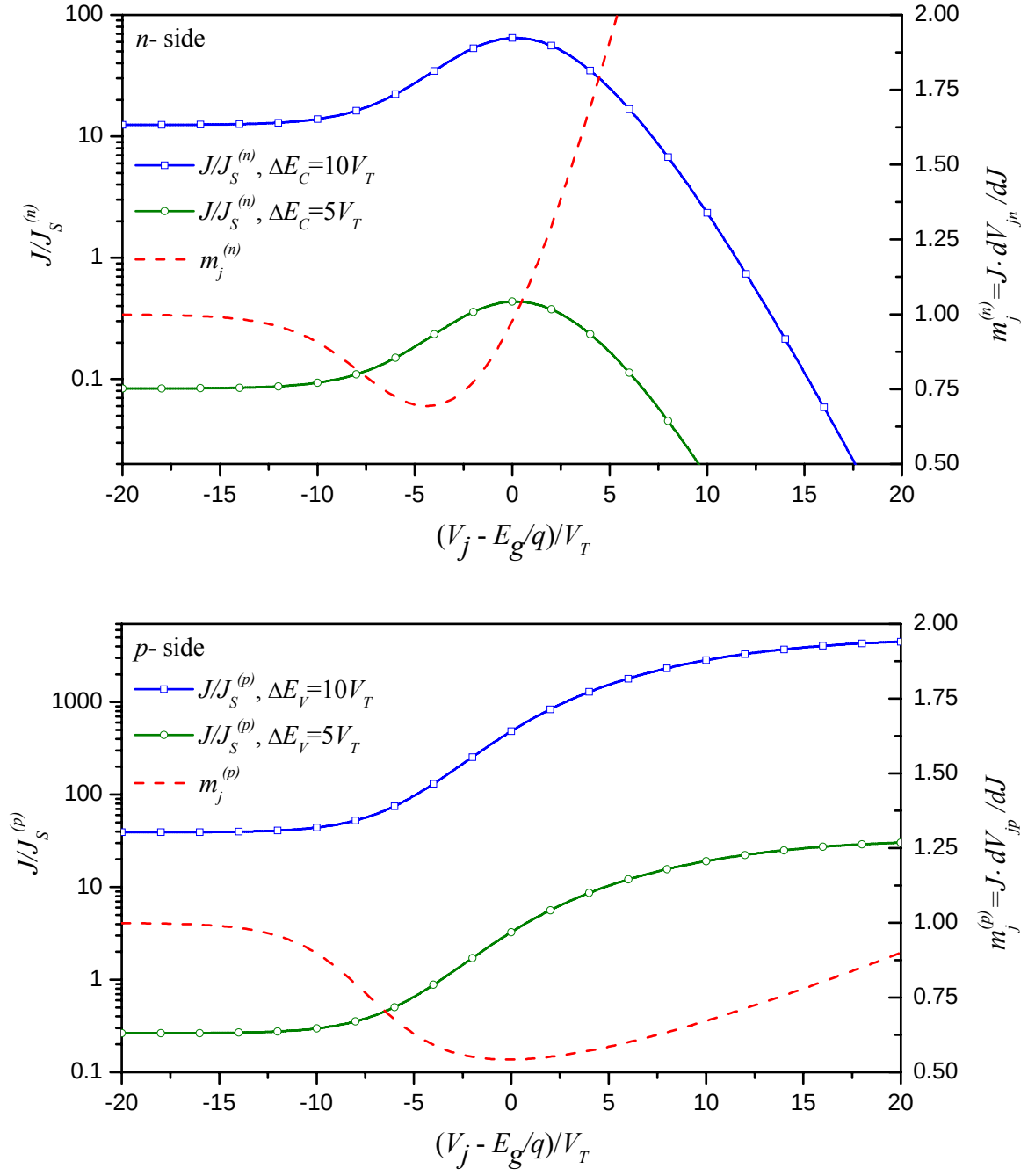


Figure 3.4: The (J/J_S) ratios with n - and p - structures and band discontinuities of $5V_T$ and $10V_T$ as function of junction voltage normalized to the bandgap energy. The corresponding junction ideality factors are also plotted. The ratio starts out with a nearly constant value at low bias voltage and keeps increasing when the corresponding ideality factor is less than 1.0, then it drops fast and approaches zero after the ideality factor is greater than 1.0.

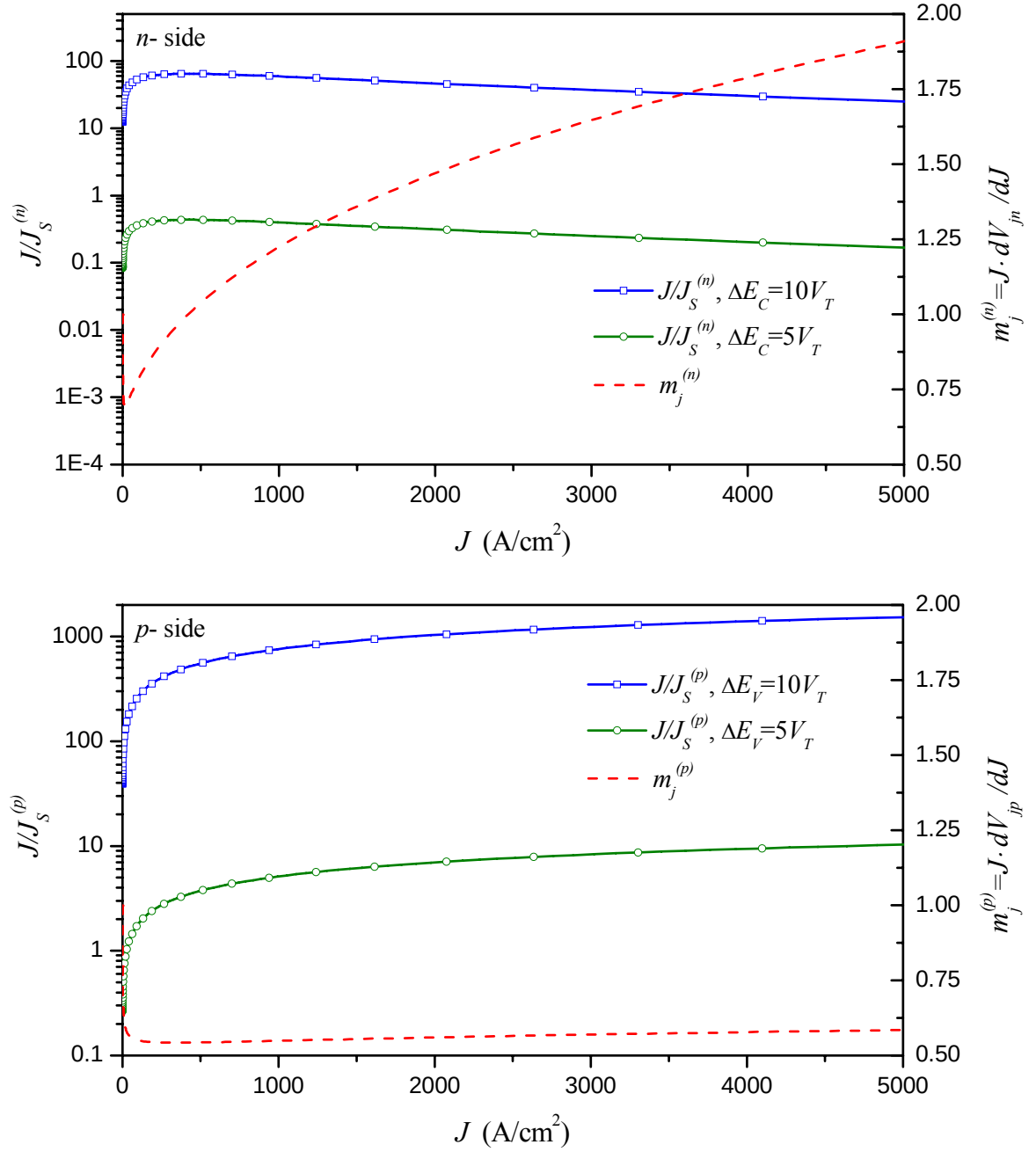


Figure 3.5: The (J/J_S) ratios with n - and p - structures and band discontinuities of $5V_T$ and $10V_T$ as function of current density ($J < 5000 \text{ A/cm}^2$). The corresponding junction ideality factors are also plotted. Note most of the corresponding junction voltages are a few V_T around E_g/q . Most of the (J/J_S) ratio is decreasing for electrons while it is increasing for holes due to the difference in the ideality factors.

3.4.3 The quasi-Fermi level difference between the cladding layer and the active region

As in Figure 3.1, the $V_{cladding}$ in this model is defined as the quasi-Fermi level difference between the cladding layer and the active region of the n - or p - side of the device. The interaction between the cladding layer and the active region is reflected in the $V_{cladding}$. With additional nonlinearity, the existence of the $V_{cladding}$ changes the electrical characteristics of the device from the junction values to new terminal properties.

In previous derivations, for either the n - or the p -cladding layers, the $V_{cladding}$ is related to terminal current as

$$J = J_S \cdot \left[\exp\left(\frac{V_{cladding}}{V_T}\right) - 1 \right] \quad (3.51)$$

where the J_S stands for $J_S^{(n)}$ or $J_S^{(p)}$, and the $V_{cladding}$ can be $V_{cladding}^{(n)}$ or $V_{cladding}^{(p)}$. Therefore,

$$V_{cladding} = V_T \cdot \ln\left(\frac{J}{J_S} + 1\right) \quad (3.52)$$

The $V_{cladding}$ with the device parameters given in Table 3.1 are calculated with this model. In Figure 3.6, the $(V_{cladding}/V_T)$ with band discontinuities of $5V_T$ and $10V_T$ for n - and p - type structures are plotted as function of junction voltage normalized to the bandgap energy. The corresponding junction ideality factors are also plotted. From Figure 3.6 and (3.52), it can be seen that the current-voltage relationships from the transport across the heterojunction transport is always nonlinear.

When $J/J_S \ll 1$ and therefore $V_{cladding} \ll V_T$,

$$V_{cladding} \approx V_T \cdot \left(\frac{J}{J_S} \right) \quad (3.53)$$

In this case, the $V_{cladding}$ is actually negligible regardless of the bias level (or the junction ideality factor m_j). Therefore, the external quasi-Fermi level in the cladding layer closely follows the internal quasi-Fermi level in the active region. The external electrical characteristics are expected to be almost identical to the junction properties.

At a low bias condition where the (J/J_S) ratio is independent of current level, the corresponding ideality factor for n - part or p - part is about 1.0, and the $V_{cladding}$ does not vary with injection level either. In this case, the external quasi-Fermi level in the cladding layer follows the internal quasi-Fermi level in the active region by a constant offset. While the external voltage is not identical to the internal junction voltage in this situation, the current derivatives are expected to be the same.

As in the (J/J_S) ratio, there are transition regions where the $V_{cladding}$ is strongly affected by a change in the dominant recombination mechanism in the active region. When the bimolecular recombination in the active region becomes stronger at higher injection level, the corresponding ideality factor in the junction begins to drop from 1.0, which means that the internal quasi-Fermi level moves slower. Meanwhile the (J/J_S) ratio and the $V_{cladding}$ increases until the ideality factor returns to 1.0. Therefore, although the internal quasi-Fermi level moves slower in the junction, the difference between the internal and the external quasi-Fermi levels increases, the net result is that the internal quasi-Fermi level can not be exactly “seen” from terminals. Similarly, when the junction ideality factor increases to values above

1.0, the quasi-Fermi level in the active region moves faster, while the $V_{cladding}$ decreases with current, corresponding to a negative differential resistance (NDR) in the cladding layer.

To conclude, in the regions where the internal (n - or p -) junction ideality factors are below or above 1.0, the trends of the $V_{cladding}$ always counteract the moving of internal quasi-Fermi level. This is because the backward thermionic emission fluxes are included in the boundary condition in the derivation of this model.

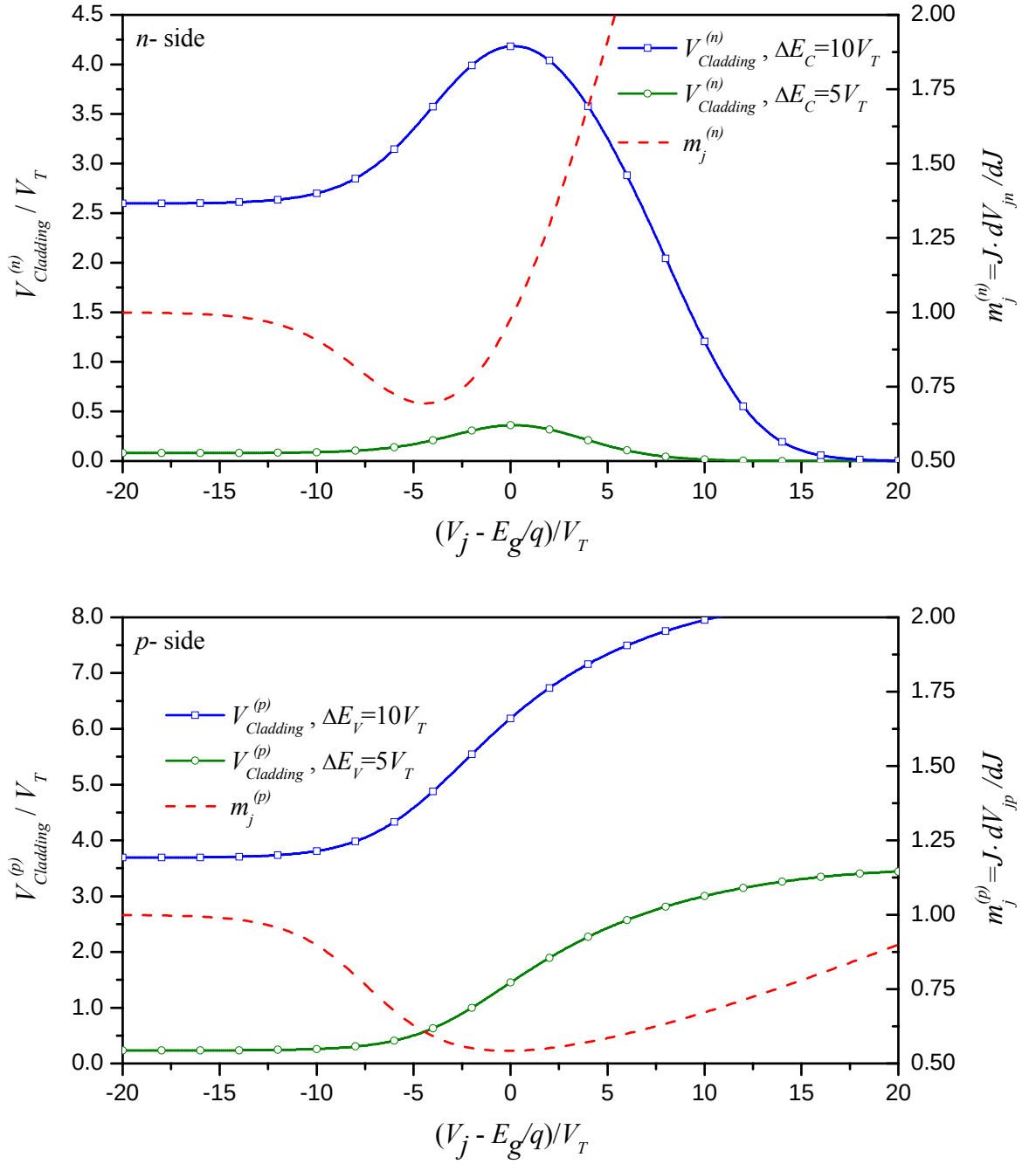


Figure 3.6: The $V_{cladding}$ with n - and p - cladding layers as function of junction voltage normalized to the bandgap energy. The corresponding junction ideality factors are also plotted. The $V_{cladding}$ increases with bias level when the corresponding ideality factor is less than 1.0 and decreases with bias level when the ideality factor is greater than 1.0.

3.4.4 The differential resistances and the fraction f_j

A. Direct calculation of the differential resistances

With the derived $V_{cladding}$, the terminal voltage can then be obtained by

$$V_{ext} = V_j + V_{cladding} \quad (3.54)$$

which has be calculated numerically. As the terminal voltage V_{ext} is offset from the junction voltage V_j by the amount of $V_{cladding}$, the corresponding current derivatives will be different.

From (3.54), the measurable differential resistance from device terminals denoted as dV_{ext}/dJ can be calculated directly by

$$\frac{dV_{ext}}{dJ} = \frac{dV_j}{dJ} + \frac{dV_{cladding}}{dJ}. \quad (3.55)$$

With the same parameters as previous used, in Figure 3.7, the dV/dJ from the terminals (dV_{ext}/dJ), the active junctions (dV_j/dJ), the cladding layers ($dV_{cladding}/dJ$) and the junction ideality factor (m_j) of n - and p - side of the double heterostructure are directly calculated from (3.55) and plotted as function of junction voltage normalized to the bandgap energy. It can be seen that the $dV_{cladding}/dJ$ are negligible before the junction voltage is close to the bandgap. The same data is plotted in Figure 3.8 but as function of current. As mentioned in Section 3.4.3, the differential resistances calculated for the cladding layer voltage drops are negative when the corresponding ideality factor is above 1.0, resulting in a smaller terminal differential resistance than the junction differential resistance. For the region where the ideality factor is less than 1.0, the $dV_{cladding}/dJ$ is positive and the terminal differential resistance is bigger than the junction value.

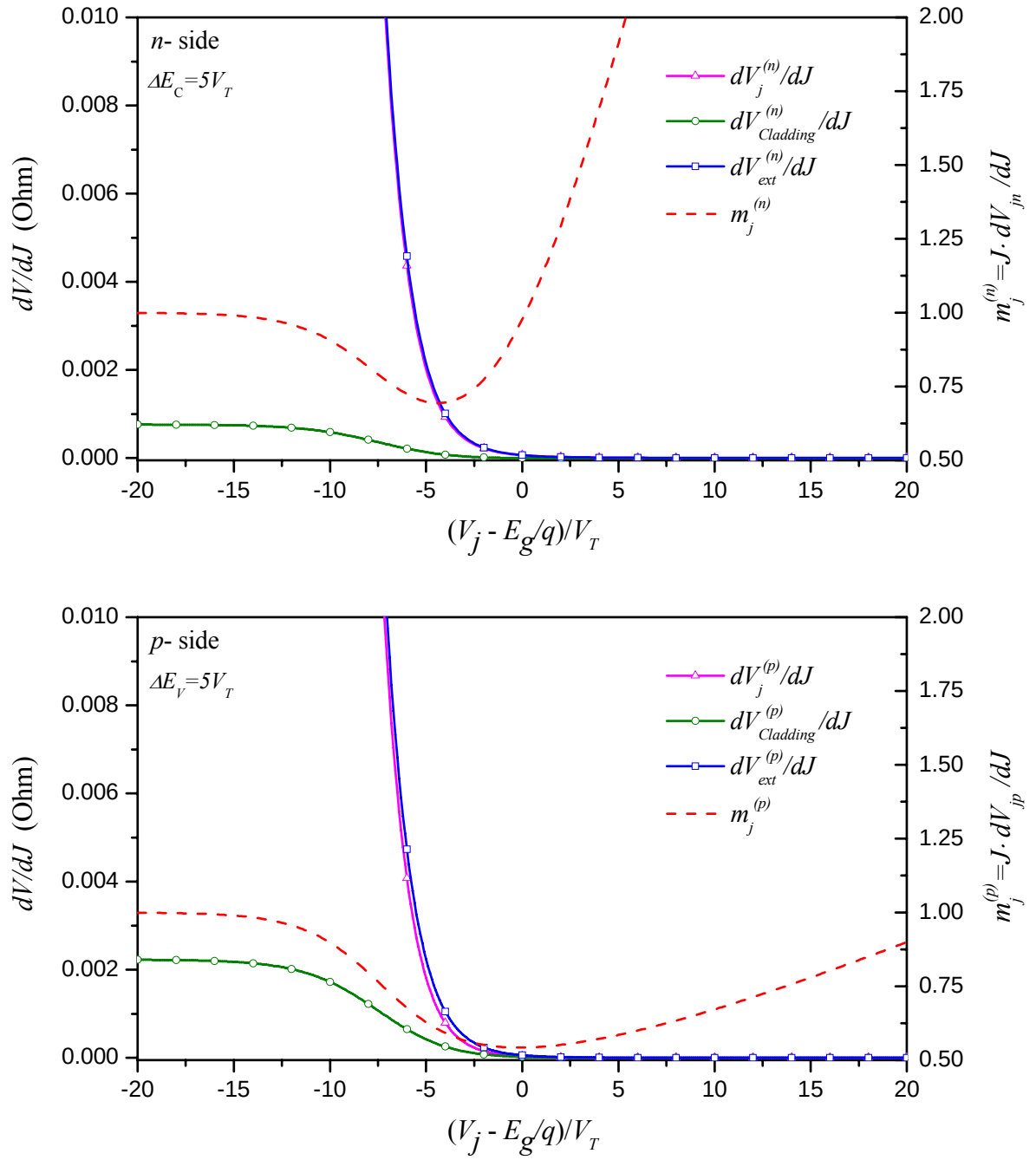


Figure 3.7: The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_j/dJ), cladding layers (dV_{cladding}/dJ) and the junction ideality factor (m_j) of n - and p - side of the structure as function of junction voltage normalized to the bandgap energy. Note that the dV_{cladding}/dJ are negligible compared to dV_j/dJ before the junction voltage is close to the bandgap.

