Band structures and optical properties of InGaNAs quantum wells

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Band Structures and Optical Properties of InGaNAs Quantum Wells

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Table of Content

Acknowledgements	i
Table of Content	ii
Summary	v
List of Figures	vii
List of Tables	xii
Chapter 1 Introduction	1
1.1 Motivation	1
1.2 Objectives	2
1.3 Major contribution of the thesis	2
1.4 Organization of the thesis	3
Chapter 2 Literature review	4
Chapter 3 Band parameters, band model, and optical gain model	8
3.1 Band parameters for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$	8
3.2 E_G and m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ by phenomenological relationship	9
3.3 E_G and m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ by BAC model	10
3.4 Strained conduction band offset ratio (Q_C)	12
3.5 10-band $\mathbf{k} \cdot \mathbf{p}$ model	19
3.6 Envelope wave function and identification of band components	22
3.7 Various $\mathbf{k} \cdot \mathbf{p}$ formalisms considered	24
3.8 Density of states and carrier density	25
3.9 Optical transition matrix elements	26
3.10 Optical gain model	28

3.11	Summary	29
Chapter 4	Band structure	30
4.1	Comparison of band structure with published literatures.....	30
4.2	Comparison of E_{eh} calculated by 10-band $\mathbf{k} \cdot \mathbf{p}$ with published emission wavelength	30
4.3	Comparison of band structure calculated by different $\mathbf{k} \cdot \mathbf{p}$ models	32
4.4	Dependence of E_{eh} and energy separation on nitrogen and indium composition	37
4.5	Dependence of energy dispersion curves on indium and nitrogen composition	42
4.6	Summary	45
Chapter 5	Density of states for quantum well.....	46
5.1	Relationship of energy dispersion curves and QW's DOS	46
5.2	Dependence of DOS and carrier density on nitrogen composition.....	49
5.3	Dependence of DOS and carrier density on indium composition.....	54
5.4	Summary	58
Chapter 6	Optical gain	59
6.1	Dependence of N_{tr} and $J_{rad(tr)}$ of QWs on nitrogen composition.....	59
6.2	Dependence of N_{tr} and $J_{rad(tr)}$ of QWs on indium composition	63
6.3	Importance of m_e^* on the calculation of band structure and optical gain	65
6.4	Dependence of dG/dN and dG/dJ_{rad} on nitrogen composition	68
6.5	Dependence of dG/dN and dG/dJ_{rad} on indium composition	71
6.6	Summary	73
Chapter 7	Barrier engineering.....	74
7.1	GaAs/GaAsP/GaAs triple barriers	75

7.2	Derivation of matrix elements for barrier potential and strain in $\mathbf{k} \cdot \mathbf{p}$	
	Hamiltonian	76
7.2.1	GaAs barrier	77
7.2.2	GaAs/GaAsP/GaAs barrier	78
7.3	Comparison of band structure and optical properties of InGaAsN QW with GaAs/GaAsP/GaAs and GaAs barriers	80
Chapter 8	Conclusion and recommendations	84
	List of Publications.....	86
	Bibliography.....	88

Summary

This thesis presents theoretical studies of electronic band structures and optical properties for compressively strained $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well (QW). We have used a realistic 10-band $\mathbf{k} \cdot \mathbf{p}$ model for the detailed calculation of band structures and have even studied the QW structure with tensile GaAs/GaAsP/GaAs compounded barrier. Strained conduction band offset ratio (Q_C) of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ was proposed. Together with band gap energy (E_G) and electron effective mass (m_e^*) based on band-anticrossing (BAC) model, we are able to predict quantum well transition energies that is reasonably close to the reported experimental values. Model-dependent prediction of transition energy (E_{eh}) and energy separation of conduction subbands were also conducted using additional 8-band and 6-band $\mathbf{k} \cdot \mathbf{p}$ models, which neglect nitrogen related energy level (E_N) and conduction-valence band interaction, respectively.

From the results of the band structures, we are able to study the dependence of two-dimensional density of states of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW, and its carrier density, on nitrogen and indium compositions of the active layers. Subsequently, the optical transition matrix elements, optical gain, and optical transparency conditions of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW are being investigated for a better understanding concerning the reduction of optical gain when higher nitrogen composition is being used for the QW active layers. In contrary to earlier reports that the reduction of optical gain and differential gain (dG/dN) in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ is due to the increase in m_e^* , we have shown that the reduction was actually due to the increased interaction between

the conduction-band state and nitrogen related energy state, which weakened the interband optical transition matrix elements. Our results will be valuable in achieving optimum design of long wavelength QW lasers based on $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$.