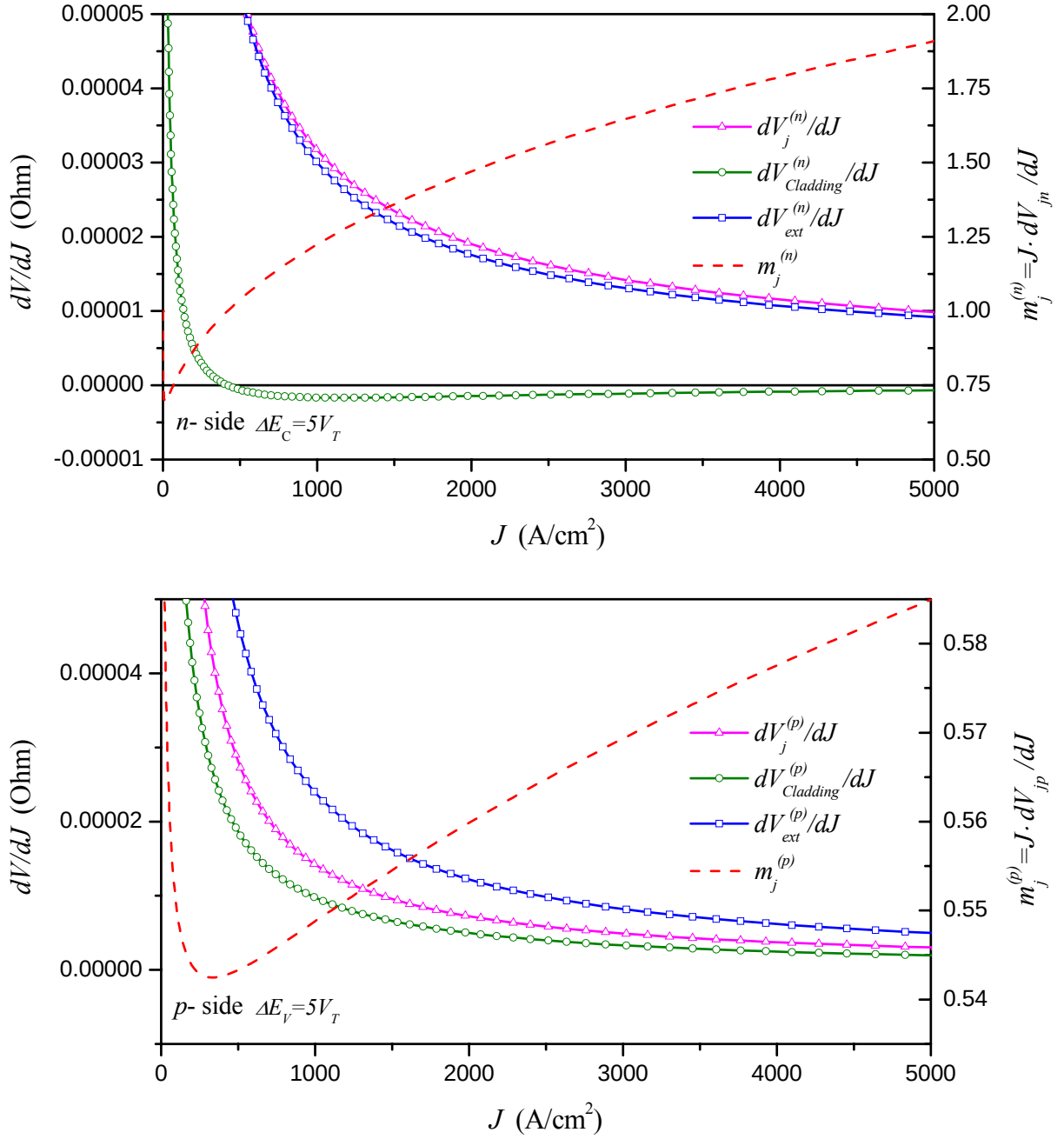


Figure 3.8: The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_j/dJ) cladding layers ($dV_{cladding}/dJ$) and the junction ideality factor (m_j) of n - and p - side of the structure as function of current. Note the differential resistances of the cladding layer are negative when the corresponding ideality factor is above 1.0.

$B. f_j$ – the fraction associated with junction for differential resistances and ideality factors

In addition to (3.55), it is found that there is a simpler analytical formulation between the external and the internal differential resistances with this model. In this section, the relationship between the differential resistances is derived and discussed.

The n - part of the structure is used as an example in the derivation. With

$$J = J_S^{(n)} \cdot \left[\exp\left(\frac{V_{cladding}^{(n)}}{V_T}\right) - 1 \right] \quad (3.56)$$

and

$$V_{ext}^{(n)} = V_j^{(n)} + V_{cladding}^{(n)}, \quad (3.57)$$

the current can be expressed as

$$J = \left[J_S^{(n)} \cdot \exp\left(\frac{-V_j^{(n)}}{V_T}\right) \right] \cdot \left[\exp\left(\frac{V_{ext}^{(n)}}{V_T}\right) - \exp\left(\frac{V_j^{(n)}}{V_T}\right) \right]. \quad (3.58)$$

As $J_S^{(n)} = q \cdot v_n \cdot N_{Cl} \cdot \exp\left(-\frac{\Delta E_C^{(n)} + V_{cf2}}{V_T}\right)$, $J_S^{(n)} \cdot \exp\left(\frac{-V_j^{(n)}}{V_T}\right)$ is independent of J if the v_n is a

constant. Differentiate the equation and it becomes

$$dJ = \left(J_S^{(n)} \cdot \exp\left(\frac{-V_j^{(n)}}{V_T}\right) \right) \cdot \frac{1}{V_T} \cdot \left[\exp\left(\frac{V_{ext}^{(n)}}{V_T}\right) \cdot dV_{ext}^{(n)} - \exp\left(\frac{V_j^{(n)}}{V_T}\right) \cdot dV_j^{(n)} \right] \quad (3.59)$$

$$\frac{V_T}{J_S^{(n)}} \cdot \exp\left(\frac{V_j^{(n)}}{V_T}\right) = \exp\left(\frac{V_{ext}^{(n)}}{V_T}\right) \cdot \frac{dV_{ext}^{(n)}}{dJ} - \exp\left(\frac{V_j^{(n)}}{V_T}\right) \cdot \frac{dV_j^{(n)}}{dJ} \quad (3.60)$$

$$\frac{dV_{ext}^{(n)}}{dJ} = \exp\left(\frac{-V_{ext}^{(n)}}{V_T}\right) \cdot \exp\left(\frac{V_j^{(n)}}{V_T}\right) \cdot \left(\frac{V_T}{J_S^{(n)}} + \frac{dV_j^{(n)}}{dJ} \right) \quad (3.61)$$

$$\frac{dV_{ext}^{(n)}}{dJ} = \exp\left(\frac{-V_{cladding}^{(n)}}{V_T}\right) \cdot \left(\frac{V_T}{J_S^{(n)}} + \frac{dV_j^{(n)}}{dJ}\right). \quad (3.62)$$

Note the same result can be achieved by differentiating the J -dependent $J_S^{(n)}$ directly. With

$$V_{cladding}^{(n)} = V_T \cdot \ln\left(\frac{J}{J_S^{(n)}} + 1\right), \quad (3.63)$$

the external differential resistance from n - side can be simplified as

$$\frac{dV_{ext}^{(n)}}{dJ} = \left(\frac{V_T}{J_S^{(n)} + J}\right) + \left(\frac{dV_j^{(n)}}{dJ}\right) \cdot \frac{1}{J/J_S^{(n)} + 1} \quad (3.64)$$

or:

$$\frac{dV_{ext}^{(n)}}{dJ} = \left(\frac{V_T}{J}\right) \cdot \left(\frac{J}{J + J_S^{(n)}}\right) + \left(\frac{dV_j^{(n)}}{dJ}\right) \cdot \left(\frac{J_S^{(n)}}{J + J_S^{(n)}}\right). \quad (3.65)$$

In (3.65), the ratio $\frac{V_T}{J}$ is the differential resistance of an ideal diode with ideality factor of

1.0 and the $\frac{dV_j^{(n)}}{dJ}$ is the differential resistance of the junction, which can be alternatively

written as $m_j^{(n)} \cdot \frac{V_T}{J}$ with $m_j^{(n)}$ being the junction ideality factor. Nevertheless, as the $\frac{J}{J + J_S^{(n)}}$

and the $\frac{J_S^{(n)}}{J + J_S^{(n)}}$ add up to unity, equation (3.65) reveals an important conclusion from this

model: the measurable terminal differential resistance is a linear combination of the

differential resistances from the junction and from the heterojunction transport.

Define the fraction which is associated with the junction f_j as

$$f_j = \frac{J_s}{J + J_s} = \frac{1}{J/J_s + 1} \quad (0 \leq f_j \leq 1), \quad (3.66)$$

the terminal differential resistance can be written as

$$\frac{dV_{ext}}{dJ} = \left(\frac{dV_j}{dJ} \right) \cdot f_j + \left(\frac{V_T}{J} \right) \cdot (1 - f_j) \quad (3.67)$$

or

$$\begin{aligned} \frac{dV_{ext}}{dJ} &= \left(\frac{m_j \cdot V_T}{J} \right) \cdot f_j + \left(\frac{V_T}{J} \right) \cdot (1 - f_j) \\ &= \left(\frac{V_T}{J} \right) \cdot [m_j \cdot f_j + (1 - f_j)] \end{aligned} \quad (3.68)$$

which indicates that the total differential resistance is equivalent to that from a diode with an ideality factor between 1.0 and m_j .

Therefore, in order that the device derivative characteristics can be “seen” from the terminals, it is desirable that the junction fraction f_j is close to unity. From (3.66), the fraction is directly related to the (J/J_s) ratio discussed in Section 3.4.2. As the (J/J_s) ratio is a function of the strength of interaction between the layers as well as the bias condition of the junction, the same dependency is expected for the f_j .

Similar to the (J/J_s) ratio which is sensitive to parameters such as band alignment, temperature, nonradiative recombination in the active region etc., the f_j is also sensitive to these parameters. With the same parameters as used in previous calculations, in Figure 3.9, the fractions from junction f_j with n - and p - structures as a function of junction voltage normalized to the bandgap energy are plotted. The corresponding junction ideality factors are also plotted. In Figure 3.9, when the band discontinuity is increased from $5V_T$ to $10V_T$ so that

the interaction between the layers is reduced, the f_j also drops dramatically. In Figure 3.10, the fraction from junction f_j with n - and p - cladding layers with different monomolecular recombination coefficients in the active region as function of junction voltage normalized to the bandgap energy are plotted. It can be seen that small nonradiative recombination lifetime in the active region reduces the fraction f_j .

The fraction f_j is also modulated by the ideality factor in the active region. When the ideality factor is about 1.0, the f_j is a constant determined by the interaction strength. The fraction f_j decreases when the ideality factor drops below 1.0, and it increase whenever the corresponding m_j is above unity. As in Figure 3.9, due to the different effective density of states for electrons and holes, the ideality factor from electrons and holes are quite different. Within the region of a few V_T around the band gap, the f_j for electrons is increasing while the f_j for holes is decreasing.

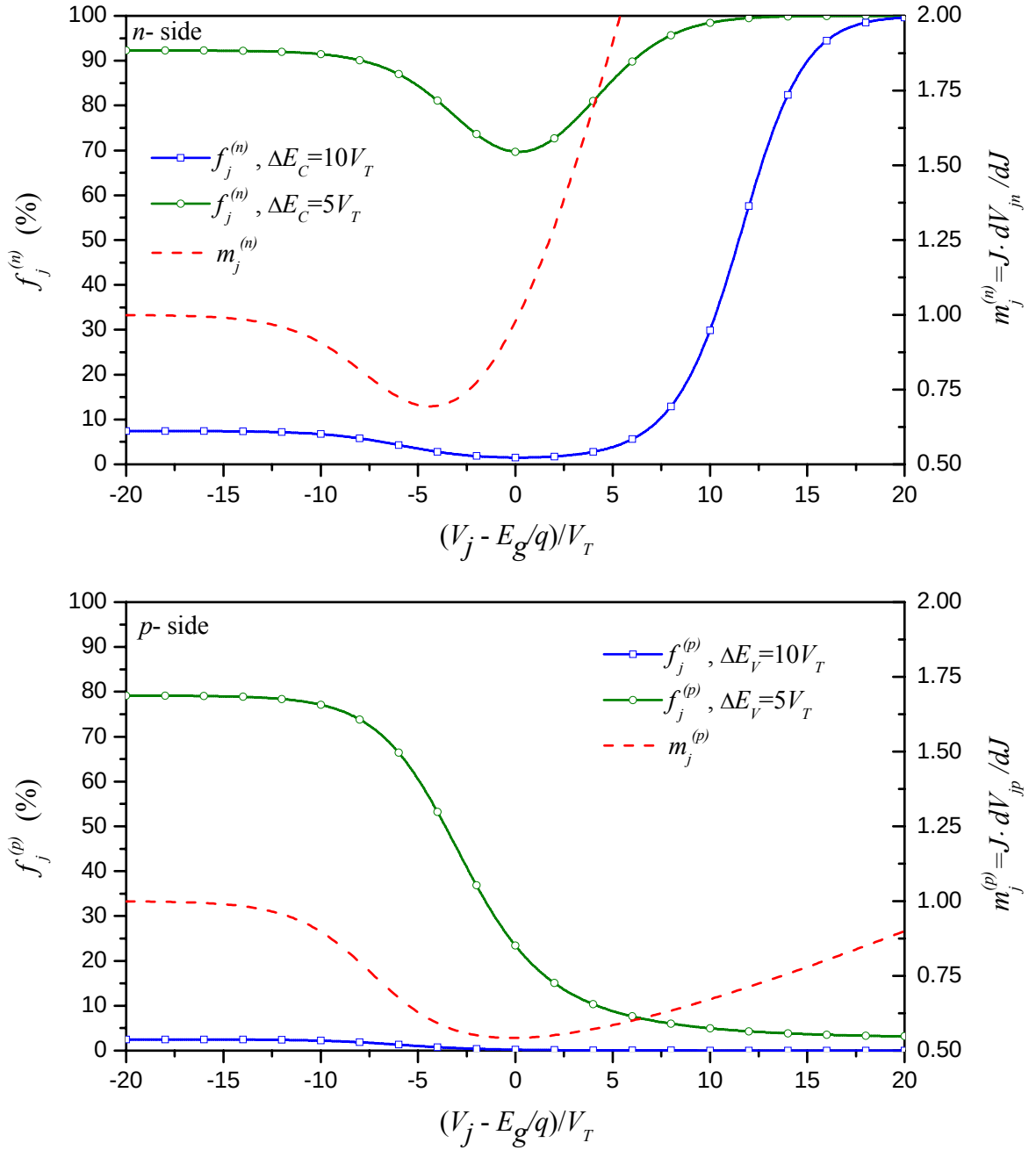


Figure 3.9: The fraction from junction f_j of n - and p - side of the structure as function of junction voltage normalized to the bandgap energy. The corresponding junction ideality factors are also plotted. The f_j starts out almost a constant, decreases with bias level until the corresponding ideality factor is greater than 1.0, and then increases to 100% at extremely high bias level.

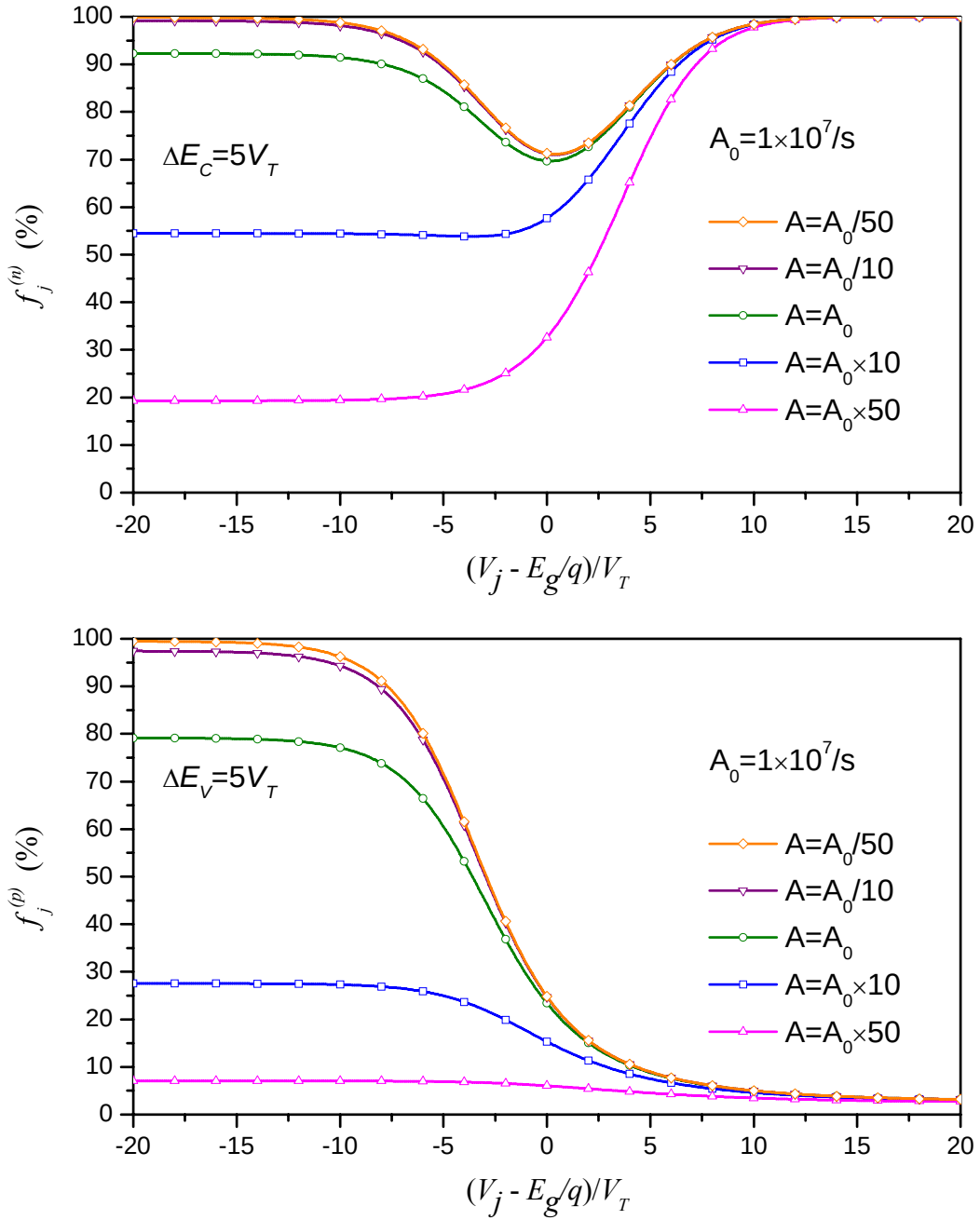


Figure 3.10: The fraction from junction f_j of n - and p - side of the structure with different monomolecular recombination coefficients in the active region as function of junction voltage normalized to the bandgap energy. Small nonradiative recombination lifetime reduces the fraction f_j . Note the different A coefficients correspond to different ideality factor curves.

C. Calculation of differential resistances and ideality factors with f_j

As shown in (3.67) or (3.68), the differential resistance from the terminals consists partially of the junction differential resistance and the remainder of V_T/J . In Figure 3.11, the dV_{ext}/dJ , dV_j/dJ , and V_T/J are plotted as function of current along with the junction fraction f_j of the n - and p - side of the double heterostructure device. It can be seen that the dV_{ext}/dJ is always between the dV_j/dJ and the V_T/J . It is closer to dV_j/dJ when the f_j is closer to 100% as for electrons. On the other hand, it is closer to the V_T/J for holes because the corresponding f_j is much smaller than 1.0. Note for the n - part as the corresponding junction ideality factor is bigger than 1.0, the external differential resistance is smaller than the junction differential resistance. While for the p - part the external differential resistance is bigger than the junction's due to the less-than-1.0 junction ideality factor.

To compare the results from a device with different strengths of interaction between the active region and the cladding layer, in Figure 3.12, the dV_{ext}/dJ , dV_j/dJ , and V_T/J are plotted as function of current for n - and p - side of the device as function of current with a band discontinuity of $5V_T$ and $10V_T$. It can be seen that the dV_{ext}/dJ is always between the dV_j/dJ and the V_T/J for both alignments. With higher band discontinuity, the strength of interaction is weaker so that the f_j is smaller, i.e. less junction properties can be seen from terminals. As a result, the dV_{ext}/dJ is closer to V_T/J for both electrons and holes.

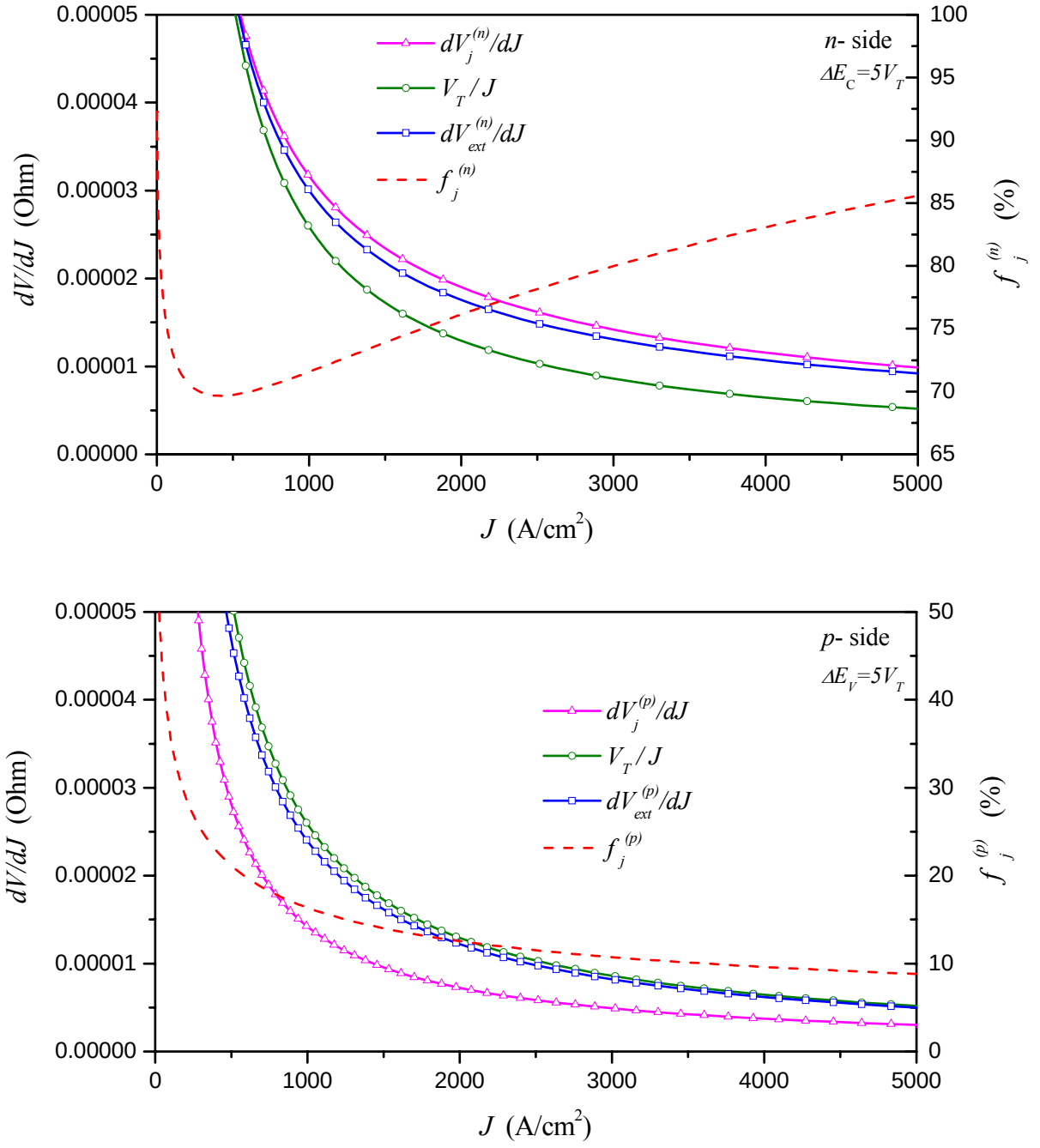


Figure 3.11: The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_j/dJ), V_T/J and the junction fraction f_j from n - and p - side of the structure as function of current. Note the dV_{ext}/dJ is always between the dV_j/dJ and the V_T/J , and it is closer to dV_j/dJ when the f_j is closer to 1.0.