List of Figures

Figure 1. Dependence of (a) bulk band gap energy and (b) electron effective mass of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material on indium and nitrogen composition.....	10
Figure 2. Compositional dependence of Q_C for $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWs.	14
Figure 3. The dependence of Q_C (InGaAsN) on indium composition for nitrogen composition from 0% to 3%.....	18
Figure 4. Energy dispersion curves for conduction and valence subbands along $[100]$ and $[110]$ crystal directions for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.	33
Figure 5. Energy dispersion curves for conduction and valence subbands along $[100]$ and $[110]$ crystal directions for a 7 nm $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.	35
Figure 6. (a) Dependence of transition energy E_{eh} for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for $\text{In}_w = 15\%$ and 35% as calculated by the 10-band model. (b) and (c) are differences of E_{eh} calculated by other models from that calculated by the 10-band model at $\text{In}_w = 15\%$ and 35% , respectively.	38
Figure 7. (a) Dependence of energy separation between the first two conduction subbands ($e2-e1$) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for $\text{In}_w = 15\%$ and 35% as calculated by the 10-band model. (b) and (c) are differences of ($e2-e1$) calculated by other models from that calculated by the 10-band model at $\text{In}_w = 35\%$ and $\text{In}_w = 15\%$, respectively.	39
Figure 8. (a) Dependence of transition energy E_{eh} for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on indium composition for $\text{N}_w = 0\%$, 2% and 4% as calculated by the 10-band model. (b) and (c) are differences of E_{eh} calculated by other models from that calculated by the 10-band model at $\text{N}_w = 2\%$ and 4% , respectively.	40

Figure 9. (a) Dependence of energy separation between the first two conduction subbands (e_2-e_1) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on indium composition for $N_w = 0\%$, 2% and 4% as calculated by the 10-band model. (b) and (c) are differences of (e_2-e_1) calculated by other models from that calculated by the 10-band model at $N_w = 4\%$ and 2%, respectively	41
Figure 10. Comparison of curvatures of e_1 and hh_1 for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%, in steps of 5%.	43
Figure 11. Comparison of curvatures of e_1 and hh_1 for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%, in steps of 1%.	44
Figure 12. (a) Energy dispersion curves for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW using 10-band $\mathbf{k} \cdot \mathbf{p}$ model. (b) Corresponding density of states in conduction band and valence band.	46
Figure 13. Constituting band components for the first three conduction subbands as calculated by the 10-band $\mathbf{k} \cdot \mathbf{p}$ model for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.	47
Figure 14. Constituting band components for the first four valence subbands as calculated by the 10-band $\mathbf{k} \cdot \mathbf{p}$ model for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.	48
Figure 15. Comparison of density of states (DOS) in conduction band versus energy for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.	50
Figure 16. Comparison of carrier density (N_c) in conduction band versus quasi-Fermi level (E_{fc}) for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.	51
Figure 17. Comparison of density of states (DOS) in valence band versus energy for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.	52

Figure 18. Comparison of carrier density (N_c) in valence band versus quasi-Fermi level (E_{f_v}) for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.	53
Figure 19. Comparison of density of states (DOS) in conduction band versus energy for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%. ..	55
Figure 20. Comparison of carrier density (N_c) in conduction band versus quasi-Fermi level (E_{f_c}) for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.	55
Figure 21. Comparison of density of states (DOS) in valence band versus energy for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.	57
Figure 22. Comparison of carrier density (N_c) in valence band versus quasi-Fermi level (E_{f_v}) for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.	57
Figure 23. Dependence of (a) transparency carrier density (N_{tr}) and (b) transparency radiative current density ($J_{rad(tr)}$) for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for various $\mathbf{k} \cdot \mathbf{p}$ models considered.	60
Figure 24. Dependence of (a) P_n^e for the first conduction subband, e1 and (b) TE-mode squared transition matrix elements for e1 to hh1 transition for various $\mathbf{k} \cdot \mathbf{p}$ models on nitrogen composition at $k = 0$ in a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well.	62
Figure 25. Dependence of (a) transparency carrier density (N_{tr}) and (b) transparency radiative current density ($J_{rad(tr)}$) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well on indium composition for various $\mathbf{k} \cdot \mathbf{p}$ models considered.	64

Figure 26. Dependence of (a) P_n^e for the first conduction subband, $e1$ and (b) TE-mode squared transition matrix elements for $e1$ to $hh1$ transition for various $\mathbf{k} \cdot \mathbf{p}$ models on indium composition at $k = 0$ in a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well.....	65
Figure 27. Dependence of maximum TE-mode differential gain (a) dG/dN and (b) dG/dJ_{rad} for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for various $\mathbf{k} \cdot \mathbf{p}$ models.....	68
Figure 28. Dependence of maximum TE-mode differential gain (a) dG/dN and (b) dG/dJ_{rad} for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well on indium composition for various $\mathbf{k} \cdot \mathbf{p}$ models.....	72
Figure 29. Schematic band diagram for the $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ multiple quantum wells with barrier formed by tensile-strain $\text{GaAs}_{0.82}\text{P}_{0.18}$ and unstrained GaAs layers.....	75
Figure 30. CW light output power versus injection current measured at room temperature (RT) for a $10 \times 1600 \mu\text{m}^2$ ridge waveguide $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ triple quantum wells.....	76
Figure 31. Schematic band diagram for InGaAsN quantum well with unstrained GaAs as barrier.	77
Figure 32. Schematic band diagram for the InGaAsN quantum well with GaAs/GaAsP/GaAs triple barriers and its origin for the derivation of matrix elements in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian.	79
Figure 33. The in-plane energy dispersion curves of $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ quantum wells with GaAs/GaAs _{0.82} P _{0.18} /GaAs barriers (solid line) and GaAs barrier	

(dashed line). (a) and (b) are the conduction and valence subbands, respectively.

.....80

Figure 34. (a) Maximum optical gain of the TE-mode as a function of the carrier

density and (b) radiative current density as a function of the carrier density for

$In_{0.35}Ga_{0.65}As_{0.985}N_{0.015}$ quantum wells.82

List of Tables

Table I.	<i>Parameters for binary compounds used in the $\mathbf{k} \cdot \mathbf{p}$ band structure calculation.</i>	8
Table II.	<i>Details of various $\mathbf{k} \cdot \mathbf{p}$ models used in this thesis</i>	25
Table III.	<i>Comparison of theoretical transition energies of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs by 10-band $\mathbf{k} \cdot \mathbf{p}$ model with experimental values.</i>	31
Table IV.	<i>Comparison of band parameters for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.96}\text{N}_{0.04}$ and $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}$.</i>	37

Chapter 1 Introduction

1.1 Motivation

Conventionally, most long-haul transmitters are manufactured using InGaAs/InP-based material systems and most uncooled lasers are based on InAlGaAs-based structures, which suffers from poor thermal stability and high leakage current due to the low carrier confinement in the conduction band. Subsequently, InGaAsN-based structure was proposed by Kondow to address these issues with the hope that laser diode emitting at 1.3 and 1.55 μm can operate without an external cooling mechanism.¹ For many years, InGaAs/GaAs structure is known to be a suitable candidate for laser emission at the 980 nm optical window. The mature processing technology for GaAs is something that is seriously desired in order to reduce the manufacturing cost for the long-wavelength laser diode, which was previously based on InP material. However, to achieve emission at 1.55 μm using InGaAs/GaAs structure will required a very high indium content in the active layer of the quantum well, which will result in high compressive strain present in the active layer and thus limiting the thickness of the active layer that can be grown pseudo-morphically. By adding nitrogen into the InGaAs layer, it is discovered that the compressive strain and the band gap energy (E_G) can be reduced concurrently. This has generated tremendous interest in the research communities to investigate many unusual material properties observed for this material, which includes the large enhancement to effective electron mass (m_e^*) and the great bowing factor observed for the band gap energy.

Chapter 1 Introduction

1.2 Objectives

This research topic is undertaken to investigate the band structures of InGaAsN quantum well and its optical properties (such as, transparency current density, transparency carrier density and differential gain) using $\mathbf{k} \cdot \mathbf{p}$ model. The results of the band structure calculation will help to determine optimum composition and structure for the InGaAsN quantum well that will emit at 1.3 or 1.55 μm . In addition, the studies on optical properties will help to further determine the structural and compositional dependence of threshold condition and differential gain, which will help to design a better laser system emitting at room temperature and low threshold current density. Model-dependent prediction is also studied using 6-band, 8-band and 10-band $\mathbf{k} \cdot \mathbf{p}$ models.

1.3 Major contribution of the thesis

This work contributes to the development of a 10-band $\mathbf{k} \cdot \mathbf{p}$ model that has been proven to be able to predict the experimentally observed emission wavelengths from InGaAsN quantum wells. Subsequently, its comparison with 8-band and 6-band model with different electron effective mass determine that the estimation of electron effective mass by the band-anticrossing (BAC) model is more accurate than that predicted by the phenomenological relationship derived from the early works. This is the first time that such an extensive and systematic comparison is conducted. Simulation of optical gain using the 10-band model also contributed to the real understanding of the reduction in optical gain when more nitrogen is present in the well layer. In contrary to the earlier understanding that the reduction in optical gain is due to the large enhancement of electron effective mass, our work shows that the

Chapter 1 Introduction

reduction is actually caused by the increased interaction between the conduction band and the non-radiative nitrogen-related states.

1.4 Organization of the thesis

In this thesis, we present the motivation, objectives, and contribution of our work in Chapter 1. A brief literature review is given in Chapter 2 to give an overview of the state of research before this work was undertaken. Theoretical band model, optical model and band parameters are described in great detail in Chapter 3. Chapter 4 will compare the transition energies calculated by 10-band $\mathbf{k} \cdot \mathbf{p}$ model to the experimental results to establish the correctness of the band model followed by the effect on prediction of transition energy and band structure by the different band models. The two-dimensional density of states and carrier density for the quantum well will be discussed in Chapter 5. Chapter 6 investigates the various optical properties as affected by the band models used in the simulations. Chapter 7 will present some theoretical findings on barrier engineering using compounded GaAs/GaAsP/GaAs barrier. Chapter 8 will sum up the entire thesis with final concluding remarks and recommendations.