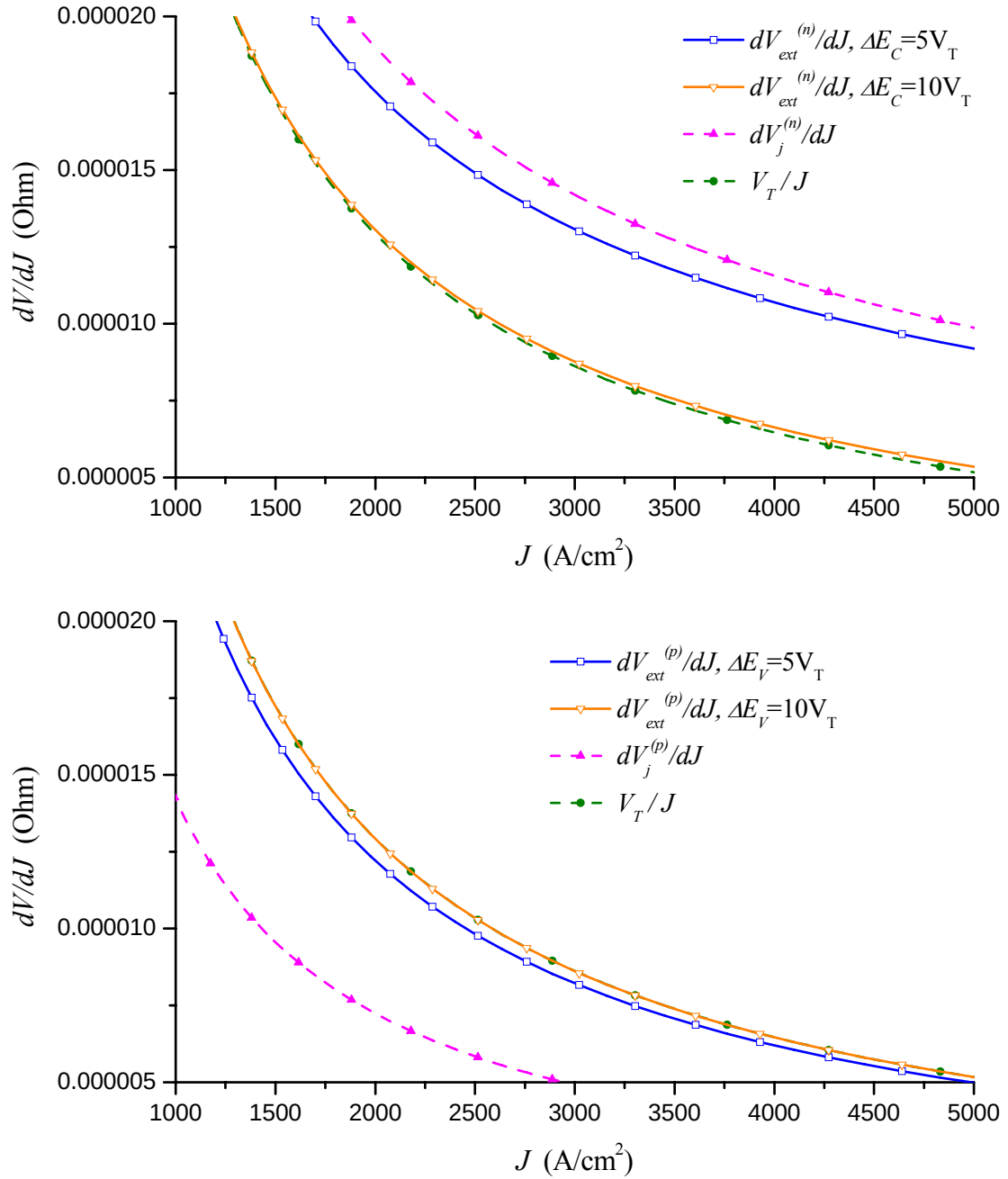


Figure 3.12: The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_i/dJ), V_T/J from n - and p - side of the structure as function of current with band discontinuity of $5V_T$ and $10V_T$. Note the dV_{ext}/dJ is always between the dV_j/dJ and the V_T/J , and it is closer to V_T/J with higher band discontinuity.

The fraction f_j (nonlinear) provides linear combination of internal components for the external differential resistance, and since the (first derivative) ideality factor is measurable through the differential resistance by

$$m_{ext} = \frac{J}{V_T} \cdot \frac{dV_{ext}}{dJ}, \quad (3.69)$$

the external ideality factor can also be associated with the internal junction ideality factors through the same fraction f_j .

For electrons or holes, as in (3.68),

$$\frac{dV_{ext}}{dJ} = \left(\frac{V_T}{J} \right) \cdot [m_j \cdot f_j + (1 - f_j)], \quad (3.70)$$

the corresponding first derivative ideality factor is

$$m_{ext} = \frac{J}{V_T} \cdot \frac{dV_{ext}}{dJ} = [m_j \cdot f_j + (1 - f_j)] \quad (3.71)$$

In Figure 3.13, the ideality factors from the terminals (m_{ext}) and the active junctions (m_j) for n - and p - side of the LED with band discontinuity of $5V_T$ and $10V_T$ as function of junction voltage normalized to the bandgap energy are plotted. It can be seen that it is a value between 1.0 (associated with the thermionic emission across the heterojunction interface) and the ideality factor of the active region (n - or p - part). With both types of carriers for a full device, it can be written as:

$$m_{ext} = (m_j) \cdot f_j + (2.0) \cdot (1 - f_j) \quad (3.72)$$

which varies between the total junction ideality factor m_j and 2.0 depending on the bias level.

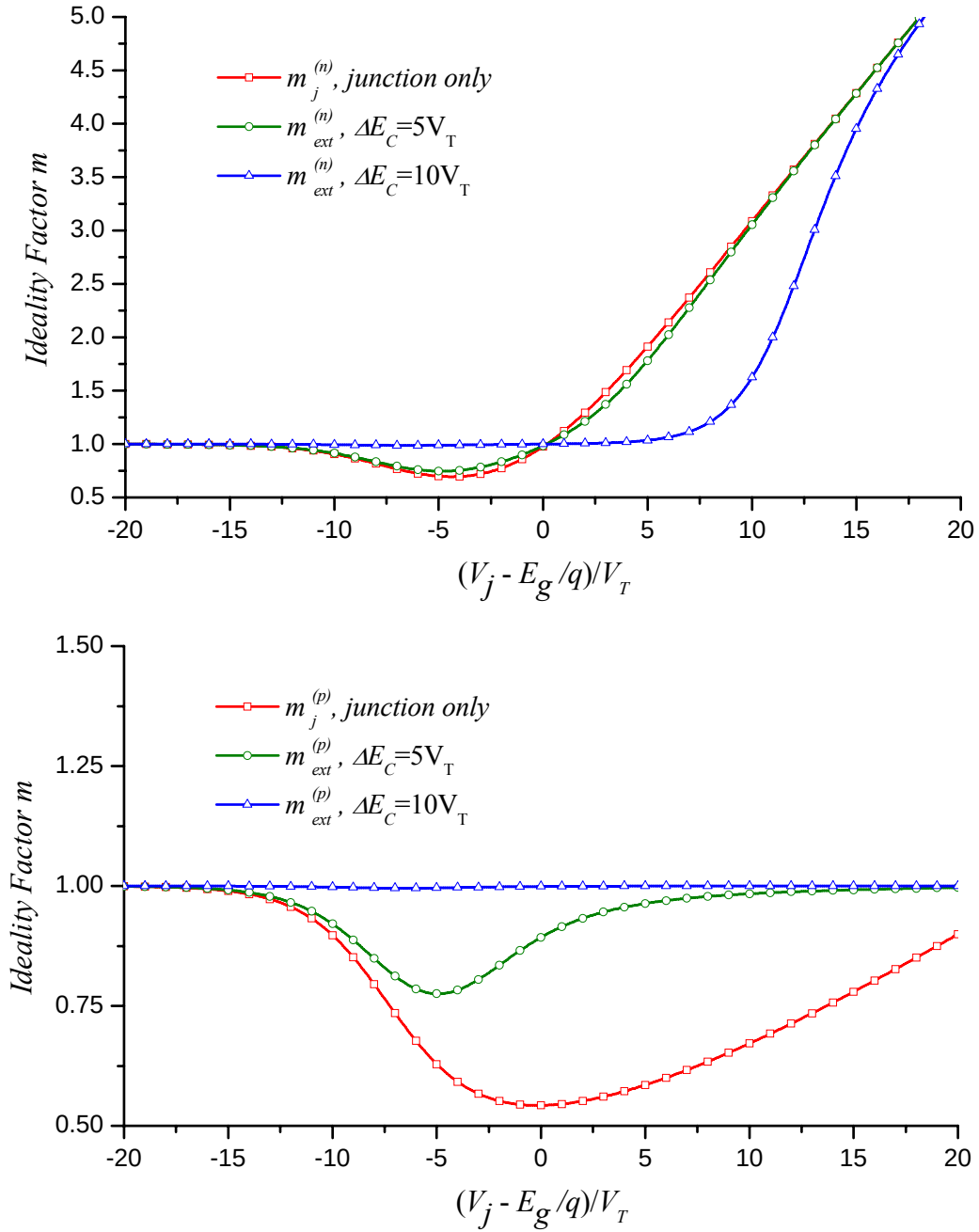


Figure 3.13: The ideality factor m from the terminals and active junctions from n - and p - side of the LED with band discontinuity of $5V_T$ and $10V_T$ as function of junction voltage normalized to the bandgap energy. The ideality factors from terminals are between 1.0 and the ideality from junction.

3.4.5 Summary

In this model, the interaction between the active region and the cladding layer is implied in the thermionic emission boundary condition between the two layers. It is sensitive to parameters such as band discontinuity and temperature.

The strength of interaction is closely related to a bias level dependent (J/J_S) ratio. At low bias level, it is a constant determined by material properties. At higher bias level, it is modulated by the corresponding ideality factor from the active junction, which reflects the speed of quasi-Fermi level separation in the active region.

Due to the backward flux of the thermionic emission, the quasi-Fermi difference between the cladding layer and the active region $V_{cladding}$ is “reactive” to the quasi-Fermi level splitting inside the active junction. The $V_{cladding}$ increases when the junction ideality factor is smaller (corresponding to slower moving of the quasi-Fermi level) and vice versa.

A nonlinear fraction f_j is found to be useful in describing the external differential resistances and the ideality factors by the linear combination of the internal components from the cladding layer and the active region. The value of f_j is always between 0 and 1 and it can also be related to device parameters and junction ideality factor. When f_j is close to 1.0, the measurements of the terminal characteristics are reflective of the junction characteristics. It is closer to 100% when the interactions between the layers are stronger.

3.5 The Simplified Laser Diode Model

3.5.1 Introduction

The internal junction quasi-Fermi level splitting is expected to saturate after lasing threshold due to the gain saturation effect in laser diodes, resulting in kinks in the junction differential resistances and ideality factors. In this section, the active region of a simple double heterostructure laser diode is constructed from the “junction” model with ABC recombination currents as described in Chapter 2, and the stimulated recombination model by Paoli [20]. Cladding layers are next to the active region as shown in Figure 3.1. The device geometry is identical to the one without stimulated emission in Section 3.4. It was shown in the previous section that the interaction between the cladding layer and the active region through thermionic emission can be strong, and as a result there can be significant differences between the electrical characteristics of the terminals and of the junction. This model is extended to describe simple double heterostructure lasers with the inclusion of the junction voltage saturation effect in the active region.

In this section, a simple double heterostructure laser diode is used as an example for a numerical calculation. The device structure and some of the parameters for the active material are shown in Figure 3.1 and Table 3.1 respectively. Additional parameters for the laser junction model as described in Chapter 2 are listed in Table 3.2.

Table 3.2: Additional parameters with the laser active region material.

Parameter	Symbol	Value/Unit
Transparency concentration	n_{tr}	$1.8 \times 10^{18} \text{ cm}^{-3}$
Saturation density of electron concentration	n_s	$2.2 \times 10^{18} \text{ cm}^{-3}$
Saturation value of quasi-Fermi level splitting	V_S	1.4742 V
Differential gain	a	$9.3 \times 10^{-17} \text{ cm}^2$

3.5.2 Interaction between the active region and cladding layer for laser diodes

As discussed in Section 3.4, the (J/J_S) ratio is an important parameter in describing the interaction between the layers. When operated as an LED, the (J/J_S) ratio starts out at a relatively constant value which is mainly determined by material parameters at a low bias junction voltage level. At the transition zone where the junction quasi-Fermi level splitting is close to the band gap energy, the ratio increases with current when the corresponding p - or n -junction ideality factor is less than 1.0 and decreases if the junction ideality factor is more than unity.

The J_S is a function of the active region bias level through V_{cf} and V_{fv} . With the introduction of laser action where the quasi-Fermi levels lock after threshold, the J_S will stop increasing with current as V_{cf} and V_{fv} no longer vary with current. Consequently, after the injection current level passes the lasing threshold, the J/J_S ratio is expected to increase linearly with current, corresponding to less interaction between the active region and the cladding layer.

The (J/J_S) ratios and the corresponding junction ideality factors (m_j) with an n - and p -structure in the laser model are plotted as function of current in Figure 3.14. The curves for

the LED without junction voltage saturation are also plotted. The abrupt change of ideality factors correspond to laser threshold. It can be seen that after threshold, the (J/J_S) ratio always increases with a constant slope with injection level. Before threshold the (J/J_S) ratio can be increasing or decreasing depending on the corresponding ideality factor. As a result, at threshold there are sudden changes or upwards kinks in the slope of the (J/J_S) ratio.

The difference between the quasi-Fermi level in the cladding layer and the active region can be obtained from the (J/J_S) ratio as

$$\frac{V_{cladding}}{V_T} = \ln \left(\frac{J}{J_S} + 1 \right) \quad (3.73)$$

Therefore, kinks are also expected in the slope of $V_{cladding}$ due to the sudden change in the (J/J_S) ratio. In Figure 3.15, $V_{cladding}$ (normalized to the thermal voltage) and the corresponding junction ideality factors (m_j) with n - and p - structure in the laser model are plotted as function of current. Note the $V_{cladding}$ increases logarithmically or linearly as function of current after threshold depending on the absolute value of the (J/J_S) ratio. In contrast, when the device operates as an LED before threshold, $V_{cladding}$ can be increasing or decreasing as function of current depending on the corresponding ideality factor. At the point of threshold there is a sudden increase in the slope of $V_{cladding}$, which corresponds to an upward kink in the $dV_{cladding}/dJ$. On the other hand, the kink from the junction dV_j/dJ is always downwards at lasing threshold, this upward change in the $dV_{cladding}/dJ$ will reduce the total kink height at the terminals.

As defined previously,

$$f_j = \frac{1}{J/J_s + 1} \quad (3.74)$$

and an increasing (J/J_s) ratio after threshold is going to reduce the fraction associated with junction f_j . The f_j and the corresponding ideality factors m_j with n - and p - structures in the laser model are plotted as function of current in Figure 3.16. The curves for the LED without junction voltage saturation are also plotted. It can be seen that for both types, the f_j always decrease with current after threshold. Similar to the (J/J_s) ratio and $V_{cladding}$, there are abrupt changes in the slopes of the f_j at threshold while their values are still continuous with current level.

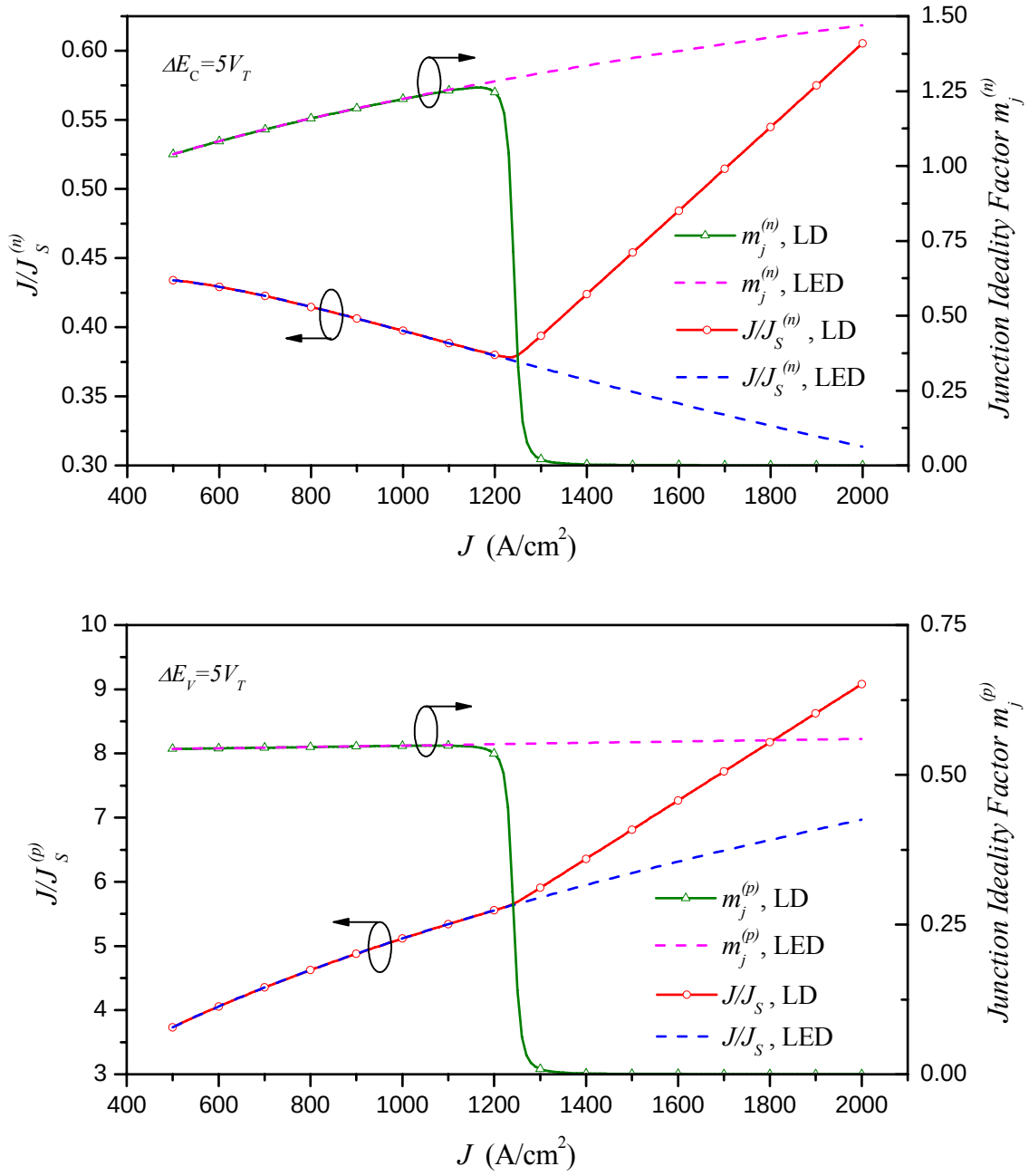


Figure 3.14: The (J/J_S) ratios and the corresponding junction ideality factors (m_j) with n - and p - structure in the laser model as function of current. Dashed lines: the (J/J_S) ratios for the LED without junction voltage saturation. Note the abrupt change of ideality factors and the slopes with the (J/J_S) ratios correspond to laser threshold.

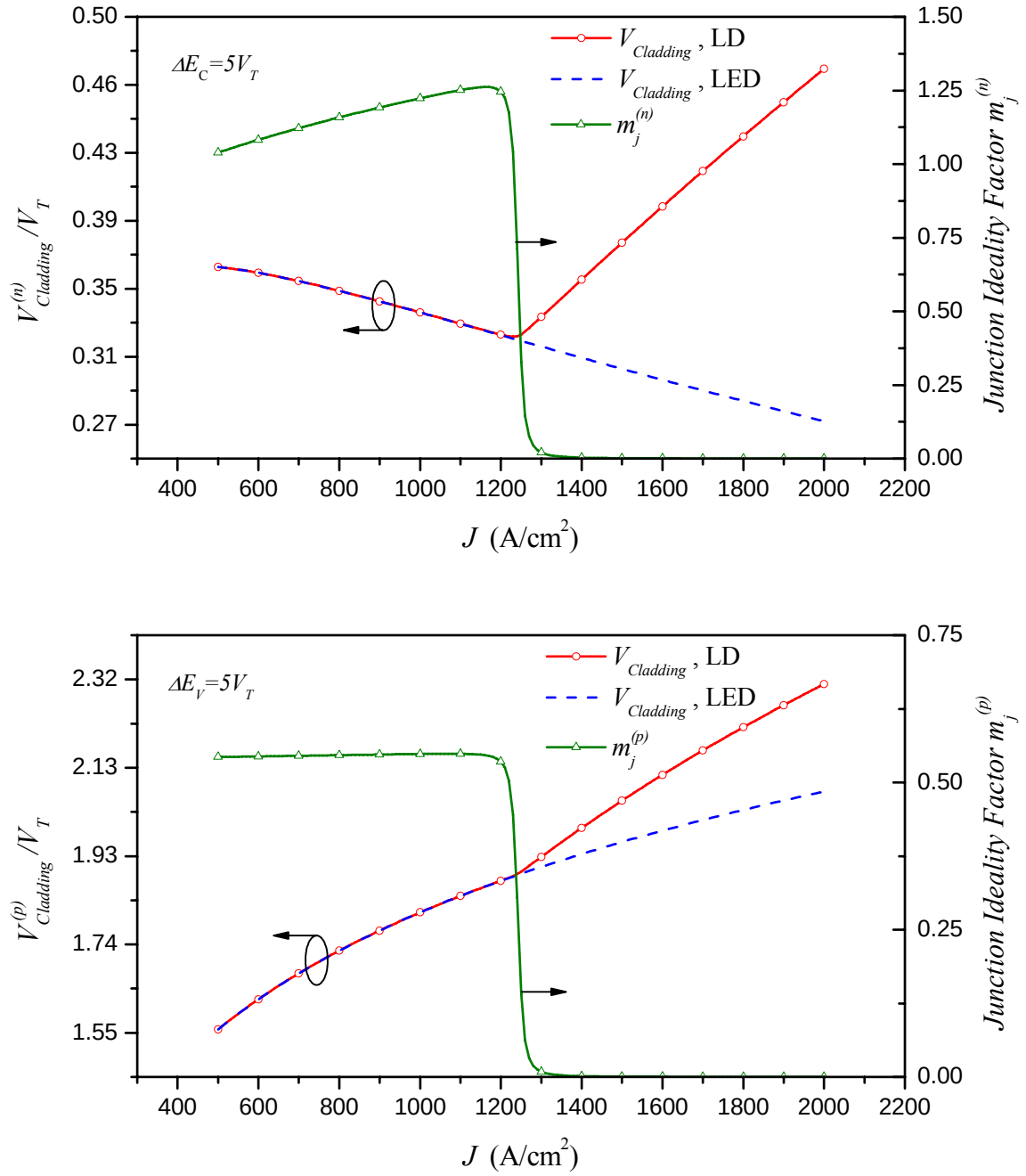


Figure 3.15: The $V_{cladding}$ normalized to thermal voltage and the corresponding junction ideality factors (m_j) with n - and p - structure in the laser model as function of current. Dashed line: the $V_{cladding}$ for the LED without junction voltage saturation. Note the abrupt drop of ideality factor and changes of slope in the $V_{cladding}$ correspond to laser threshold.