Chapter 2 Literature review

Over the past decade, research effort based on $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material has captured the attention of the research community. Since its introduction, $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ system has the potential of replacing $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{P}_y/\text{InP}$ system as the conventional long-wavelength laser emitter in long-haul communication links.¹ Not only that samples were grown by both molecular beam epitaxy (MBE) and metal organic chemical vapor deposition (MOCVD) to explore the possibility of achieving $1.3\ \mu\text{m}^{2-10}$ and near $1.55\ \mu\text{m}^{11-18}$ emissions, but also various theories were proposed in an attempt to predict the compositional dependence of the $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ bulk material. In the area of QW laser fabrication, the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QW has been shown to exhibit very low threshold current density due to the presence of compressive strain in the well layer under lattice mismatch.^{19,20} However, the compressive strain will build up when more indium is added to the well layer to increase the emission wavelength and thus imposing a limit to the thickness of the QW. By adding nitrogen atom into the matrix to form $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$, it was found to further reduce the band gap energy and simultaneously reduce the compressive strain in the well layer. The ability to grow a thicker layer of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ due to its reduced compressive strain in the well region as compared to the $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ quantum well (QW) has also enabled it to be used in the GaAs-based photodetector and solar cell.²¹ Although QW laser using $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ has demonstrated the ability to exhibit desirable low threshold current density (J_{th}) of $390\ \text{A}/\text{cm}^2$ at $1.3\ \mu\text{m}$ emission,²² and potentially reduce manufacturing cost due to its compatibility with matured processing techniques of GaAs, the possibility of using it in the $1.55\ \mu\text{m}$ has very much depended on the understanding of its material properties. This special material exhibits very different

Chapter 2 Literature review

behaviours, including the larger than normal band-gap energy (E_G) bowing factor and enhancement of electron effective mass (m_e^*) by the addition of nitrogen atom.

Experimentally, emission wavelength over the range of 1.00 to 1.55 μm has been demonstrated using InGaAsN/GaAs QW structure.²³ More researches are focusing on the effect of annealing on the undesired blueshift of emission wavelength of InGaAsN/GaAs^{24,25} and the addition of antimony (Sb) to form the InGaAsNSb active layers.^{26–29} Apart from QW lasers, InGaAsN was also used to fabricate p-i-n solar cell,³⁰ metal-semiconductor-metal photodetector,³¹ and even as channel layer in high electron mobility transistor.³²

Recently, the band-anticrossing (BAC) model has been employed to explain the modification to E_G ,³³ m_e^* ,³⁴ and pressure-induced shifting of conduction band edge³⁵ when nitrogen atoms are added into $\text{In}_x\text{Ga}_{1-x}\text{As}$ to form $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ alloys. The dependence of E_G on nitrogen composition has been predicted very well by the BAC model, which states that the large reduction of the fundamental band-gap energy of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ is due to the repulsion between a localized nitrogen-related energy level (E_N) and the extended conduction band (E_C) of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ host matrix.³⁵ To date, the BAC model is used extensively and successfully in the prediction of E_G of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ with low indium composition and $\text{GaAs}_{1-y}\text{N}_y$.^{35–37} However, it was discovered that the interaction between E_N and E_C depends not only on the nitrogen composition (y), but it is also a function of indium composition (x). Consequently, the rate of reduction of band-gap energy with respect to nitrogen composition (dE_G/dy) decreases when the indium composition increases, as the downward shift of

Chapter 2 Literature review

E_C with respect to valence band maximum (VBM) is greater than that of E_N .³³ Therefore, the next question is whether m_e^* in the conduction band would show the same kind of weakened dependence on nitrogen composition when indium composition in the well is being increased. This is important to the study since the technologically important 1.3 μm emission will require the indium composition to be in the range of 30% to 40%. The validity of this weakened enhancement will undoubtedly affect the prediction of transparency conditions of QWs, which will be assessed in this thesis.

In order to understand the performance figure of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ system, various studies have been undertaken using $\mathbf{k} \cdot \mathbf{p}$ method, which include, the performance of InGaAsN/GaAs semiconductor optical amplifiers emitting at 1.3 μm (with 6-band model in the valence band plus BAC in the conduction band),³⁸ the comparison of material gain of InGaAsN/GaAs with InGaAsP/InGaAsP (with different compositions in the well and barrier layers) and InGaAs/AlInGaAs (4-band model in the valence band plus BAC in the conduction band),³⁹ nitrogen-induced modification to the gain characteristics (10-band model for both valence and conduction bands),^{40,41} interdiffusion in InGaAsN/GaAs QW (8-band model with phenomenological m_e^*),⁴² and also the effect of adding nitrogen into the GaAs barrier (6-band model in the valence band and single band in the conduction band).⁴³ Despite reducing the need for additional computing requirements by using various assumptions to simplify the simulation, either by flattening of the band structure using large m_e^* or neglecting conduction band (CB) and valence band (VB) interaction, we are aware that these simplified $\mathbf{k} \cdot \mathbf{p}$ models (other than the 10-band model) may not give an accurate

Chapter 2 Literature review

prediction of the real material properties. Furthermore, we were doubtful whether the presence of CB and VB interaction would yield different results to some of the early findings in these literatures, or whether a heavier m_e^* predicted by the phenomenological model⁴⁴ would be able to give agreeable results with the supposedly most complete and realistic 10-band $\mathbf{k} \cdot \mathbf{p}$ model. Therefore, it is of great importance that these doubts be clarified to ascertain that whether simplified models are to be used for future investigation of material properties on III-N-V compounds.

Chapter 3 Band parameters, band model, and optical gain model

3.1 Band parameters for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$

In band structure calculation, band parameters play a significant part in getting accurate results. The band parameters of the parental binary compounds (GaAs, InAs, GaN, and InN) used in our calculations at 300K are taken from Ref. 45 and are listed in Table I.

Table I. Parameters for binary compounds used in the $\mathbf{k} \cdot \mathbf{p}$ band structure calculation.

Quantity	Unit	GaAs	InAs	GaN	InN
a_0	Å	5.6533	6.0583	4.50	4.98
Δ	eV	0.341	0.390	0.017	0.006
a_c	eV	-7.17	-5.08	-2.20	-1.85
a_v	eV	-1.16	-1.00	-5.20	-1.50
b	eV	-2.0	-1.8	-2.2	-1.2
c_{11}	GPa	122.1	83.29	293.0	187.0
c_{12}	GPa	56.6	45.26	159.0	125.0
γ_1^L	--	6.98	20.00	2.67	3.72
γ_2^L	--	2.06	8.50	0.75	1.26
γ_3^L	--	2.93	9.20	1.10	1.63
E_p	eV	28.8	21.5	25.0	25.0

The parameters for ternary $\text{In}_x\text{Ga}_{1-x}\text{As}$ and quarternary $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ are interpolated as follows:

$$P(\text{In}_x\text{Ga}_{1-x}\text{As}) = (1-x)P(\text{GaAs}) + xP(\text{InAs}), \quad (1)$$

Chapter 3 Band parameters, band model, and optical gain model

$$P(\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y) = (1-x)(1-y)P(\text{GaAs}) + x(1-y)P(\text{InAs}) \\ + (1-x)yP(\text{GaN}) + xyP(\text{InN}). \quad (2)$$

However, for band gap energy (E_G) and electron effective mass (m_e^*) of $\text{In}_x\text{Ga}_{1-x}\text{As}$, we have included the bowing parameters for the ternary compound,⁴⁵

$$E_G(\text{In}_x\text{Ga}_{1-x}\text{As}) = (1-x)E_G(\text{GaAs}) + xE_G(\text{InAs}) - 0.477x(1-x), \quad (3)$$

$$m_e^*(\text{In}_x\text{Ga}_{1-x}\text{As}) = (1-x)m_e^*(\text{GaAs}) + xm_e^*(\text{InAs}) - 0.0091x(1-x). \quad (4)$$

3.2 E_G and m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ by phenomenological relationship

In the earlier stage of research for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material, due to the scarcity of experimental data, Chow *et al.* proposed a phenomenological relationship for E_G and m_e^* of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ that was fitted to E_G of 1.05eV and m_e^* of $0.14m_0$ for $\text{In}_{0.07}\text{Ga}_{0.93}\text{As}_{0.98}\text{N}_{0.02}$,⁴⁴

$$E_G(\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y) = E_G(\text{In}_x\text{Ga}_{1-x}\text{As}) - 69\text{eV} \times \Delta e(x, y), \quad (5)$$

$$m_e^*(\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y) = m_e^*(\text{In}_x\text{Ga}_{1-x}\text{As}) + 18.1667m_0 \times \Delta e(x, y). \quad (6)$$

The dependence of E_G and m_e^* of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ on indium and nitrogen compositions, using Eqs. (5) and (6), are plotted in Figure 1 as dotted-dashed lines. As observed, the dependence is linear in both E_G and m_e^* .

Figure 1. Dependence of (a) bulk band gap energy and (b) electron effective mass of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material on indium and nitrogen composition.

Solid lines are results calculated using BAC model and Eqs. (10) and (11). Dashed lines are results calculated using BAC model and Eqs. (8) and (9). Dotted-dashed lines are results calculated using the phenomenological relationship in Eqs. (5) and (6).