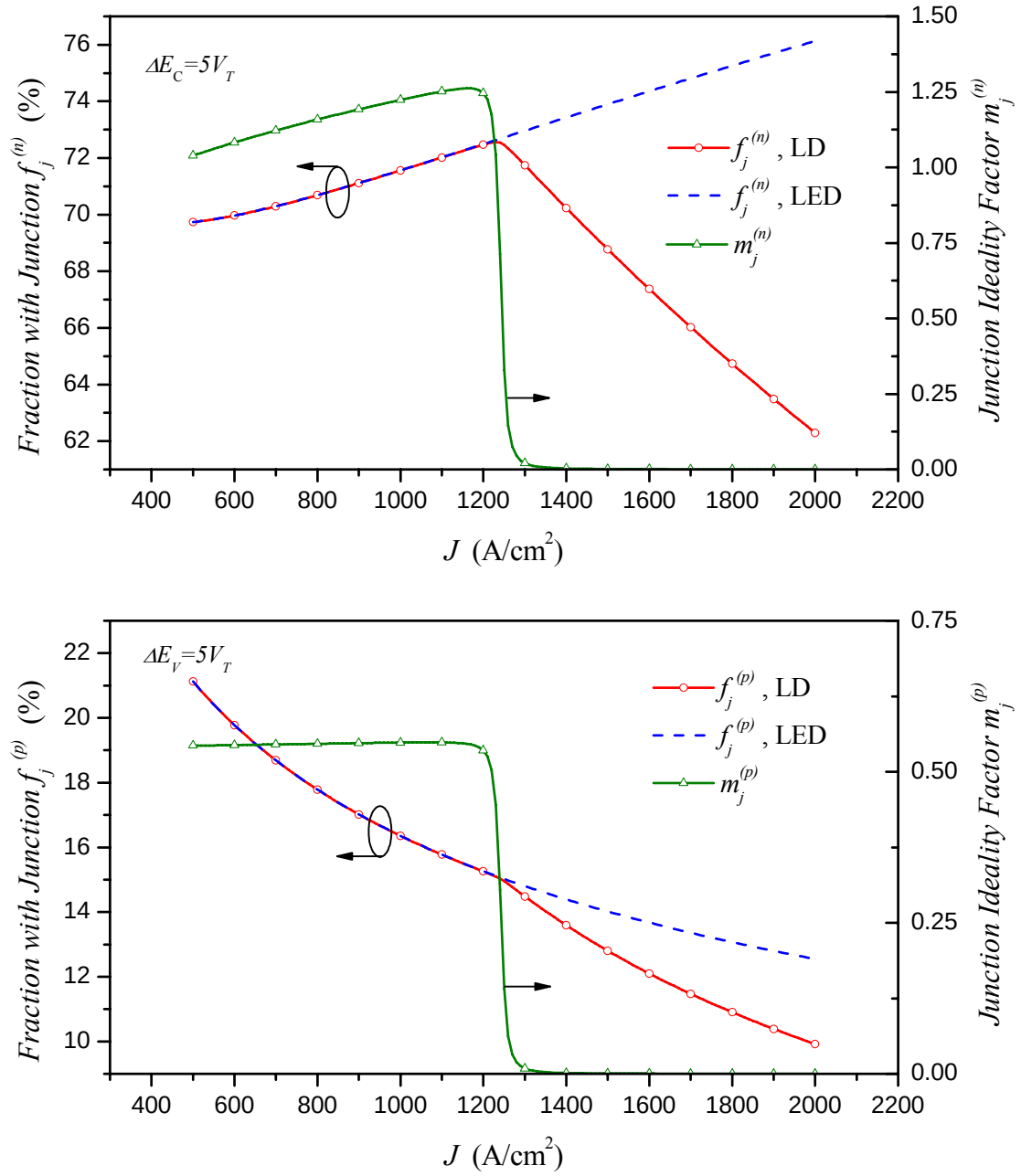


Figure 3.16: The f_j and the corresponding ideality factors m_j with n - and p - structures in the laser model as function of current. The curves for the LED without junction voltage saturation are also plotted. Note there are abrupt changes in the slopes of the f_j at threshold and the f_j always decrease with current after threshold. A decreasing f_j makes it more difficult to observe what is happening at the junction when measuring the terminal characteristics.

3.5.3 Differential resistances and the ideality factors for laser diodes

The fraction associated with junction f_j can be used to describe the terminal differential resistances and ideality factors by the linear combination of values from the junction and the cladding layers as in the LED model described in Section 3.4. The terminal differential resistance for the n - or p - side of the device is given as

$$\frac{dV_{ext}}{dJ} = \left(\frac{V_T}{J} \right) \cdot [m_j \cdot f_j + (1 - f_j)]. \quad (3.75)$$

At threshold, assuming that the fraction associated with junction is $f_{j,th}$, the corresponding junction ideality factor diminish abruptly from $m_{j,th}$ to zero, the kink in the differential resistance from the terminal is

$$\left. \frac{dV_{ext}}{dJ} \right|_{J_{th}^+} - \left. \frac{dV_{ext}}{dJ} \right|_{J_{th}^-} = - (m_{j,th}) \cdot \left(\frac{V_T}{J} \right) \cdot (f_{j,th}) \quad (3.76)$$

It can be seen that the differential resistance right after threshold is always smaller than the one right before threshold, or the kink direction is always downwards with this model. The external kink height is different from the internal value with the fraction $f_{j,th}$. Since the factor $f_{j,th}$ is always less than unity, the kink heights detected at the terminals are smaller than the one solely from the internal active region.

After threshold, from (3.75) the total differential resistance becomes

$$\left. \frac{dV_{ext}}{dJ} \right|_{J > J_{th}} = \left(\frac{V_T}{J} \right) \cdot (1 - f_j) \quad (3.77)$$

with non-constant f_j . As the f_j is decreasing after threshold, the $(1 - f_j)$ will increase with current after threshold. Nonetheless, it can be simplified to

$$\left. \frac{dV_{ext}}{dJ} \right|_{J > J_{th}} = \frac{V_T}{J_S + J} \quad (3.78)$$

which decreases with bias level after threshold. The trend of the decreasing differential resistances is also modified from $m_j \cdot \frac{V_T}{J}$ ($\sim \frac{1}{x}$) before threshold to $\frac{V_T}{J_S + J}$ ($\sim \frac{1}{x + x_0}$) after threshold.

The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_j/dJ), cladding layers ($dV_{cladding}/dJ$) and the junction fraction f_j for the n - and the p - side of the simple laser model are plotted as function of current in Figure 3.17. The curves for the LED without junction voltage saturation are also plotted in dashed lines for comparison. The kinks in the differential resistances indicate the lasing threshold. It can be seen that the non-unity f_j reduces the terminal kink height at laser threshold and creates a slowly decreasing differential resistance after threshold.

In Figure 3.18, the dV/dJ from the junction and from the terminals with band discontinuities of $5V_T$ and $10V_T$ for the n - and the p - side of the laser model are plotted as function of current. The case of $10V_T$ (compared to $5V_T$) for the band discontinuity corresponds to a much smaller interaction between the layers. This also dramatically reduces the kink height at lasing threshold so that it is barely visible as shown in the curves with triangle symbol. In this situation it is no longer possible to detect laser thresholds by finding the kinks in the differential resistances.

The terminal ideality factors can be calculated from measured differential resistance by

$$m_{ext} = \frac{J}{V_T} \cdot \frac{dV_{ext}}{dJ} = [m_j \cdot f_j + (1 - f_j)] \quad (3.79)$$

Before threshold, the obtained ideality factor from the n - or the p - side of the device is between the junction value m_j and 1.0 as discussed in the LED model. Assume that right before threshold, the fraction associated with junction is $f_{j,th}$ and the corresponding junction ideality factor is $m_{j,th}$. The junction ideality factor diminishes abruptly to zero right after threshold, and the corresponding downward kink in the terminal ideality factor associated with lasing threshold is therefore

$$m_{ext}|_{J_{th}^+} - m_{ext}|_{J_{th}^-} = -(m_{j,th}) \cdot (f_{j,th}) \quad (3.80)$$

Equation (3.80) indicates that, as with the differential resistance, a reduction of kink height in the ideality factor to the fraction of $f_{j,th}$ occurs.

The terminal ideality is not a constant after threshold. Instead of dropping to zero as within the junction, the measurable value from the terminals is

$$m_{ext}|_{J > J_{th}} = 1 - f_j \quad (3.81)$$

which increases with current after threshold since the f_j is decreasing after threshold.

In Figure 3.19, the ideality factors of the junction (m_j) and of the terminals (m_{ext}) with band discontinuities of $5V_T$ and $10V_T$ in the n - and the p - side structure of the laser model are plotted as function of current. The kink heights at the laser thresholds are dramatically reduced with less interaction between the active region and the cladding layer. After threshold, the terminal ideality factor increases with current level and approaches 1.0.

To summarize, the LED model which takes into account of the interaction between the cladding layer and the active region of double heterostructure devices through thermionic emission across the heterojunction boundary is extended to a simple laser model with the inclusion of junction quasi-Fermi level saturation. The model predicts that less interaction between the active region and the cladding layer will result in reduced kink heights in the differential resistances and the ideality factors as measured at the terminals at laser threshold. It is also responsible for decreasing differential resistances and increasing ideality factors after threshold.

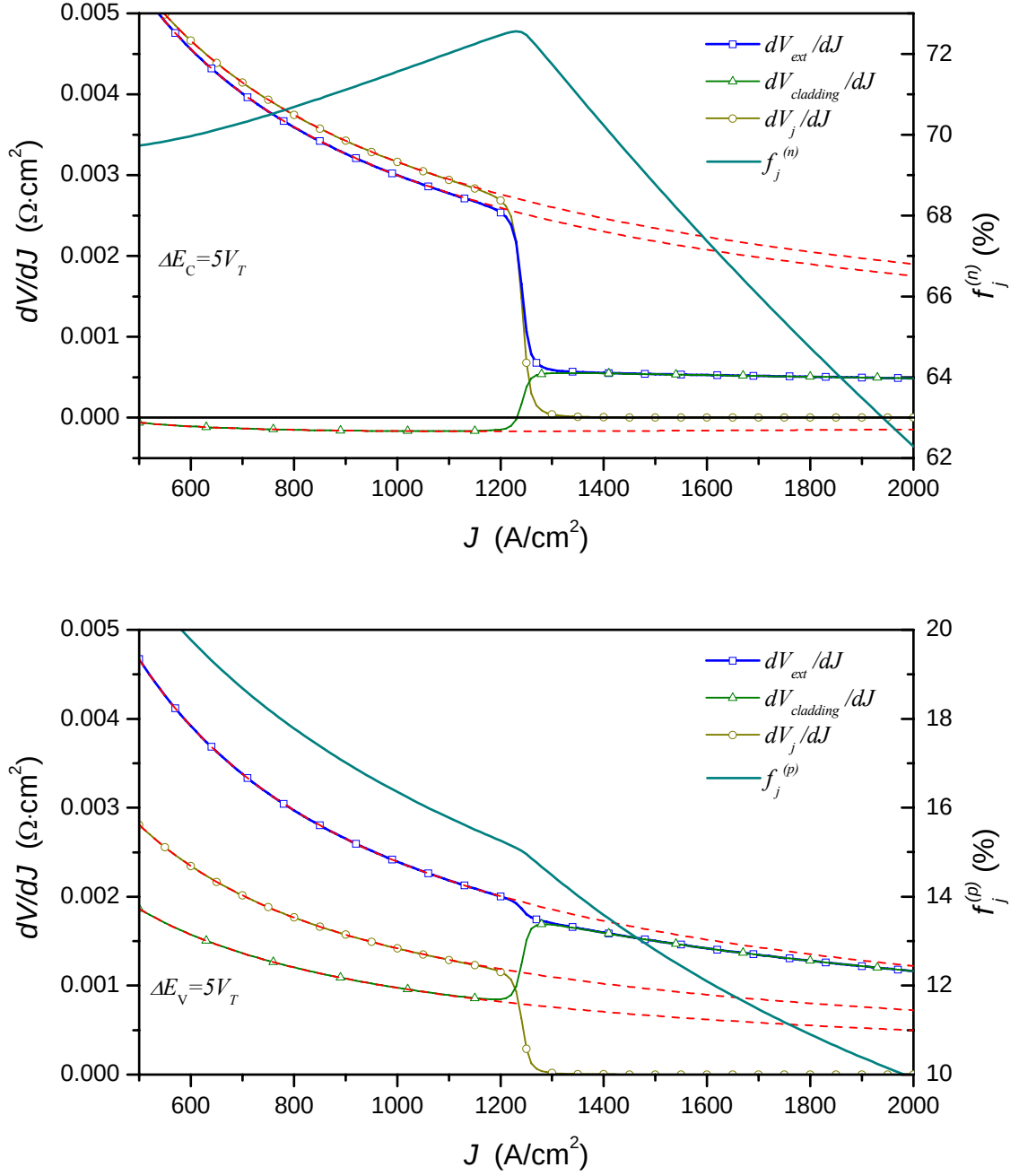


Figure 3.17: The dV/dJ from the terminals (dV_{ext}/dJ), active junctions (dV_j/dJ), cladding layers (dV_{cladding}/dJ) and the junction fraction f_j from n - and p - side of the simple laser model as function of current. The curves for the LED without junction voltage saturation are also plotted in dashed lines for comparison. The non-unity f_j reduces the terminal kink height at laser threshold and creates decreasing differential resistance after threshold.

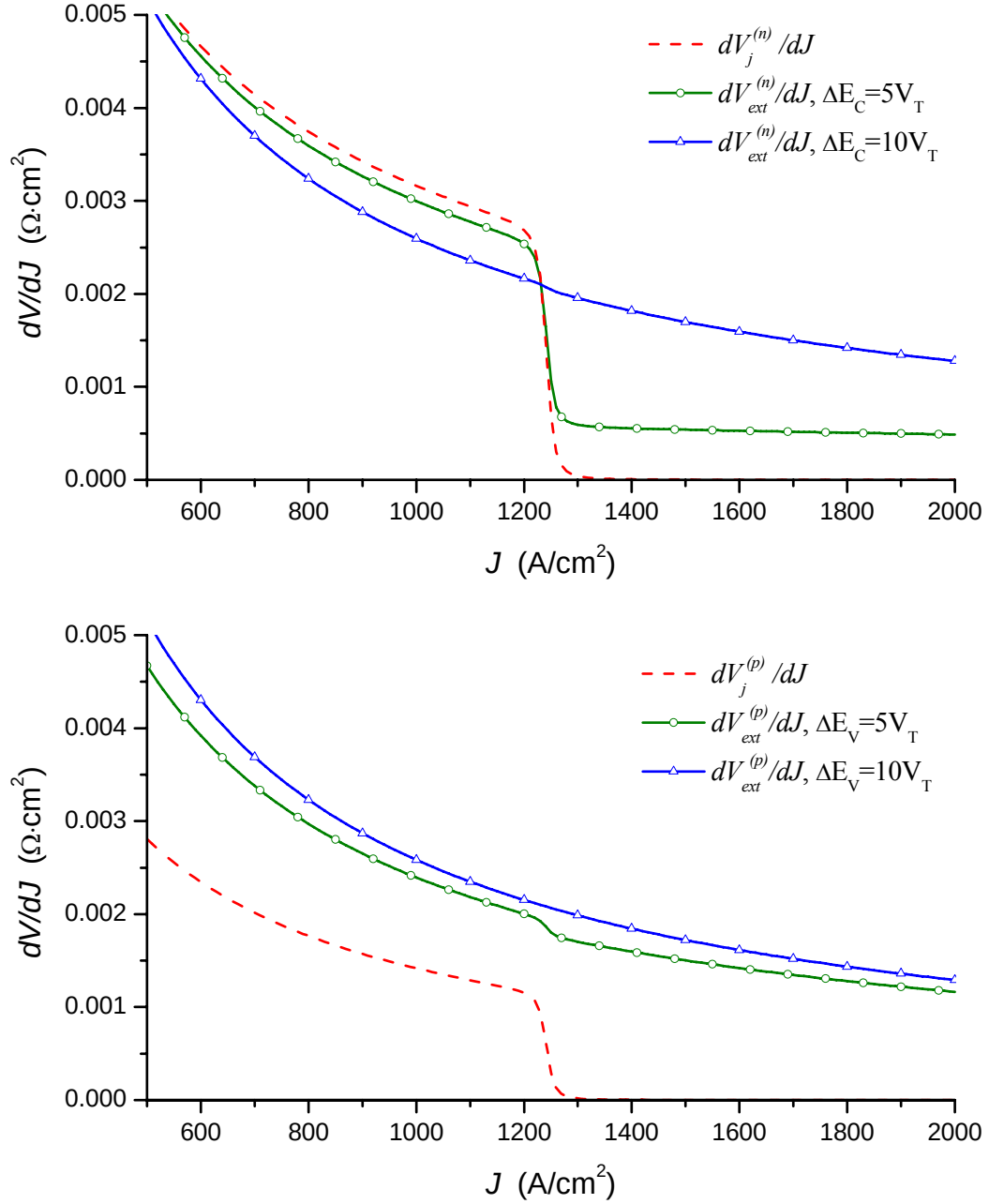


Figure 3.18: The dV/dJ from junction and from the terminals with cladding layers band discontinuities of $5V_T$ and $10V_T$ of n - and p - side of the laser model as function of current. The smaller interaction between the layers with the $10V_T$ discontinuity in the structure dramatically reduces the kink height at lasing threshold so that it is barely visible (the curves with triangle symbol).

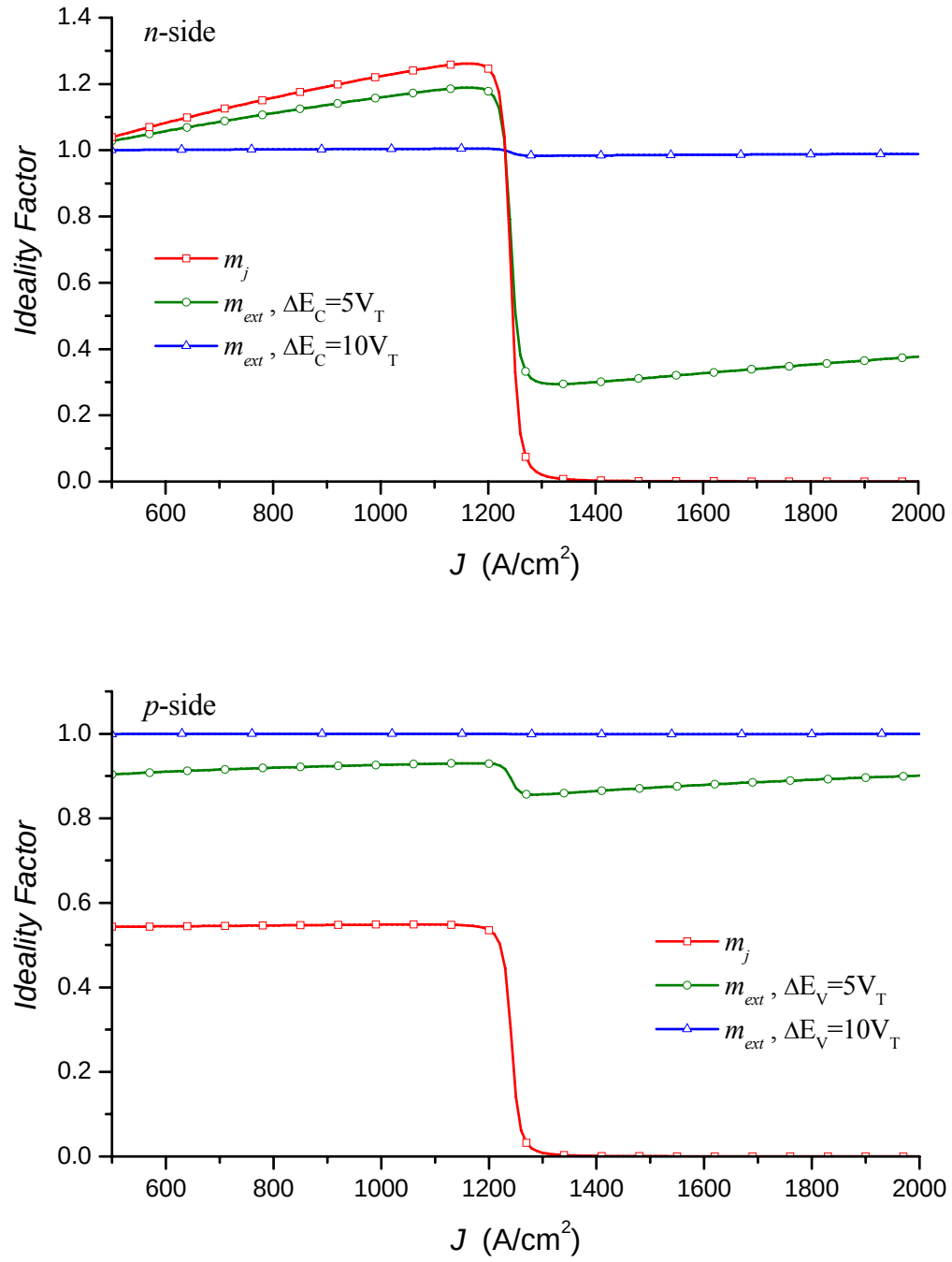


Figure 3.19: The ideality factors of the junction (m_j) and of the terminals (m_{ext}) with band discontinuities of $5V_T$ and $10V_T$ for the n - and the p - side of the laser model as function of current.