3.3 E_G and m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ by BAC model

Using the BAC model, E_- which is taken to be the fundamental band gap energy (E_G)

for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ is given by,^{33,35}

$$E_- = \frac{1}{2}[(E_N + E_C) - \sqrt{(E_N - E_C)^2 + 4V_{NC}^2 y}], \quad (7)$$

where y is the nitrogen composition in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$. E_N is the parameter which characterizes the position of the nitrogen-induced energy level with respect to the valence band maximum (VBM), while V_{NC} is the matrix element measuring the strength of interaction between the extended E_C and the localized E_N . E_C is the conduction band edge of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ host matrix and is calculated using Eq. (3).

There are two sets of E_N and V_{NC} available. The first set has been proven to agree very well with experimental E_G in $\text{GaAs}_{1-y}\text{N}_y$,^{36,37}

Chapter 3 Band parameters, band model, and optical gain model

$$E_N = 1.65(1 - x) + 1.44x - 0.38x(1 - x), \quad (8)$$

$$V_{NC} = 2.7(1 - x) + 2.0x - 3.5x(1 - x), \quad (9)$$

where x is the indium composition in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$.

As more experimental data is reported in the literature, Duboz *et al.* proposed a prediction of E_G for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ which takes into consideration the statistical local nitrogen environment.³³ This second set is able to yield better agreement with $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ in the range where indium is 30% to 40%,

$$E_N = 1.65 + 0.25x - 0.56x, \quad (10)$$

$$V_{NC} = 2.4(1 - x) + 1.75x. \quad (11)$$

m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ as predicted by the BAC model is given by,^{36,46}

$$m_e^*(\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y) = 2m_e^*(\text{In}_x\text{Ga}_{1-x}\text{As}) \left/ \left(1 - \frac{E_C - E_N}{\sqrt{(E_C - E_N)^2 + 4V_{NC}^2 y}} \right) \right. \quad (12)$$

In addition to the value of E_G and m_e^* predicted by the phenomenological relationship (Eqs. (5) and (6)), in Figure 1, the BAC results calculated using Eqs. (10) and (11) are shown in solid lines, while the results calculated using Eqs. (8) and (9) are shown in dashed lines. In this thesis, we will use Eqs. (10) and (11) for our simulations, unless otherwise stated, not only because of the good agreement obtained in Ref. 33, but also based on the comparison of the calculation using our 10-band $\mathbf{k} \cdot \mathbf{p}$ model with the experimental values of measured photoluminescence wavelengths which will be presented in the next chapter.

Chapter 3 Band parameters, band model, and optical gain model

From Figure 1, it can be observed that the phenomenological relationship generally predicted lower E_G and heavier m_e^* than the BAC model. Both E_G and m_e^* as predicted by BAC model depend not only on the nitrogen composition but also the indium composition. As the indium composition increases, the enhancement of E_G and m_e^* by the addition of nitrogen atom is reduced significantly, due to the increase in separation between E_N and E_C .

3.4 Strained conduction band offset ratio (Q_C)

Strained conduction band offset ratio (Q_C) is defined as the ratio of the band discontinuity in the conduction band to the total discontinuity at the interface of an heterostructure. In the situation of compressive strain, Q_C is

$$Q_C = \frac{\Delta E_C}{\Delta E_C + \Delta E_{hh}}, \quad (13)$$

where ΔE_C is the discontinuity in the conduction band and ΔE_{hh} is the valence band edge after considering the energy shifting caused by the compressive strain. Although Q_C is also an important band parameter for detailed studies of band structure, thus far, there is no attempt in using the BAC model to explain quantitatively and qualitatively the experimental values of Q_C of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs. Heroux *et al.* has formulated the valence band offset for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$.³⁴ However, their focus was on the correct assignment of optical transitions observed in the experiments. It is strongly believed that since the BAC model is able to predict the lowering of conduction band edge of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material, it should be able to aid in the

Chapter 3 Band parameters, band model, and optical gain model

estimation of Q_C of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs (hereafter denoted as $Q_C(\text{InGaAsN})$) from Q_C of $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWs (hereafter denoted as $Q_C(\text{InGaAs})$).

Whenever the issue of the band lineup in a heterostructure is discussed, there will always be controversies involved, with some even suggesting that band lineup of lattice-mismatched heterostructure made up of polar semiconductors is sensitive to the atomic configuration at the interface.⁴⁷ However, in this thesis, it will be treated as a band parameter best determined phenomenologically from the experimental data. Figure 2 shows the compositional dependence of $Q_C(\text{InGaAs})$ fitted from reported values,^{48–61} by assuming that Q_C is independent of temperature. Although Joyce *et al.* has performed similar work,⁶² more recent data has been added into Figure 2. The dashed line shows the least-squared fit performed on the collected values. The equation for the dashed line is

$$Q_C(\text{In}_x\text{Ga}_{1-x}\text{As}) = \begin{cases} 0.4 & \text{for } x \leq 0.05 \\ -8.3885x^2 + 3.8417x + 0.2424 & \text{for } 0.05 < x < 0.18 \\ 0.66 & \text{for } x \geq 0.18 \end{cases} \quad (14)$$

However, recent measurements using capacitance voltage (C-V) and deep-level transient spectroscopy (DLTS) techniques, and analyzed by an empirical $sp^3d^5s^*$ nearest-neighbour tight-binding model has shown that Q_C for InAs/GaAs is about 0.70.⁶³ Therefore, the curve has been adjusted to take this into consideration. It will be shown later that $Q_C(\text{InGaAs})=0.7$ for $x > 25\%$ is indeed preferred for better prediction by the method proposed here. The equation for the solid line is

Chapter 3 Band parameters, band model, and optical gain model

$$\begin{aligned}
Q_C(\text{In}_x\text{Ga}_{1-x}\text{As}) = & \\
& 0.40 & \text{for } x \leq 0.05 \\
& -6.7677x^2 + 3.4276x + 0.2642 & \text{for } 0.05 < x < 0.25 \\
& 0.70 & \text{for } x \geq 0.25
\end{aligned} \tag{15}$$

Figure 2. Compositional dependence of Q_C for $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWs. When experimental errors are not reported in original works, a value of ± 0.05 is assumed.

From $Q_C(\text{InGaAs})$, the position of the unstrained band edges of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer can be determined by considering the energy splitting shifting caused by the compressive or tensile strain. Under compressive strain, the unstrained conduction band edge will shift upwards by

$$\delta E_C = 2a_c(1 - c_{12}/c_{11})e_{xx}, \tag{16}$$

while the valence band edge will shift downwards by

$$\delta E_V = 2a_v(1 - c_{12}/c_{11})e_{xx} - b(1 + 2c_{12}/c_{11})e_{xx}. \tag{17}$$

Chapter 3 Band parameters, band model, and optical gain model

a_c and a_v are the hydrostatic deformation potential for conduction and valence band, respectively. b is the shear deformation potential. c_{11} and c_{12} are the elastic stiffness constants. $e_{xx} = (a_s - a_w)/a_w$ is the in-plane strain, a_s and a_w are the lattice constants for the substrate material and the well layer, respectively. The direction in which both δE_C and δE_V are shifted are considered with respect to the absolute positive electron energy. It is assumed that the unstrained valence band offset of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer is not affected by the incorporation of nitrogen atom, consistent with the formalism proposed in Ref. 34, except that in this thesis, the contribution of the hydrostatic component of the strain has been considered separately for the conduction and valence band. The presence of the nitrogen atom merely promotes the interaction of nitrogen resonant states with $\text{In}_x\text{Ga}_{1-x}\text{As}$ conduction band and reduces the fundamental unstrained E_G of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$, according to Eq. (7). The original form of Eq. (11) is

$$V = V_{Ga}(1 - x) + V_{In}x, \quad (18)$$

where V_{Ga} and V_{In} are 2.4 eV and 1.75 eV, respectively.³³ The original form of Eq. (10) is

$$E_N = E_{Ga} + i(E_{In} - E_{Ga})/4 - x\beta, \quad (19)$$

where $E_{Ga} = 1.65$ eV, $E_{In} = 1.9$ eV, $\beta = 0.56$ eV.³³ i describes the statistical number of indium atom neighbours in the vicinity of the nitrogen atom and $i = 4x$ for an as-grown sample. For annealed samples, it is assumed that on average, one additional indium atom will come in the close vicinity of the nitrogen atoms. In the latter case, x is being replaced by $x + 0.25$ in Eq. (18), and i is being replaced by $i + 1$ in Eq. (19). With these information, the position of the band edges of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ can be calculated. Generally, ΔE_{hh} of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ is smaller than ΔE_{hh} of $\text{In}_x\text{Ga}_{1-x}$

Chapter 3 Band parameters, band model, and optical gain model

x As/GaAs with similar indium composition since the addition of nitrogen reduces the compressive strain. ΔE_C is larger in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ than in $\text{GaAs}_{1-y}\text{N}_y/\text{GaAs}$ because the presence of indium introduces additional band gap energy lowering.