3.6 Conclusions

In this chapter, the nonlinear resistances introduced by majority carrier injection from the device terminals to the active region in simple double heterostructure light emitting diode or a laser diode are investigated through a semi-analytical current-voltage model. The model is based on a classical drift-diffusion formulation for the bulk cladding layers and a thermionic emission mechanism for carrier transport across abrupt heterojunction interfaces. Various assumptions such as a flat-band condition in the active region and negligible carrier overflow were assumed in the derivation.

The characteristics of the voltages, differential resistances and ideality factors are different between the active region and the terminals with this model. The differences vary with injection level and they are found to be dependent on the interaction between the active region and the confining layers. The strength of interaction is closely related to an injection level dependent (J/J_S) ratio. At a low bias level, the ratio is a constant determined by material properties. It is sensitive to parameters such as band discontinuity and temperature. At a higher bias level, the ratio is modulated by the corresponding ideality factor from the active junction, which reflects the speed of quasi-Fermi level separation in the active region. The quasi-Fermi level movement in the active region is slower when the corresponding junction ideality factor is smaller than 1.0 where the interaction between the layers is smaller. On the other hand, the strength of interaction is stronger when the junction ideality factor is greater than 1.0.

The interaction between the layers is implied in the thermionic emission boundary condition for heterointerfaces in this model. Due to the backward flux of the thermionic emission, the quasi-Fermi difference between the cladding layer and the active region $V_{cladding}$ is “reactive” to the quasi-Fermi level splitting inside the active junction. The $V_{cladding}$ increases when the junction ideality factor is smaller (corresponding to slower moving of the quasi-Fermi level) and vice versa.

The nonlinearity is accompanied by the junction properties being only partially reflected at the device terminals. The measured differential resistances and the ideality factors at device pins are normally only a fraction of the contribution from the active region, and the remainder of the terminal characteristics is from the cladding layers. A nonlinear fraction f_j is found to be useful in describing the external differential resistances and the ideality factors by the linear combination of the internal components from the cladding layer and the active region. The value of the f_j is always between 0 and 1, and it can also be related to device parameters and junction ideality factors which are related to the bias level. When f_j is close to 100% then the terminal differential resistances and ideality factors are closer to the junction values when the interactions between the layers are stronger. It is nontrivial to design a device whose derivative characteristics can be mostly measured from its terminals.

The LED model was extended to a simple laser model with the inclusion of junction quasi-Fermi level saturation in the active region. The model predicts that less interaction between the active region and the cladding layer will result in reduced kink heights in the differential resistances and the ideality factors at laser threshold. Although the junction quasi-Fermi level splitting is saturated after threshold, a decrease in the differential resistance and an increase

in the terminal ideality factor can be observed as a result of the contribution from the interaction between the cladding layer and the active region. A reduction in the differential resistance kink height at threshold is always accompanied by the decrease of differential resistance after threshold from this model.

Chapter 4

Numerical Modeling of the Carrier Overflow Effects on the Differential Resistance of Simple Double Heterostructure Laser Diodes

4.1 Introduction

The interaction between the active region and the cladding (or the confinement) layer of double heterostructure LEDs and LDs were analyzed through the current-voltage equation derived with the thermionic emission boundary condition in the semi-analytical model described in Chapter 3. As mentioned previously, this semi-analytical model is based on various assumptions and simplifications. In order to obtain more realistic results, in this chapter, the differential resistances and the ideality factors of the same device geometries are

analyzed through a self-consistent numerical approach that makes possible the inclusion of recombination in the cladding layer and the over-barrier minority carrier leakage.

Carrier confinement has always been an important issue for semiconductor opto-electronic devices such as LEDs and LDs. The mechanisms and effects of carrier leakage over blocking layers have been extensively studied analytically, numerically and by experiments on various devices and material systems [69-94]. The carrier spillover is practically not avoidable. Spillover in laser diodes not only deteriorates device efficiency and increases threshold current density, it also creates a nonlinear light-current relationship, decreases the characteristic temperature T_0 , limits the maximum modulation frequency and output power, reduces the reliability and shortens device lifetime. In this chapter it will be shown that the leakage currents also affect the differential resistances and therefore the ideality factors of laser diodes.

Some important physics including 1) thermionic emission at a heterojunction interface, 2) drift-diffusion transport within bulk semiconductor and 3) quantum mechanical tunneling at the heterojunction interface have to be considered in order to model the over-barrier leakage. So far there is no analytical model that can take into accounts all these mechanisms and the transport of both majority carrier and minority carriers even for the simplest one-dimensional problem.

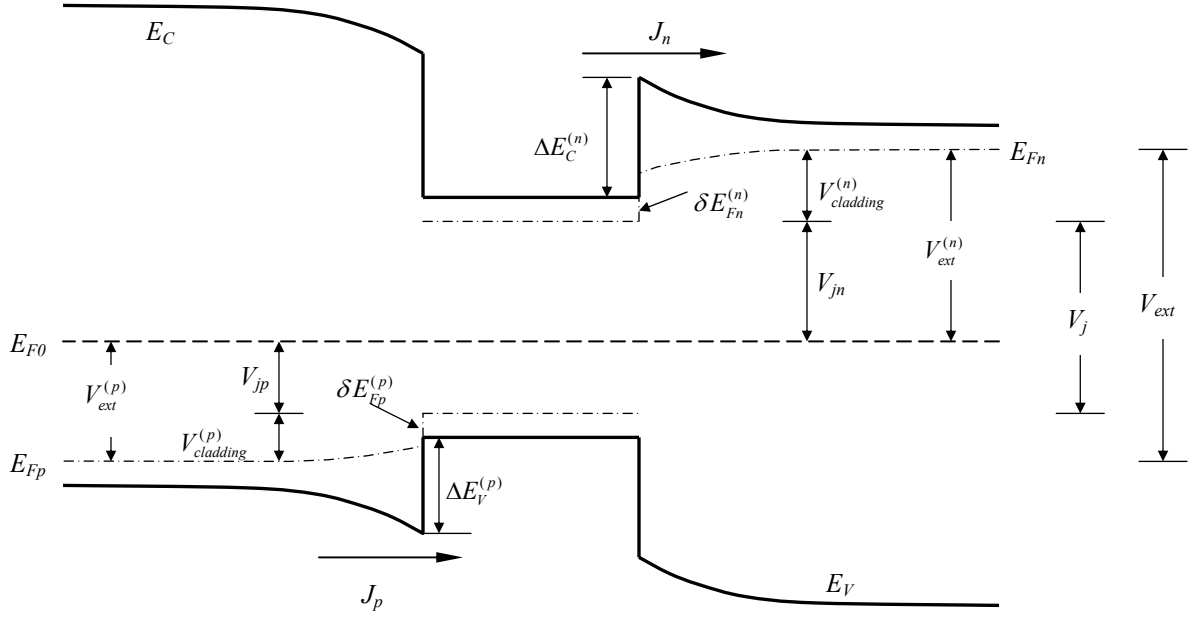
Commercial simulators are available and normally the entire device is simulated instead of the leakage problem over a barrier. Numerical simulation of a simple laser diode or light-emitting diode is complicated, and the simulation requires a tremendous amount of computation because of the coupling between electrical, optical and thermal equations. On

the other hand, the motivation of our approach is to identify the primary physical processes that affect the differential resistance and the ideality factor of a diode. Therefore, instead of accurately predicting the electrical and optical behavior of a designed or fabricated diode with complete input parameters, our focus is to include the capability of incorporating the key physical effects and obtaining the general trends and tendencies of the behaviors from the underlying physics.

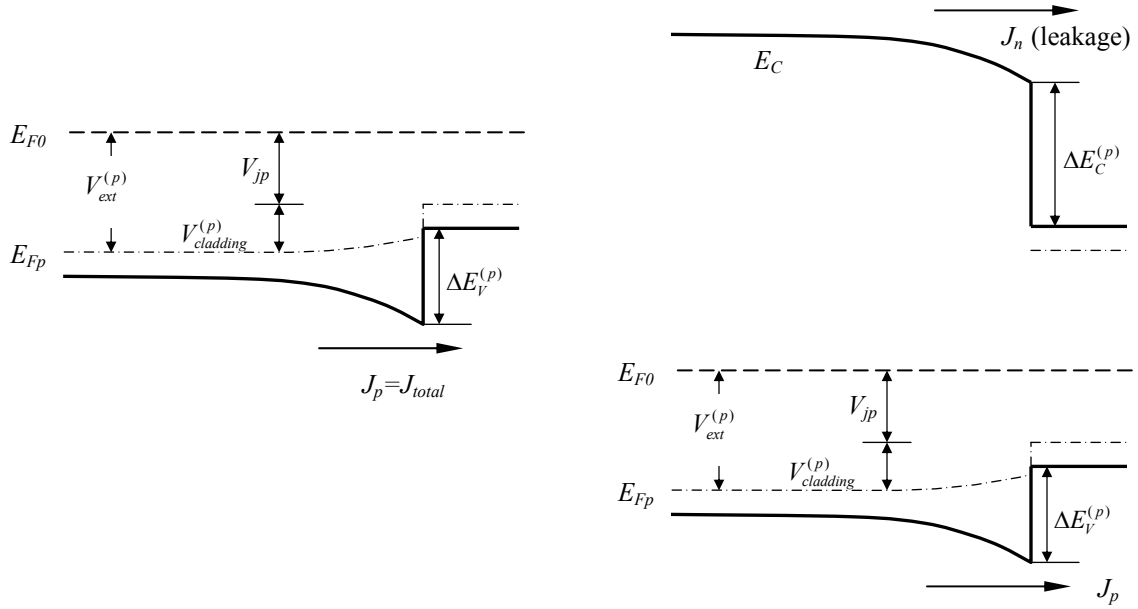
To minimize the computational load, the numerical simulator is simplified as follows. First, it is restricted to only one spatial dimension. While the spatial effects such as current spreading and spatial hole burning (SHB) in modern LEDs and Vertical-Cavity Surface-Emitting Lasers (VCSELs) are obviously not negligible, they can possibly be simulated using the lumped circuit model (e.g. resistor-diode networks) [95] with the simulated one-dimensional device as circuit elements. Second, most of the physics in the model is kept phenomenological. For example, the electrical-optical interaction in the active region of a laser diode is modeled through the classical electron and photon rate equations. The recombination mechanisms are described with $A/B/C$ coefficients whenever possible. Third, the model is further simplified to only half of the device, i.e. the p - or the n - side result can be obtained without running the full-device simulation. In previous chapters, it was shown that the ideality factors from the recombination mechanisms in the active region and that from the majority carrier injection through heterointerfaces can both be separated into n - (electron) and p - (hole) parts. The problem is solvable in a self-consistent manner for half of this one-dimensional device using the additional thermionic boundary condition for minority carriers, and assuming that the quasi-Fermi level splitting in the uniform active region and

the majority current at the boundary are known. With these simplifications, the computational cost of the simulation is greatly reduced while the primary physics can be easily identified in studying their effects on the differential resistance and the ideality factor characteristics. The simplification and the difference between the models are illustrated in Figure 4.1.

The implementation of a self-consistent one-dimensional (1-D) numerical model is described in Section 4.2. With the described numerical model, the effects which were not included in Chapter 3 such as the recombination in the cladding and the over-barrier minority carrier leakage currents are taken into account in the simulation. Results are shown and compared with the semi-analytical model in Section 4.3. Important parameters that affect the leakage currents are discussed. Simulation of the effects of the leakage current on the terminal differential resistances are demonstrated and compared with experiment data. Conclusions are presented in Section 4.4.



(a) A simple double heterostructure device at high-biased condition.



(b) The *p*-side heterointerface for the semi-analytical model in Chapter 3.

(c) The structure for numerical simulation in this chapter.

Figure 4.1: Simplification of the numerical simulation. (a) A simple double heterostructure device at high-biased condition. (b) The *p*-side heterointerface for the semi-analytical model in Chapter 3. (c) The structure for numerical simulation in this chapter.

4.2 The Numerical Model

The simulated structure is a p -cladding layer with an Ohmic contact on one side and an active region on the other side. In theory, either the p - or n - cladding layer can be chosen in the simulation, while normally the p -cladding layers draw more attention. Compared with n - type material, it is in general more difficult to dope the p - type material with a high concentration of dopants, more challenging to make a good Ohmic contact, and the valence band structure is much more complicated. Therefore, the modeling of the hole current is more challenging and richer in important effects. As mentioned before, the simulator is not intended for accurate prediction and the model is mainly phenomenological. The assumptions for this model are described below.

4.2.1 Assumptions for the numerical simulation

First, without taking into accounts the individual sub-bands in the valence band and the indirect minima in the conduction bands, single electron and hole effective density of states are used along with parabolic E - k relationship in the model. Then band-filling and the carrier concentrations can then be calculated with the Fermi-Dirac integral.

The simulation is performed only at high injection conditions in the active region, which is the same condition as previously used for the semi-analytical model. The internal junction quasi-Fermi level splitting is significant so the free carrier concentrations of both carrier types are high and the active region is assumed homogeneous. The active layer band-bending is assumed negligible and the quasi-Fermi levels as well as the conduction and the valence

band diagram are flat across the entire active region. Charge neutrality is also assumed for the double heterostructure devices. For devices whose active regions are quantum wells, it has been pointed out that charge neutrality may not be met in the active region even at high injection levels [111]. The recombination currents in the active region follow the models described in Chapter 2, i.e. monomolecular, bimolecular and Auger recombinations with $A/B/C$ coefficient respectively, along with stimulated emission in lasers derived from the classical rate equations [20] are taken into account.

The main problem to solve is actually the bulk cladding layer, where the classical drift-diffusion transport model is applied. Unlike the semi-analytical model where the recombination events in this layer are neglected and the full depletion approximation is used, in this numerical model, the recombinations in this layer can be included and the band-bending in this layer is not necessarily quadratic.

The same thermionic-field emission formulation as in Chapter 3 is used for the boundary of heterojunction interface. As the simulation is performed on only half of the device, the boundary condition at this interface is critical to ensure the existence of the solution and the convergence of the simulation. The other boundary of the simulated structure is an ideal Ohmic contact, which is a Dirichet type of condition for the differential equations. Details on the treatment of the boundary conditions will be presented in Section 4.2.3.

4.2.2 The drift-diffusion formulation of the cladding layer

With the flat-band approximation for the active region and the phenomenological recombination and rate-equation models for the gain medium, the cladding layer next to this layer becomes the main body of the numerical simulation. When using the self-consistent drift-diffusion (DD) simulation, the quadratic assumption of band-bending is not required and the results are expected to be more realistic. Nevertheless, with the inclusion of recombinations in the cladding layer, the effects from the additional current path and the minority carriers overflow leakage currents can be investigated.

In this model the conventional one-dimensional (1-D) drift-diffusion (DD) approach [96, 101] is used to describe carrier transport within the cladding layer. The set of three coupled transport equations are Poisson's equation and the continuity equations for electrons and holes. We use the electrostatic potential V_{ep} , the electron quasi-Fermi level V_n and the hole quasi-Fermi level V_p as the independent variables. For simplicity, the cladding layer material is assumed to be homogeneous. Only Shockley-Read-Hall (SRH) recombination with a single trap level in the cladding layer is considered and the trap level is assumed to be the same as the intrinsic level. In 1-D and steady-state, the equations are given as

$$\frac{d^2 V_{ep}}{dx^2} + \frac{q}{\epsilon} \cdot (p + N_D^+ - n - N_A^-) = 0 \quad (4.1)$$

$$\frac{dJ_n}{dx} - q \cdot R^{SRH} = 0 \quad (4.2)$$

$$\frac{dJ_p}{dx} + q \cdot R^{SRH} = 0 \quad (4.3)$$

where ϵ is the permittivity of cladding layer material. n and p are the free electron and hole densities. N_A^- , N_D^+ are the ionized acceptor and donor concentrations. Electron and hole current densities J_n and J_p are expressed as

$$J_n = -q\mu_n n \frac{dV_{ep}}{dx} + qD_n \frac{dn}{dx} \quad (4.4)$$

$$J_p = -q\mu_p p \frac{dV_{ep}}{dx} - qD_p \frac{dp}{dx} \quad (4.5)$$

where μ_n and μ_p are the electron and hole mobilities, D_n and D_p are the electron and hole diffusion coefficients, respectively. Free carrier densities are calculated using Fermi-Dirac statistics. The electron and hole concentrations, without individually taking into account the multiple sub-bands, are given by

$$n = N_C \cdot \mathcal{F}_{1/2} \left(-\frac{E_C / q - V_{ep} - V_n}{V_T} \right) \quad (4.6)$$

$$p = N_V \cdot \mathcal{F}_{1/2} \left(-\frac{V_p + V_{ep} - E_V / q}{V_T} \right) \quad (4.7)$$

where $\mathcal{F}_{1/2}$ is the Fermi integral of order 1/2 defined as

$$\mathcal{F}_{1/2}(\xi) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}}{1 + \exp(x - \xi)} dx \quad (4.8)$$

The E_C , E_V are the conduction and valance band edges. N_C , N_V are the effective density of states of electrons in the conduction band and holes in the valance band. The ionized acceptor and donor concentrations N_A^- , N_D^+ are obtained from total acceptor and donor concentrations N_A , N_D by

$$N_A^- = \frac{N_A}{1 + 4 \cdot \exp\left(-\frac{V_p + V_{ep} - E_V / q - E_A / q}{V_T}\right)} \quad (4.9)$$

$$N_D^+ = \frac{N_D}{1 + 2 \cdot \exp\left(-\frac{E_C / q - V_{ep} - V_n - E_D / q}{V_T}\right)} \quad (4.10)$$

where E_A , E_D are the ionization energies of the acceptors and donors, respectively. The Shockley-Read-Hall recombination rate is given by

$$R^{SRH} = \frac{n \cdot p - n_i^2}{\tau_{p0}(n + n_i) + \tau_{n0}(p + p_i)} \quad (4.11)$$

where n_i is the intrinsic carrier concentration and τ_{n0} , τ_{p0} are the carrier lifetime for electrons and holes, respectively.

4.2.3 Treatment of the boundary conditions

There are two boundaries for the simplified cladding layer structure as shown in Figure 4.1 part (c). The first is an p -contact for hole injection and we model it as an ideal Ohmic contact where charge neutrality and thermal equilibrium are assumed. This is a Dirichet boundary condition for the differential equations. The second boundary is the cladding/active layer interface. The importance of the heterojunction transport over this interface on the differential resistances and the ideality factors has been demonstrated in Chapter 3. In the semi-analytical model, only the majority carrier (and therefore the corresponding quasi-

Fermi level) in the cladding layer needs to be considered, while in this numerical model, both carrier distributions and quasi-Fermi levels will be calculated self-consistently.

Within the cladding layer, there are three independent variables $\{V_{ep}, V_n, V_p\}$. In the active layer, V_n and V_p with respect to their thermal equilibrium values are known if the recombination currents are given. However, the V_{ep} is unknown and it cannot be predicted solely from the active material model. Therefore, the boundary condition for the drift-diffusion equations is not explicit. Nevertheless, there are three independent equations that can be used as the boundary conditions for this interface and they will be explained as follows.

First, the thermionic emission current of holes at the boundary can be written as:

$$J_p^{TE} = q \cdot \left(p_1 \cdot v_{p1} - p_2 \cdot v_{p2} \cdot \left(\frac{m_{p1}^*}{m_{p2}^*} \right) \cdot e^{-\frac{\Delta E_V^{(p)}}{V_T}} \right) \quad (4.12)$$

where the subscript 1 means p -cladding layer boundary and 2 means the active layer boundary.

The same hole current within the cladding layer is governed by the drift-diffusion equation (4.5). Therefore, at the boundary the drift-diffusion current can be set equal to the thermionic emission current:

$$J_p^{TE} = J_p^{DD} \quad (4.13)$$

Similarly, for the minority carrier current at the boundary, the thermionic current is given by:

$$J_n^{TE} = q \cdot \left(n_2 \cdot v_{n2} \cdot \left(\frac{m_{n1}^*}{m_{n2}^*} \right) \cdot e^{-\frac{\Delta E_C^{(p)}}{V_T}} - n_1 \cdot v_{n1} \right) \quad (4.14)$$

Equating this to the drift-diffusion current and we get

$$J_n^{TE} = J_n^{DD} \quad (4.15)$$

In addition to these two equations, we assume that the majority carrier current density right at the boundary is another input parameter:

$$J_p = J \text{ (input)} \quad (4.16)$$

When most of the injected holes recombine in the active region without leaking into the n -cladding layer, the boundary hole current can be assumed equal to the recombination current in the active layer. The justification for this assumption is that holes typically have a large effective mass, a large density of states, and as such, the thermionic emission of holes over the barrier of a typical valance band discontinuity will be negligible.

To conclude, with the assumption of flat-band in the active region, a structure with only a cladding layer next to an active region becomes numerically solvable. A mixed boundary condition is used for the heterojunction interface to solve the drift-diffusion equations in the cladding layer. Self-consistency is reached when the above three equations (4.13), (4.15) and (4.16) along with the main drift-diffusion equations (4.1), (4.2) and (4.3) are all satisfied.

4.2.4 Numerical methods

A program has been written in the MATLAB script to implement the simulation of the device structure described above. Parameters such as the geometry, material and the doping

of the cladding layer and the active layer are stored in files and they are loaded upon simulation.

To solve the system of nonlinear equations, each equation is first converted to a set of finite difference equations at all the spatially discretized mesh points. The classical Scharfetter-Gummel scheme [102] is used for the discretization.

Then the coupled partial differential equations are solved in a decoupled iteration loop [97, 99], or the Gummel iteration scheme [103]. We first assume that the V_n and V_p values at all the mesh points are known and solve the Poisson equation for V_{ep} , then the V_n are solved with the electron continuity equation assuming V_{ep} and V_p are known numbers. Finally the V_p can be obtained in the same method with the hole continuity equation. Within each loop, a discretized equation is solved using Newton-like method [98, 100, 104-110, 112-120]. After all the three equations are solved separately, the program goes back to first equation for the next iteration loop. It will stop when the difference of the values between each loop falls below the desired error.

4.3 Simulation Results

In this section, simulations of electrical characteristics of a p -cladding layer next to an active region with the numerical model described in the previous section are presented. For the cladding layer, unlike the semi-analytical model in which only the resistance from the heterojunction transport is considered, in the numerical model, the bulk series resistance of the layer, the SRH recombination within the layer and the over-barrier minority carrier

leakage currents are added and their effects on the differential resistance are presented. The same recombination model as in the semi-analytical model is used for the active region, i.e. the active layer is still neutral while “leaky” in the numerical model.

4.3.1 Simulation parameters

A structure of a p -cladding layer next to an active layer is constructed and the geometry is listed in Table 4.1. Unless mentioned otherwise, the electron, hole and lattice temperatures of the device are consider the same with a value of 300K. The active region and the cladding layer parameters are listed in Table 4.2 and Table 4.3 respectively. The bandgap energy difference between the two layers ΔE_g is 0.375eV and the default value of the band offset ratio $\Delta E_C/\Delta E_V$ is 60:40.

Table 4.1: Device geometry of the ideal double heterostructure laser used in the simulation.

Name	Value	Unit
<i>p-Cladding layer thickness</i>	1.0	μm
<i>Active layer thickness</i>	0.15	μm
<i>Active layer area</i>	300×10	μm^2

Table 4.2: Active layer parameters used in the simulation.

Parameter	Symbol	Value/Unit
Bandgap	E_g	1.42 eV
Electron effective mass	m_e^*	0.067 m_0
Hole effective mass	m_h^*	0.48 m_0
Conduction band effective density of states	N_C	$4.42 \times 10^{17} \text{ cm}^{-3}$
Valance band effective density of states	N_V	$8.47 \times 10^{18} \text{ cm}^{-3}$
Acceptor concentration	N_A	0
Donor concentration	N_D	0
Transparency concentration	n_{tr}	$1.8 \times 10^{18} \text{ cm}^{-3}$
Saturation density of electron concentration	n_s	$2.2 \times 10^{18} \text{ cm}^{-3}$
Saturation value of quasi-Fermi level splitting	V_S	1.4742 V
Differential gain	a	$9.3 \times 10^{-17} \text{ cm}^3/\text{m}$
Nonradiative recombination coefficient	A	$1 \times 10^7 \text{ s}^{-1}$
Bimolecular recombination coefficient	B	$0.8 \times 10^{10} \text{ cm}^3/\text{s}$
Auger recombination coefficient	C	$1 \times 10^{-30} \text{ cm}^6/\text{s}$

Table 4.3: Cladding region parameters used in the simulation.

Parameter	Symbol	Value/Unit
Bandgap	E_g	1.798 eV
Electron effective mass	m_e^*	0.086 m_0
Hole effective mass	m_h^*	0.52 m_0
Conduction band effective density of states	N_C	$6.42 \times 10^{17} \text{ cm}^{-3}$
Valance band effective density of states	N_V	$9.65 \times 10^{18} \text{ cm}^{-3}$
Acceptor concentration	N_A	$1 \times 10^{18} \text{ cm}^{-3}$
Donor concentration	N_D	0
Acceptor ionization energy	E_A	60 meV
Donor ionization energy	E_D	5.8 meV
Permittivity	ϵ	12.24 ϵ_0
Electron lattice mobility	μ_n	$2260 \text{ cm}^2/\text{V}\cdot\text{s}$
Hole lattice mobility	μ_p	$185 \text{ cm}^2/\text{V}\cdot\text{s}$

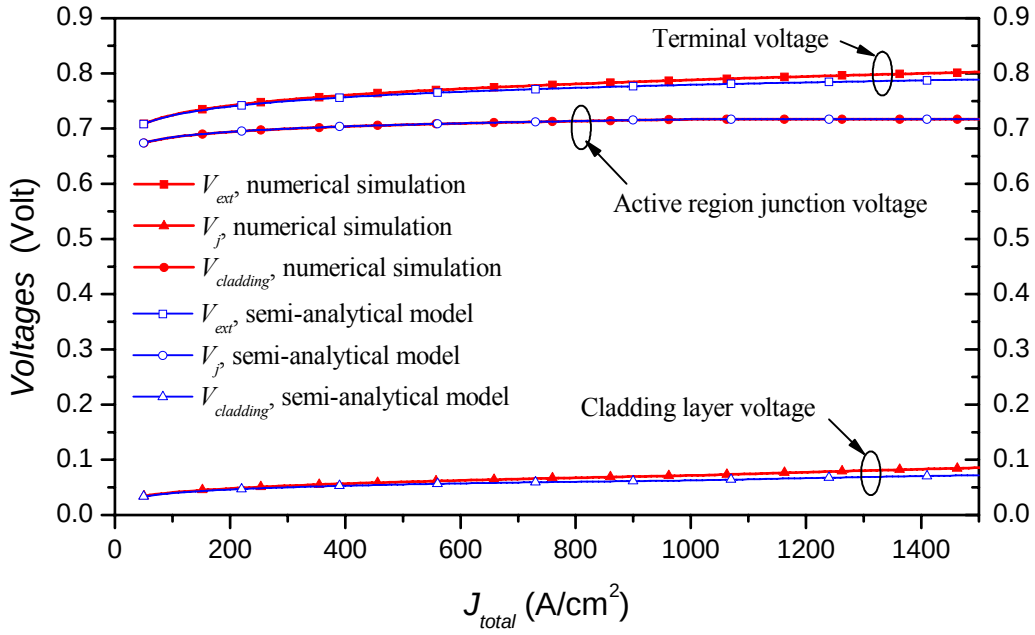


Figure 4.3: Numerical simulation results of current-voltage characteristics of the p -side structure. The results from the semi-analytical model are plotted for comparison.

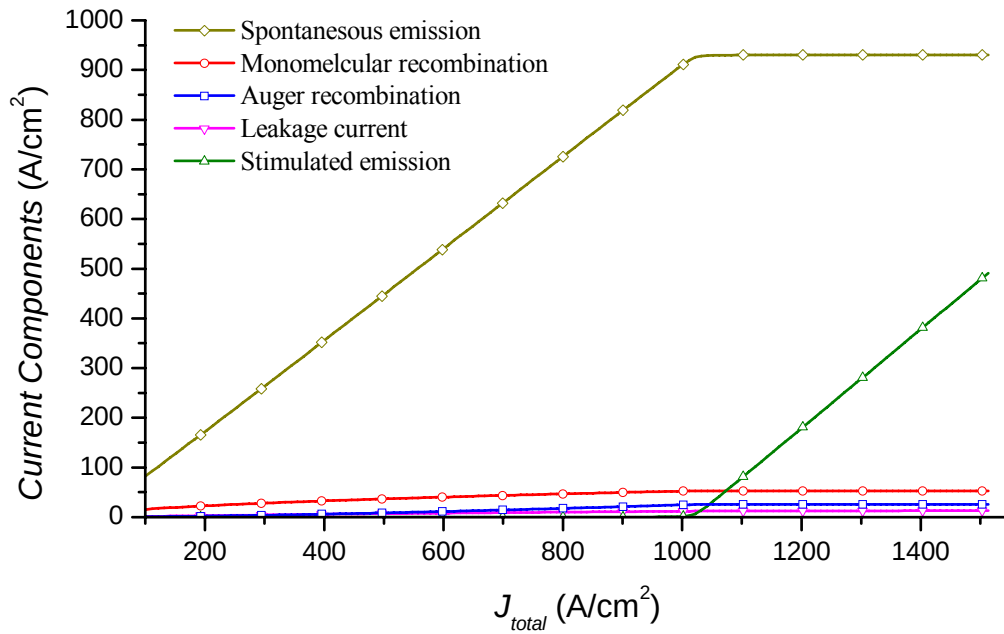


Figure 4.4: Current components as function of total current with the default parameters.

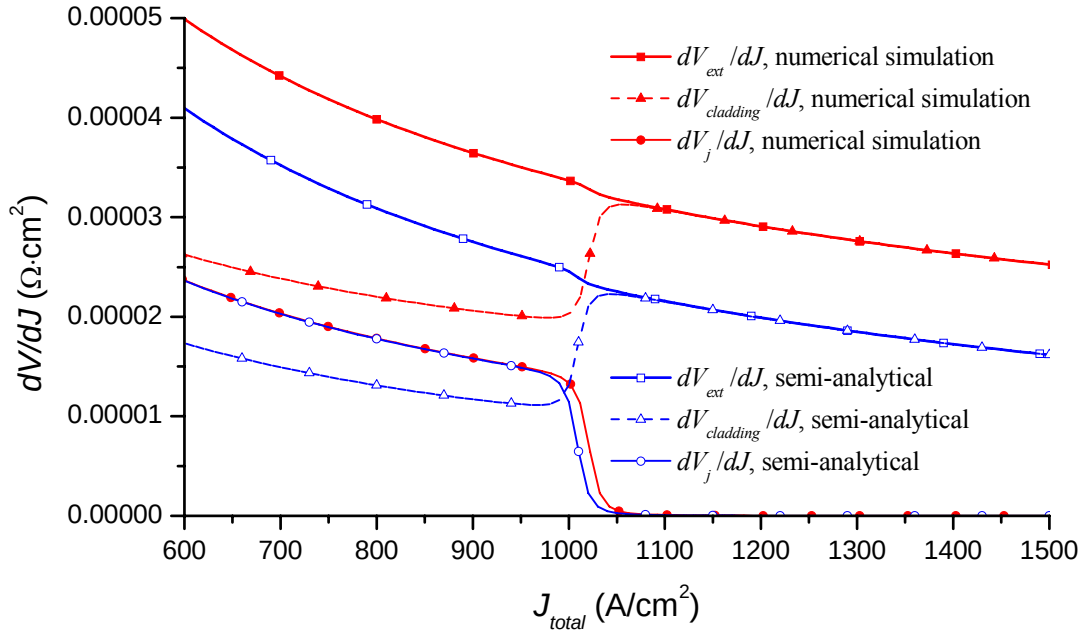


Figure 4.5: The differential resistances from terminal, junction and cladding layer as function of total current with the default parameters. The rapid change in dV/dJ corresponds to the laser threshold.

4.3.2 The electrical characteristics with the default parameters

A. The current-voltage characteristics

With the parameters given as above, the calculated J - V characteristics of the p -side structure are shown in Figure 4.3. The calculations from the semi-analytical model are also plotted. Both models use the same active region model, i.e. the junction voltage will saturate after threshold current of about 1000 A/cm^2 . From Figure 4.3, it can be seen that the inclusion of the cladding layer body resistance slightly increases the cladding layer voltage drop and therefore the terminal voltage. However, the active region junction voltages as functions of total currents from the two models are almost equal to each other. With the inclusion of leakage current, in the active region for the semi-analytical model,

$$J_{total} = J_{recombination} \quad (4.17)$$

while for the numerical model,

$$J_{total} = J_{recombination} + J_{leakage} \quad (4.18)$$

If the leakage is significant, there will be an offset in the J_{total} axis for the junction voltage. In Figure 4.3, the difference cannot be noticed and therefore with those simulation parameters, the leakage currents are actually negligible.

B. The current components

The individual current components including the spontaneous emission, the monomolecular and the Auger recombination, the stimulated emission and the leakage currents as functions of the total current are plotted in Figure 4.4.

From Figure 4.4, it can be seen that the recombination corresponding to the $A/B/C$ coefficients as well as the leakage current are almost saturated after threshold, while the stimulated emission current increases linearly with total current. Again it can be seen that the leakage current is not significant with the given material parameters. At the lasing threshold, most of the injected carriers go into the spontaneous recombination (about 90.6%) and only 1.2% of the total currents leak into the p -cladding layer.

C. The differential resistances

The simulated differential resistances of the p -cladding layer next to an ideal junction are plotted in Figure 4.5. The results from the semi-analytical model are also plotted. Compared

with the semi-analytical model, the inclusion of the cladding layer body resistance in the numerical simulation obviously moves the curves upwards. Ideally the difference between the two sets of differential resistances would be the body resistance determined by the Ohm's law. This value is estimated as follows.

The body resistance of the cladding layer R_{c0} is

$$R_{c0} = \frac{1}{\sigma} \cdot \frac{L}{A} = \frac{1}{q \cdot \mu_p \cdot p} \cdot \frac{L}{A} \quad (4.19)$$

where σ is the conductivity, L is the cladding layer length, A is the cladding layer area, p is the activated hole concentration and μ_p is the hole mobility. The derivative of the cladding layer Ohmic voltage drop is then

$$\frac{dV_{c0}}{dJ} = R_{c0} \cdot A = \frac{1}{\sigma} \cdot L = \frac{1}{q \cdot \mu_p \cdot p} \cdot L \quad (4.20)$$

At thermal equilibrium and the parameters as given previously, the activated hole concentration is $3.8 \times 10^{17} \text{ cm}^{-3}$ in the cladding layer, $\mu_p = 185 \text{ cm}^2/\text{V}\cdot\text{s}$ and $L = 1 \mu\text{m}$, the differential resistance from the bulk resistance is calculated to be $8.9 \times 10^{-6} \Omega \cdot \text{cm}^{-2}$.

From Figure 4.5, after lasing threshold, the difference between the differential resistances from the numerical model and the semi-analytical model is about $9.0 \times 10^{-6} \Omega \cdot \text{cm}^{-2}$, which is close to this value. However, it is not linear and the nonlinearity is more significant before the lasing threshold. It changes from about $8.4 \times 10^{-6} \Omega \cdot \text{cm}^{-2}$ to about $8.7 \times 10^{-6} \Omega \cdot \text{cm}^{-2}$. The smaller but increasing differential resistance might come from the existence of the depletion region around the heterojunction boundary. Nevertheless, the overflowed minority carriers

are expected to increase the conductivity of the cladding layer and therefore the resistance of this layer is expected to be smaller than that from hole only conduction.

4.3.3 The over-barrier leakage currents

A. The effects of band alignment on the carrier leakage

The default band offset ratio $\Delta E_C/\Delta E_V$ is 60:40 with a band gap difference ΔE_g 0.375eV. This ratio is artificially changed with other parameters remaining intact in order to see its effect on the leakage current. Simulation results of leakage currents as function total injection current with band offset ratios of 80:20, 60:40, 40:60 and 20:80 are plotted in Figure 4.6. The ratios correspond to conduction band discontinuities of 11.6, 8.7, 5.8 and 2.9 times the thermal energy $q \cdot V_T$ (25.85meV at room temperature) respectively.

Below laser threshold, it can be seen that the component of leakage current increase rapidly as the conduction band discontinuity decreases. This is not surprising as the carriers in the active region that are free to move to the cladding layer are those high-energy electrons who can overcome the barrier ΔE_C . If the Boltzmann distribution applies, this part of electron density will be proportional to $\exp(-\Delta E_C / q \cdot V_T)$. When the conduction band discontinuity is big enough compared to the thermal energy $q \cdot V_T$, the leakage current is negligible. With a small conduction band discontinuity, the leakage current component becomes significant with respect to the total device terminal current, which also increases the threshold current value.

After lasing threshold, it is observed that the leakage current still increases with the total current, however with a smaller slope than that before threshold. With smaller leakage, the after-threshold slope is smaller and vice versa. From Figure 4.6, when the blocking layer is effective with enough barrier height ($\Delta E_C/\Delta E_V$ of 60:40 and 80:20), the leakage currents are small and barely increase after threshold.

From Figure 4.6, it can also be seen that the leakage with $\Delta E_C/\Delta E_V$ of 60:40 is small while the one with $\Delta E_C/\Delta E_V=40:60$ is fairly strong. The current components as function of total current are plotted in Figure 4.7. In the following simulations, structures with these two band offset ratios will be used to represent “insignificant” and “significant” leakage respectively.

B. The effects of doping concentration on the over-barrier leakage

It has been noticed that a low doping concentration in the cladding layers will increase the leakage current [51, 87, 94]. The leakage currents of the device structure with $\Delta E_C/\Delta E_V=40:60$, 60:40 and acceptor dopant concentrations of 10^{17} , 10^{18} and 10^{19} are plotted as functions of terminal current in Figure 4.8.

It can be seen that the leakage current increases with decreasing dopant concentration, and it is more significant at lower doping concentrations. Within the cladding layer, the carrier transport is mainly determined by the drift-diffusion process in the numerical model. The effect from the doping concentration can be explained by the drift component. With the same majority carrier current density $J = \sigma \cdot E$ in the neutral region of the cladding layer, smaller

doping will result in a higher electric field within this region, which in turn increases the minority carrier current or the leakage.

Although the drift conduction in the cladding layer does not have the same huge impact on the amplitude of the leakage current with the given parameters as does the barrier height, it does create an easily detectable influence. In Figure 4.8, the leakage currents at threshold corresponding to different doping concentrations have differences of about 10% to 20% for both band alignments.

C. The effects of cladding layer thickness on the over-barrier leakage

With the drift-diffusion process in the cladding layer, the thickness of the cladding layers are also expected to have impacts on the leakage currents through diffusion currents. When the confinement layer is thin, the diffusion component of the leakage current will be strong. It also reduces the confinement effects on the optical field and increases free carrier absorption and therefore the loss for the lasing mode. Thicker cladding layers will reduce the diffusion currents but increase the body resistance and also the Joule heating. Simulation results of the leakage currents with cladding layer lengths of 0.5 μm , 1.0 μm and 5.0 μm are shown in Figure 4.9 for the band offset ratio of 60:40 and 40:60. It can be seen that the cladding layer length has only minor impact on the amplitude of the leakage currents. The optimization of the thickness may be focused more on the effects from Joule heating, optical confinement, dopant diffusion problem and etc.

D. The effect of nonradiative recombination lifetime on the over-barrier leakage

The nonradiative recombination lifetime of either the active layer or the cladding layer will decrease with higher defect density (from crystal growth or aging). Simulation is performed assuming the monomolecular recombination coefficient in the active region is ten times the default value and the results are plotted in Figure 4.10. The shorter monomolecular lifetime in the active layer increases the amount of nonradiative recombination current and therefore the threshold current. Compared with that from the default parameters, the leakage current at threshold only increases a small amount due to higher total current and thus the electrical field in the cladding layer.

When the nonradiative lifetime is shorter in the cladding layer instead of the active layer, it has stronger effect on the leakage current. Simulation results with different SRH recombination lifetimes and band offset ratio $\Delta E_C/\Delta E_V=60:40$ and $40:60$ are plotted in Figure 4.11. It can be seen that with both alignments and other parameters, an order of magnitude change in the life time can change the leakage current about 25 percent.

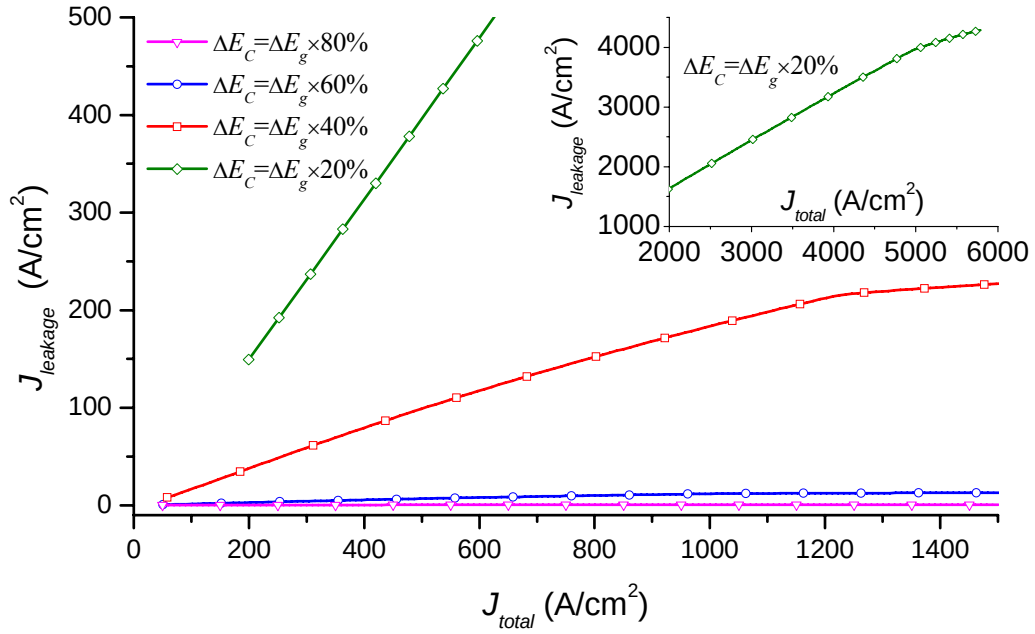


Figure 4.6: The leakage currents with different band offsets as the function of total current. Inset: the curve with $\Delta E_C = \Delta E_g \times 20\%$ at high currents. Note the slopes are reduced at laser thresholds.

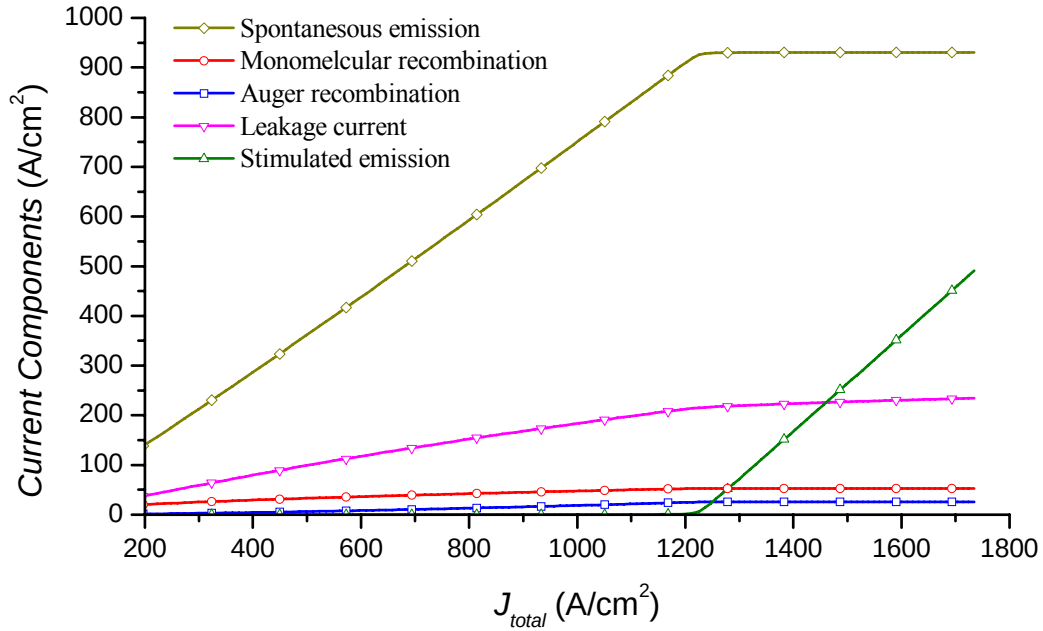
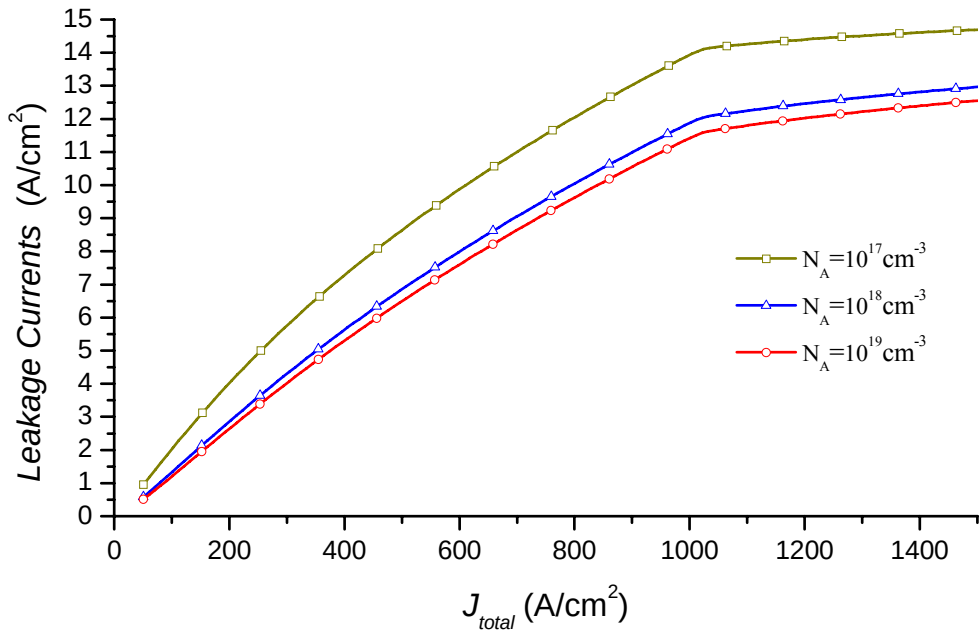
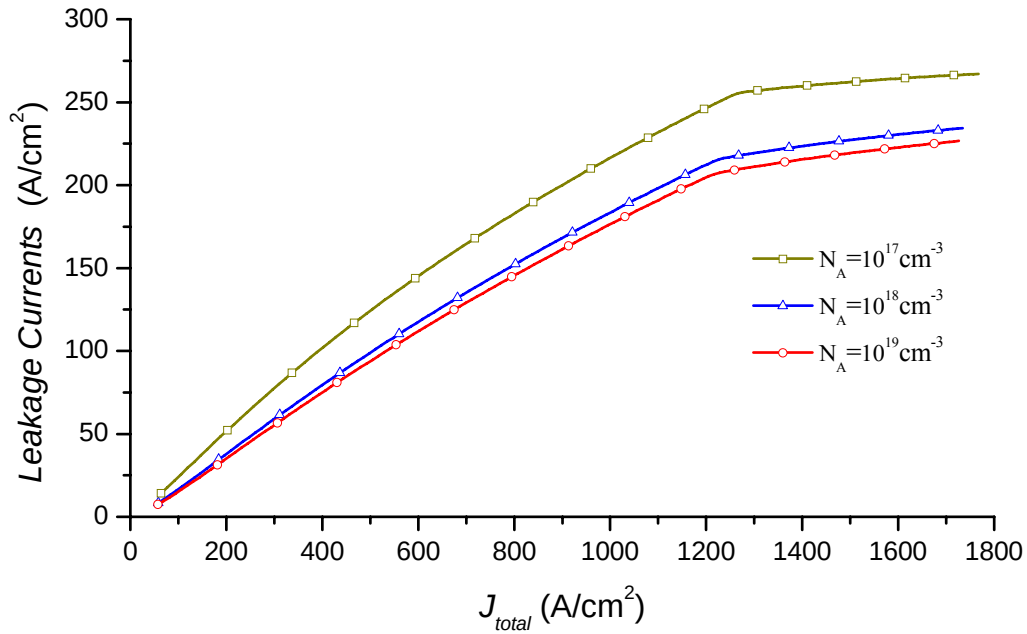


Figure 4.7: Current components with $\Delta E_C / \Delta E_V = 40:60$. Note the component of leakage is much stronger than that with the default parameters.

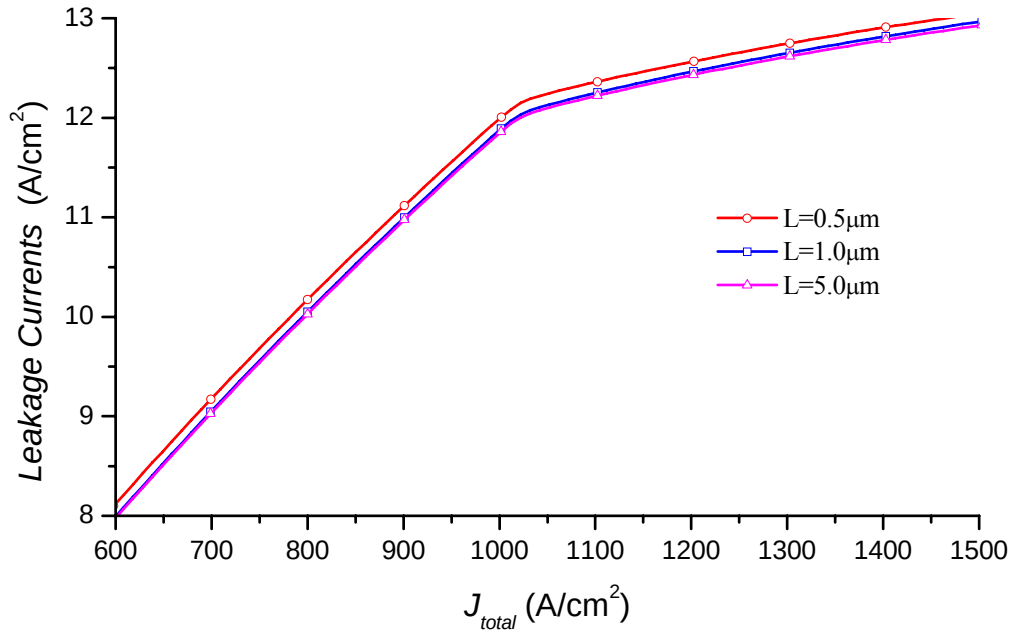


(a) $\Delta E_C/\Delta E_V = 60:40$

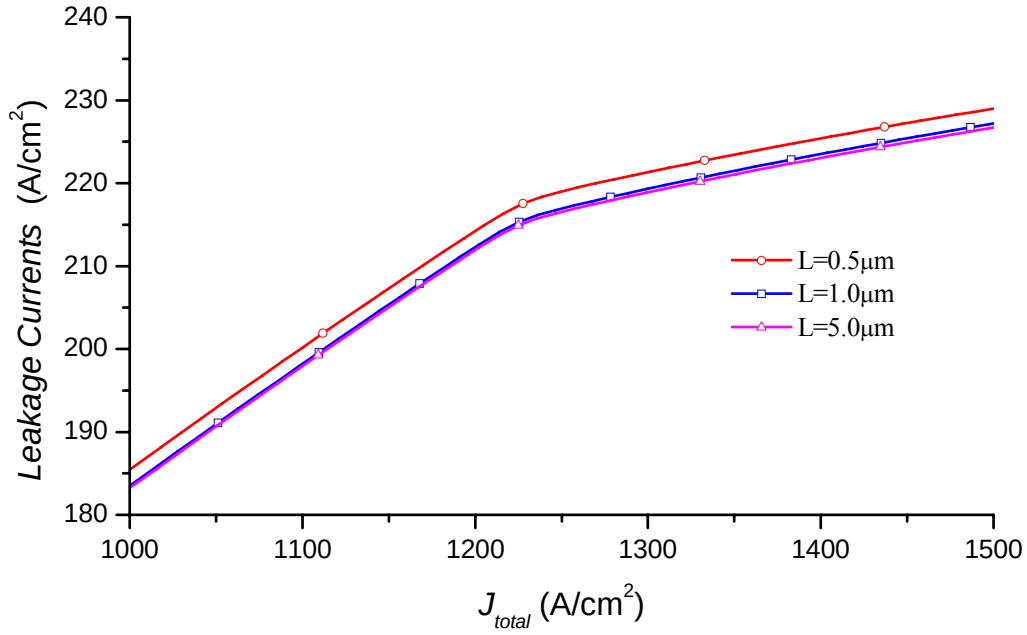


(b) $\Delta E_C/\Delta E_V = 40:60$

Figure 4.8: The leakage currents with different doping concentrations as the function of total injection currents. (a) $\Delta E_C/\Delta E_V = 60:40$. (b) $\Delta E_C/\Delta E_V = 40:60$. Note the vertical scales and the threshold values are different due to the leakage currents.

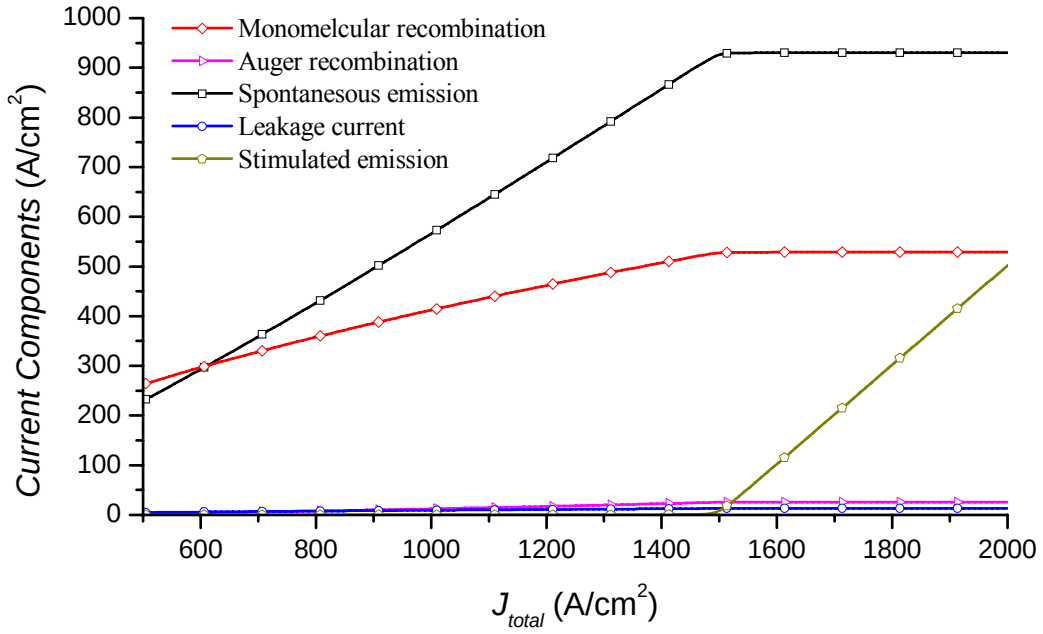


(a) $\Delta E_C/\Delta E_V=60:40$.

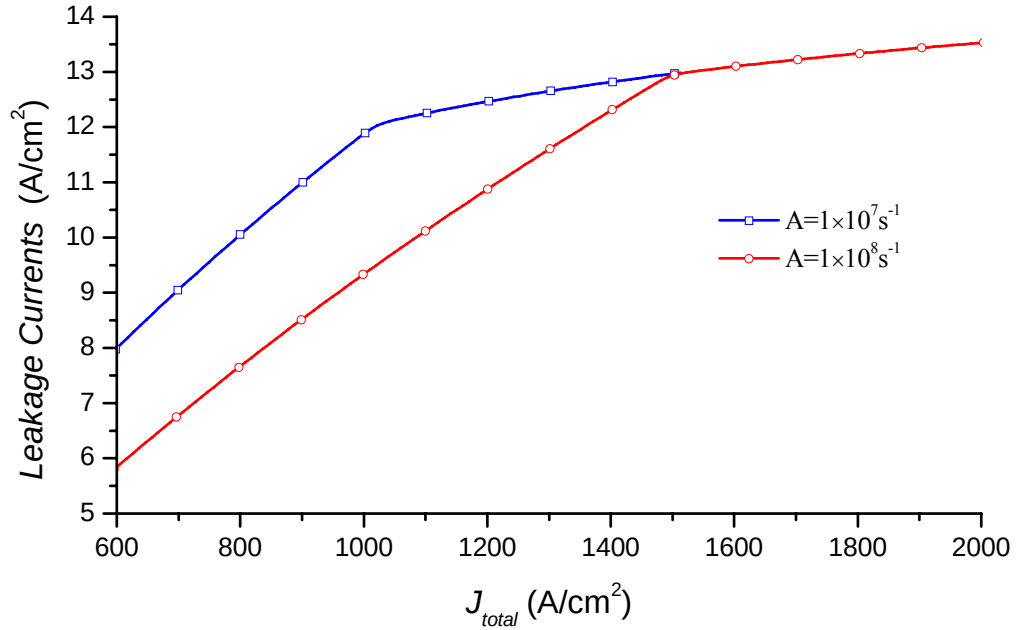


(b) $\Delta E_C/\Delta E_V=40:60$.

Figure 4.9: The leakage currents with different cladding layer thickness as the function of total injection currents. (a) $\Delta E_C/\Delta E_V=60:40$. (b) $\Delta E_C/\Delta E_V=40:60$. Note the difference in vertical scales.

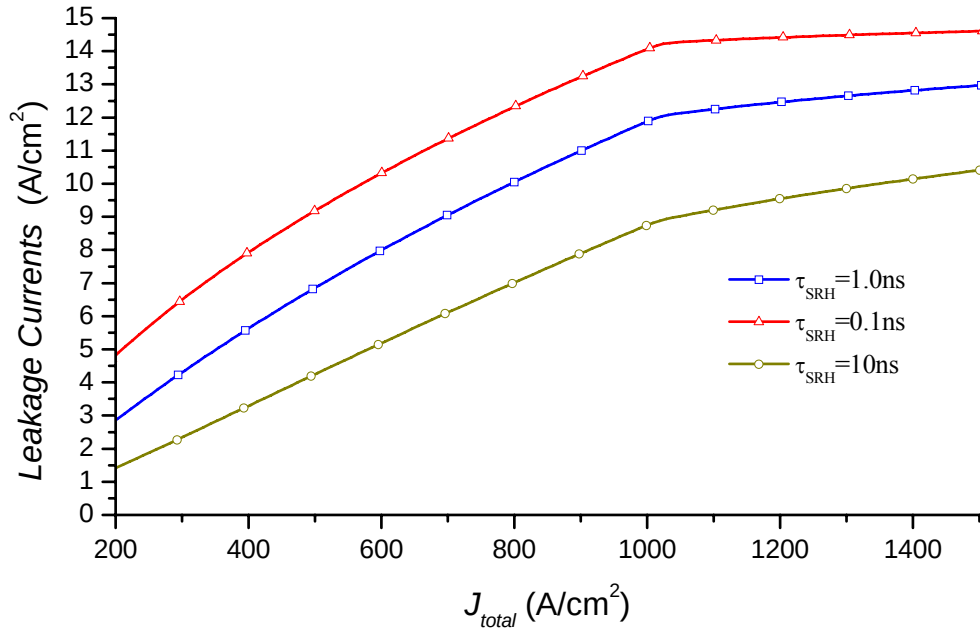


(a) Current components as function of total current.

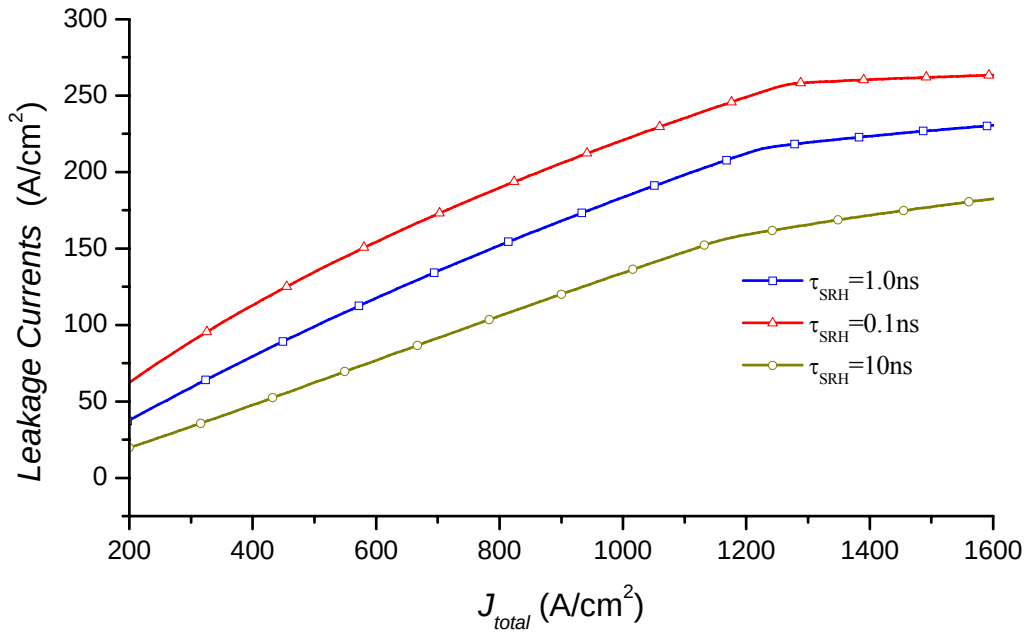


(b) The leakage currents with the two monomolecular coefficients.

Figure 4.10: Monomolecular recombination coefficient of the active region is increased to 10 times the default value. (a) Current components as function of total current. (b) The leakage currents with the two coefficients.



(a) $\Delta E_C/\Delta E_V = 60:40$.



(b) $\Delta E_C/\Delta E_V = 40:60$.

Figure 4.11: The leakage currents with different SRH recombination lifetimes as the function of total currents. (a) $\Delta E_C/\Delta E_V = 60:40$. (b) $\Delta E_C/\Delta E_V = 40:60$.

4.3.4 The effect of leakage on the differential resistance

A. Simulation of differential resistances with different band alignments

The differential resistances with different band offset ratio are plotted in Figure 4.12. When the leakage is not significant at threshold compared to the total current, the result is similar to that from Chapter 3 with the semi-analytical model, i.e. the dV/dJ from the terminals tends to be higher with smaller barrier height, accompanied by a plateau or decreasing trend after lasing threshold.

When the leakage becomes important, there are some new features revealed with the numerical model compared to the simple semi-analytical model. First, the threshold current increases with leakage current as $J_{total} = J_{recombination} + J_{leakage}$ in this model. For a band alignment with the band offset ratio $\Delta E_C/\Delta E_V = 20:80$, the threshold current density is increased from the junction value of 1000 A/cm² to the terminal value of about 5000 A/cm² as shown in the inset of Figure 4.12.

Second, the large amount of minority carriers will cause the “conductivity modulation” effect and reduce the differential resistance of the cladding layer. This can be seen in Figure 4.12 comparing the dV/dJ curves between that with a $\Delta E_C/\Delta E_V$ ratio of 20:80 and 40:60.

Third, the kink polarity at the lasing threshold can reverse, i.e. the direction of the differential kink is normally downwards, but it can become upwards when the over-barrier leakage current is significant. The semi-analytical model in Chapter 3 suggests that when the interaction between the cladding layer and the active region through thermionic emission is weak, the differential resistance kink at lasing threshold will diminish and the terminal

current-voltage relationship is mainly determined by the cladding layer instead of the active layer. With the inclusion of the leakage current,

$$\frac{\Delta V_{ext}}{\Delta J_{total}} = \frac{\Delta V_{ext}}{\Delta J_{recombination} + \Delta J_{leakage}} \quad (4.21)$$

before and after threshold, the ΔV and the $\Delta J_{recombination}$ do not change a lot while the $\Delta J_{leakage}$ may become much smaller because the slope of the $J_{leakage}$ is reduced after threshold as shown in Figure 4.5. As a result, the differential resistance can increase at lasing threshold.

Therefore, the kink polarity is affected by the leakage current as well as the strength of interaction between the cladding layer and the active region. When the interaction is weak and the leakage is strong, it is possible to observe an upward kink in the differential resistance at lasing threshold. When the band alignment is changed by decreasing the $\Delta E_C/\Delta E_V$ ratio in the simulation, this creates more leakage current and reduces the interaction between the two regions simultaneously, which facilitates the observing of a positive kink in the differential resistances using numerical simulation. With real devices made from certain material systems, arbitrarily changing this $\Delta E_C/\Delta E_V$ ratio is unlikely, and it can only be changed under extreme conditions such as unusual temperatures or hydrostatic pressure.

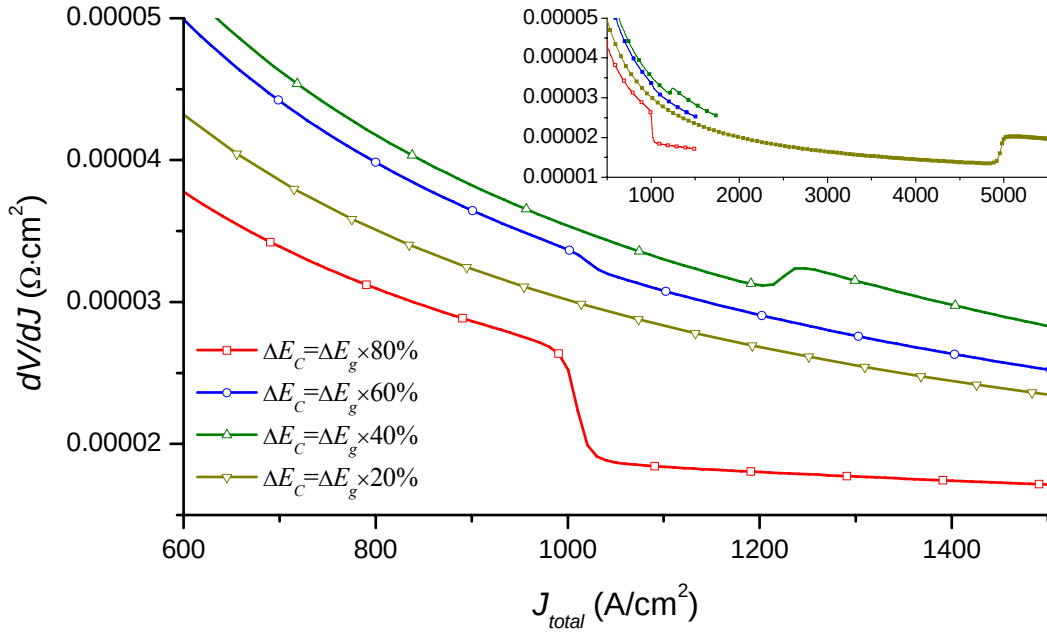


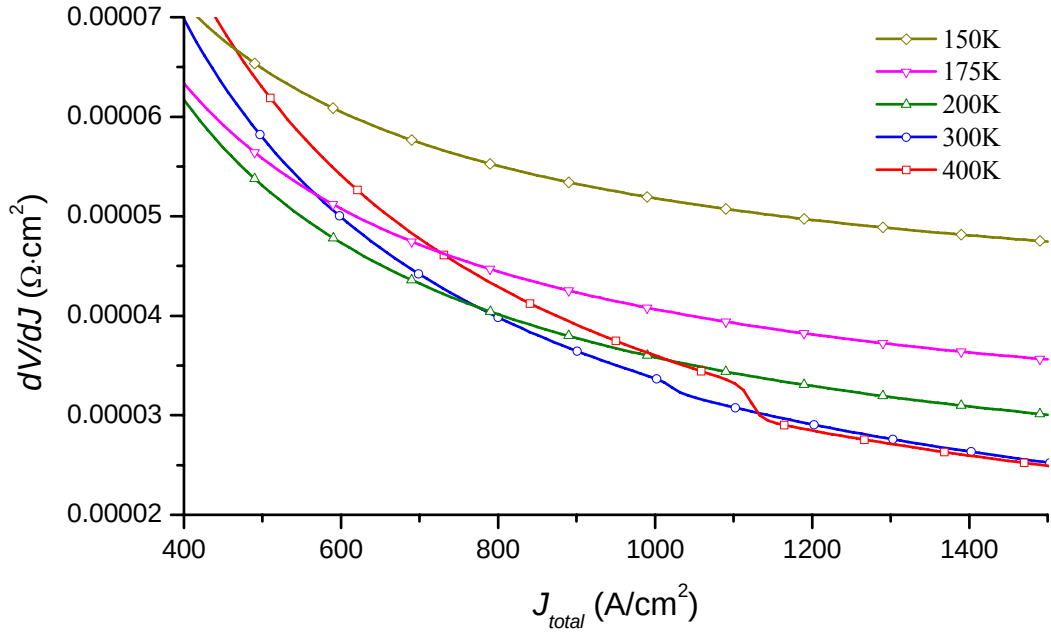
Figure 4.12: The calculated differential resistances with different band offset ratio as the function of total injection currents. Inset: rescaled figure to show the threshold and kink with $\Delta E_C = \Delta E_g \times 20\%$.

B. Simulation of the temperature effects on the differential resistances

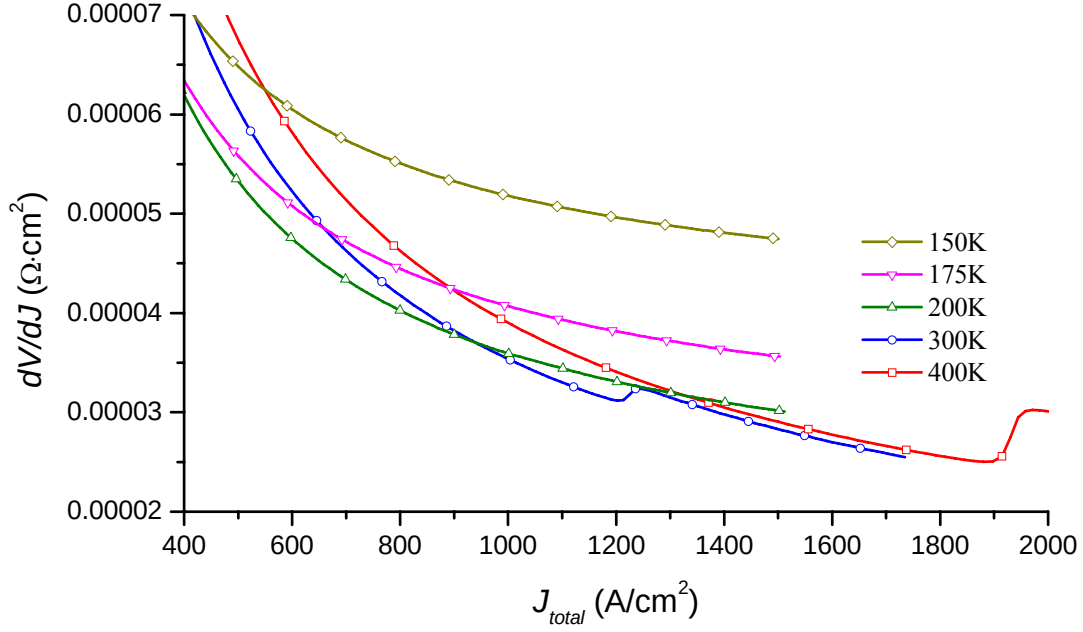
One method to change the leakage current and the strength of the interaction between the cladding layer and the active layer at the same time is to modify the operation temperature of a given device. In contrast to artificially changing the band offset ratio where the two factors are adjusted in an opposite direction, modifying the temperature will change the factors in the same direction, i.e. either increase or decrease both the strength of interaction and the leakage current at the same time. This suggests an experimental method for verifying the theoretical results.

When the device lattice temperature is changed, many parameters such as the bandgap of both layers, carrier mobilities, the gain medium properties or even the band alignment between layers will be affected. However, these parameters do not change dramatically, so for simplicity, the simulation considers mainly the temperature dependency of the carrier distribution function.

The simulated differential resistances with different temperatures and the band offset ratios of $\Delta E_C/\Delta E_V=60:40$ and $40:60$ are plotted in Figure 4.13. It can be seen that with the given parameters at lower temperature, the kink height at threshold tends to become smaller and eventually disappear for both alignments. However, when the temperature is increased, the kinks with smaller leakage will become more downward, and kinks with higher leakage will become more upward.



(a) $\Delta E_C/\Delta E_V = 60:40$.



(b) $\Delta E_C/\Delta E_V = 40:60$.

Figure 4.13: The calculated differential resistances at different temperatures as a function of total current. (a) $\Delta E_C/\Delta E_V = 60:40$. (b) $\Delta E_C/\Delta E_V = 40:60$. Note when the temperature is increased, the kinks with smaller leakage will become more downward, and kinks with higher leakage will become more upward.

C. Low temperature experimental data

As mentioned above, the differential resistance kink polarity at lasing threshold is determined by the leakage and the interaction between the layers defining the heterojunction through thermionic emission. Most practical laser diodes at room temperature will have downward kinks as the leakage should be quite small. From previous analysis, for those devices at low temperature, the kinks at lasing threshold may either disappear or become upwards depending on the leakage currents. To observe this effect, we measured some laser diodes over a range of low temperatures.

The laser diode is model #D650-5 manufactured by NVG, Inc. It is an index guided MQW structure laser with lasing wavelength of about 650nm and output power of 5mW. The diode is installed in a test fixture inside a Dewar and cooled by nitrogen gas. The temperature is measured by a thermocouple placed close to the laser case and the emitted light is collected by a multi-mode optical fiber. The electrical and optical measurements are done using a custom-built derivative measurement instrument that has been described in details elsewhere [15, 16, 17].

The measured differential resistances at different temperatures are plotted in Figure 4.14. Around room temperature, the difference resistance has a “normal” downwards kink at lasing threshold. When the temperature decreases, the kink height first increases slightly and then decreases as the temperature is lowered. Around 200K the kink can barely be found and therefore the lasing threshold can no longer be detected from a differential resistance

measurement. When the temperature drops to even lower values, kink polarity is reversed and upwards steps can be seen.

The lasing thresholds values are measured from the optical derivative dL/dI and they are plotted as the function of temperature in Figure 4.15. The characteristic temperature T_0 is estimated to be about 85K at high temperatures ($>270\text{K}$) and 160K at low temperatures.

The differential resistance kink values $\Delta R_d = \left(\left. \frac{dV}{dI} \right|_{I_{th}^+} - \left. \frac{dV}{dI} \right|_{I_{th}^-} \right)$ are plotted as the function

of temperature in Figure 4.16. The values estimated from the threshold current by

$\Delta R_d = m \cdot \frac{V_T}{I_{th}}$ with $m=1$ are also plotted for comparison. It can be seen that the kink heights

calculated from I_{th} are not close to the measurement values in most of the cases. The discrepancy is not surprising because the assumptions used to derive the simple kink height values did not include sufficient physics to account for the majority carrier injection and minority carrier leakage.

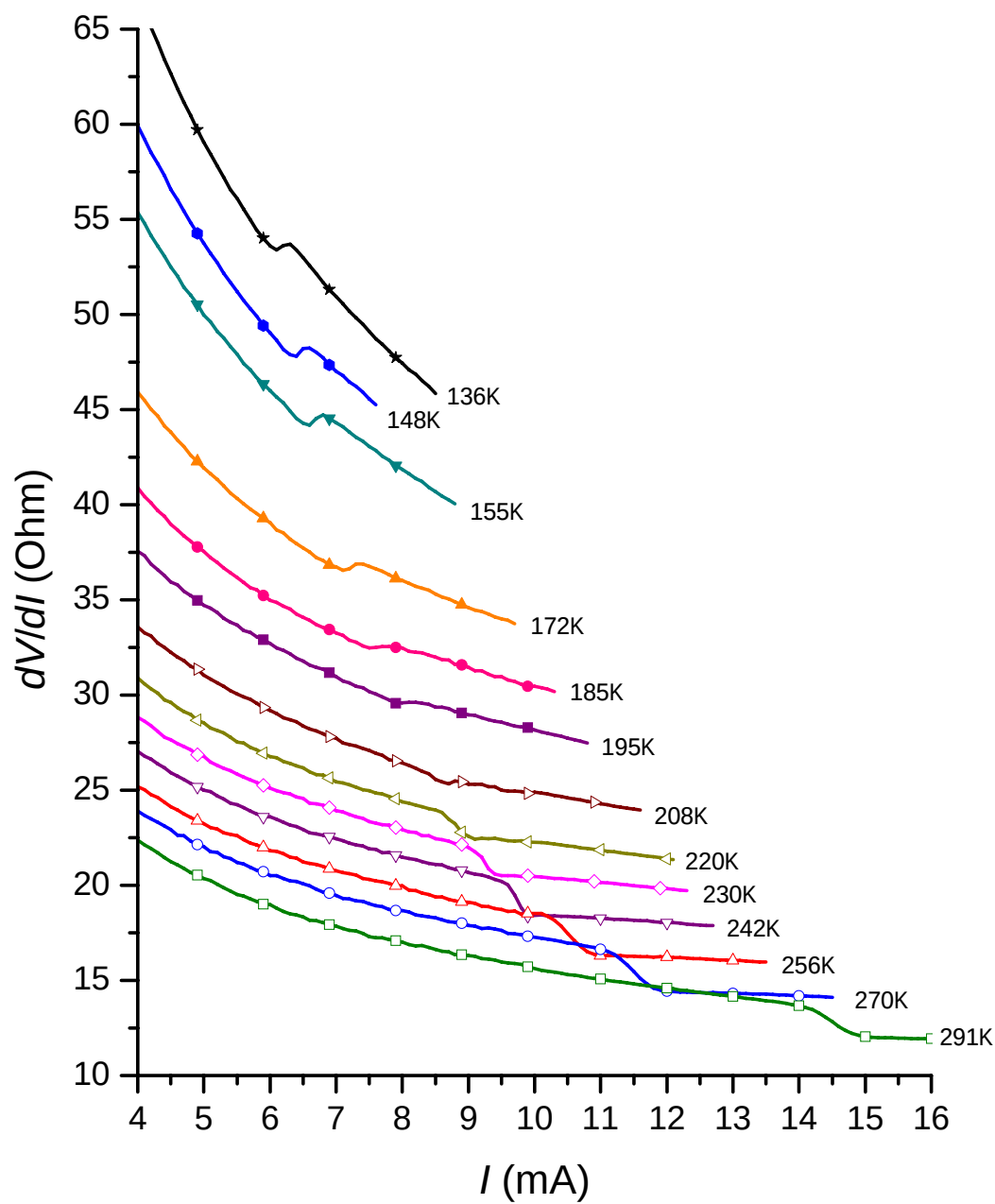


Figure 4.14: The measured differential resistances at different temperatures as the function of total current. Note the lasing threshold may correspond to downwards, upwards or zero kink in the dV/dI curve.

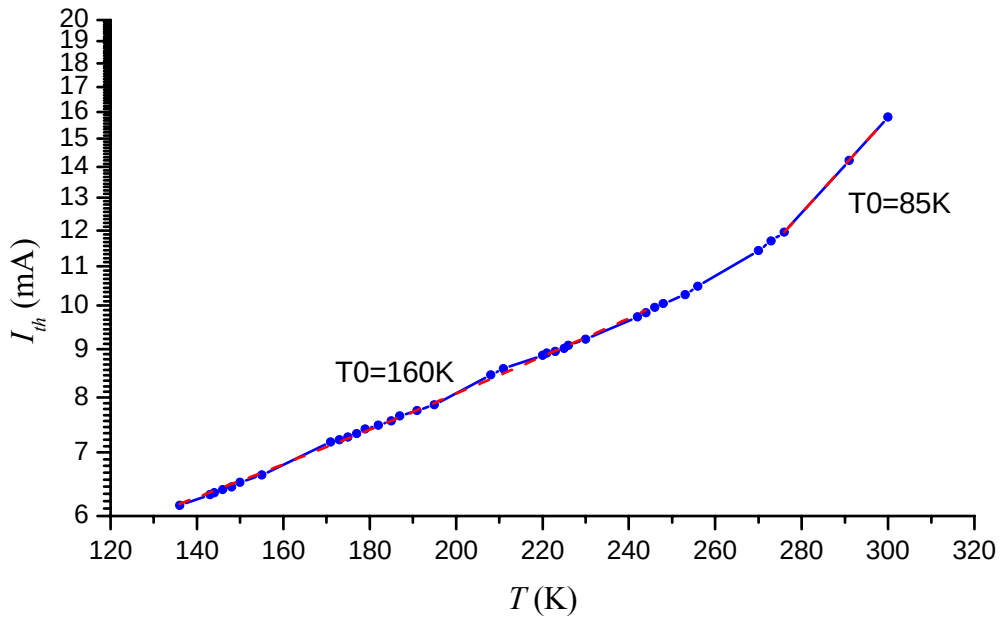


Figure 4.15: The measured threshold currents as the function of temperature.

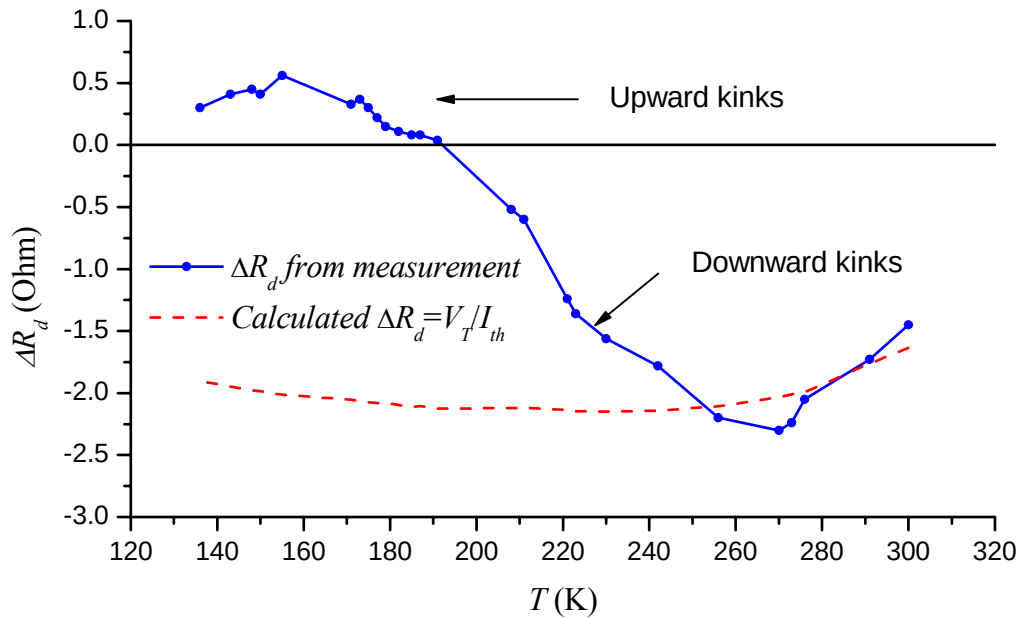


Figure 4.16: The measured differential resistance kink as the function of temperature.

4.4 Summary

A self-consistent numerical model is implemented for the cladding layer of a simple double heterostructure laser diode under high injection conditions where flat-band conditions in the active region next to the cladding layer can be assumed. The numerical model is based on the classical drift-diffusion formulation with mixed thermionic emission boundary conditions on the heterojunction interface. With this model, the gain medium and the cladding layer characteristics can be calculated separately. Important physics such as different recombination mechanisms within both layers as well as the overflow minority carrier leakage mechanisms are taken into account.

Properties of over-barrier leakage currents are studied with the numerical model and important parameters affecting the leakage currents are identified. The effects of the leakage currents on the differential resistances are simulated with the numerical model and the low temperature experiments. It is found that there are two main factors determining the differential kink polarity and the height at lasing threshold. The first is the strength of interactions between the cladding layer and the active region through thermionic emission and the second is the amount of minority carrier leakage currents at lasing threshold.

Chapter 5

Conclusions and Future Work

5.1 Conclusions

In this work, modeling and measurement of the differential resistance and ideality factors in heterostructure light emitting diodes and laser diodes were presented. The measurements were done using differential resistance spectroscopy based on analog modulation and phase sensitive detection. The modeling was performed by sequentially adding more physical processes in order to determine which physical mechanisms are required to explain the measured characteristics of the device.

The first step in the modeling was to develop the relation between the ideality factors solely from recombination currents in the device active region and the electrical derivatives.

The ideality factor is usually considered as a constant measured from the slope of the semi-log scaled current versus voltage ($\ln(I)$ - V) plot. It can also be more directly measured from the electrical derivatives with the series resistance being extracted at the same time. The ideality factor associated with a single recombination current pathway with power-law dependency on the carrier concentration was derived. It is found to have a fixed value inversely proportional to the power factor at low bias conditions. The ideality factor is no longer a constant at high injection level, and the values obtained from different orders of derivative measurements on the same diode are not identical due to the current dependent local ideality factor. Non-constant “derivative ideality factors” were introduced and they correspond to the ideality factors obtained from the different orders of derivative measurements. At a high injection level, the ideality factor with a single recombination mechanism was shown to increase with current due to the significant difference between the Boltzmann and the Fermi-Dirac distribution function in the band filling. When multiple recombination mechanisms exist at the same time in the active region such as with the *ABC* model, changes in the ideality factors can be observed when the additional recombination paths become significant. Instead of using the traditional constant ideality factor as the key parameter, we emphasized the variable ideality factor as an important parameter to indicate dominant recombination path(s) in the active region and device bias condition. Ideality factors measured from some commercial LEDs and LDs showed agreement between the model and the real device measurements, and we proposed the use of this model for parameter extraction and indication of device quality.

In addition to the recombination currents in the active region of a LED or LD, the differential resistance and ideality factor were also found to be significantly affected by the process of majority carrier injection from the device terminals to the active region. A semi-analytical model in which the interaction between the cladding layer and the active region is implied in the thermionic emission boundary conditions for heterojunction interfaces was proposed to investigate the effects of majority carrier injection. Analysis showed that the majority carrier injection creates additional nonlinear resistance, and the nonlinearity is accompanied by the junction properties being only partially reflected at the device terminals, i.e. the measured differential resistances and the ideality factors at the device pins are only a fraction of the contribution from the active region, and the remainder of the terminal characteristics is from the cladding layers. A nonlinear fraction f_j was found to be useful in describing the external differential resistances and the ideality factors by the linear combination of the internal components from the heterojunction transport and the active region. The value of the f_j is always between 0 and 1, and it can also be related to device parameters and junction ideality factors, which are related to the bias level. It is nontrivial to design a device whose derivative characteristics can be mostly measured from its terminals.

The LED model was extended to a simple laser model with the inclusion of junction quasi-Fermi level saturation in the active region upon laser threshold. The model predicts that less interaction between the active region and the cladding layer will result in reduced kink heights in the differential resistances and the ideality factors at threshold. Although the junction quasi-Fermi level splitting is saturated after threshold, a decrease in the differential resistance and an increase in the terminal ideality factor can be observed as a result of the

contribution from the interaction between the cladding layer and the active region. A reduction in the differential resistance kink height at threshold is always accompanied by the decrease of differential resistance after threshold from this model. Experiments were performed on LEDs and LDs at low temperature where the interaction through thermionic emission is reduced. Results showed qualitative agreement with the proposed model in the trends of the ideality factors and the differential resistances as a function of temperature.

To investigate the effects from minority carrier overflow in addition to the majority carrier injection, a simplified one dimensional (1-D) self-consistent numerical model was proposed and implemented. Properties of over-barrier leakage currents were studied with the numerical model and important parameters affecting the leakage currents can be identified with this simplified model. Simulations of the effects of minority carrier leakage on laser terminal differential resistances were demonstrated and compared with experiment data. It was found that there are two main factors determining the differential kink polarity and the height at lasing threshold. The first is the strength of interactions between the cladding layer and the active region through thermionic emission and the second is the amount of minority carrier leakage currents at lasing threshold.

This work has made possible the modeling of semiconductor optoelectronic devices with relatively simple parameters and methods. The theoretical and numerical calculations also correlated many experimentally observed features with specific physical mechanisms. The correlation between the electrical/optical derivative measurements and device physics was shown to be a helpful tool for experimentalists to understand and characterize complex devices.

5.2 Future Work

Electrical and optical derivative measurement techniques are an old tool but relatively under-utilized due to the lack of theoretical support. This work has provided the theoretical basis to correlate the many features experimentally observed with specific physical mechanisms. The success of this work provides encouragement that additional physical mechanisms could be included to extend the applicability of the modeling to more complex devices. Mechanisms that could be included in the analytical model include: the simple “recombination model” for the active region with lower dimensions (2-D and 1-D, e.g. quantum wells and quantum dots); a simple model for current spreading effects; the tunneling effect at heterojunction boundaries; the phenomenological carrier capture/escape model with quantum well devices, and; other conduction mechanism such as the space-charge-limited (SCL) conduction in devices. Mechanisms that could be included in the numerical model include more sophisticated calculations of recombination in the active region; carrier transport with multiple sub-bands; piezoelectric field effects at heterointerfaces, and; the electrical and optical spatial non-uniformity effects. It is the hope of this author that this approach will enable the experimentalists to understand and characterize complex devices with relatively simple methods.

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