To evaluate the correctness of the abovementioned method, comparison has been made with the experimental value reported. Although the reported values of Q_C (InGaAsN) appear to be scattered, it will be shown later that they are within the limit of experimental errors from the method mentioned here. Hettrich *et al.* has obtained Q_C of about 0.80 (at 4 K) from *in situ* annealed $\text{In}_{0.38}\text{Ga}_{0.62}\text{As}_{0.985}\text{N}_{0.015}/\text{GaAs}$ multiple quantum wells (MQWs) with well width from 2.5 nm to 9 nm.⁶⁴ In our opinion, this is the most accurate measurement available since it is a known fact that the variation of transition energies (E_{eh}) is most sensitive to Q_C at narrow well widths. After considering the annealing effect,³³ where the indium atom will statistically gain one more atom, and temperature dependence of E_G , the theoretical Q_C obtained is 0.77 (at 4 K). To verify the initial assumption that Q_C is independent of temperature, the calculation performed at 300 K yields Q_C of 0.77. Meanwhile, Miyamoto *et al.* reported ΔE_C of 0.3 – 0.4 eV for $\text{In}_{0.26}\text{Ga}_{0.74}\text{As}_{0.988}\text{N}_{0.012}/\text{GaAs}$ QW, determined from well-width dependence of absorption edge wavelength,⁶⁵ compared to our calculated value of 0.32 eV. Xin and Tu reported ΔE_C of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ increased from 0.26 eV to 0.56 eV when nitrogen composition increased from 0% to 3%.⁶⁶ However, from the proposed method, ΔE_C of 0.23 eV to 0.47 eV is obtained for the similar range of concentration. The minor discrepancy in the ΔE_C can be attributed to the approximation used in the fitting in Ref. 66. The finite-square-well model and the linear interpolation of the effective masses used in their calculation could have

Chapter 3 Band parameters, band model, and optical gain model

overestimated the position of the conduction band edge from e_1 , the first excited energy level in the conduction band. Therefore, significantly higher ΔE_C was predicted. Nevertheless, the trend of the variation of ΔE_C between their values and the proposed method is pretty consistent.

However, estimation by the proposed method does differ with some reported data. Pan *et al.* reported Q_C of 0.45, 0.75, and 0.80 for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs with indium composition of 10%, 20%, and 30%, respectively, and Q_C was independent of nitrogen composition from 0.35% to 1%.⁶⁷ Our method estimated Q_C of 0.69, 0.73, 0.73 (for nitrogen composition of 0.35%) and 0.80, 0.80, 0.77 (for nitrogen composition of 1%) over the same range of indium compositions (10%, 20%, and 30%, respectively). It is observed that good agreement is obtained for indium compositions of 20% and 30%. The dependence of $Q_C(\text{InGaAsN})$ on indium composition for various concentration of nitrogen is plotted in Figure 3. In Figure 3, it can be observed that $Q_C(\text{InGaAsN})$ for different nitrogen compositions are merging at higher indium composition ($>25\%$), although ΔE_C continues to increase (see inset of Figure 3). It is caused by the smaller rate of reduction in E_G of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ due to the larger energy separation between E_N and E_C of $\text{In}_x\text{Ga}_{1-x}\text{As}$ for increasing indium composition (thus smaller interaction between the two).³³ Coupled with increase in strain introduced by higher indium compositions (thus larger δE_C and δE_V), $d(\Delta E_C)/dx$ is actually decreasing at a rate faster than $d(\Delta E_V)/dx$ (where ΔE_V is ΔE_{hh} or ΔE_{lh}) whenever $Q_C(\text{InGaAs})$ is held constant. The same reason also causes a dip in $Q_C(\text{InGaAsN})$ for $x < 5\%$ when $Q_C(\text{InGaAs})$ is equal to 0.4. The closely-

Chapter 3 Band parameters, band model, and optical gain model

spaced values of $Q_c(\text{InGaAsN})$ for $x > 25\%$ could be the reason for the observed independence of Q_c on nitrogen composition. For indium composition of 10%, fitted values from Pan *et al.* vary significantly from ours. However, it is believed that Q_c cannot be independent of nitrogen composition at indium composition of 10%. Otherwise, it would imply a significant shift of unstrained valence band edge of $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ when nitrogen is being added, which contradicts the prediction by the BAC model that the incorporation only modifies the conduction band of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$.

Figure 3. The dependence of $Q_c(\text{InGaAsN})$ on indium composition for nitrogen composition from 0% to 3%. Inset shows the corresponding conduction band discontinuity (ΔE_c) of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ strain QWs.

Although it is never the intention of this thesis to resolve the contradictory issue of band lineup of $\text{GaAs}_{1-y}\text{N}_y/\text{GaAs}$ QWs, it should be pointed out that the proposed

Chapter 3 Band parameters, band model, and optical gain model

method consistently gives a type-I prediction with Q_c of about 0.92 for GaAs_{0.03}N_{0.97}/GaAs QW, which is very close to the reported value of 0.95 estimated by C-V measurements.⁶⁸

3.5 10-band $\mathbf{k} \cdot \mathbf{p}$ model

The 10-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian ($H_k + H_s$) for strained bulk semiconductor, which takes into account the energy levels from nitrogen-induced band, conduction band (CB), heavy hole (hh), light (lh), and spin-orbit split-off (so) bands is formed from 8-band Hamiltonian⁶⁹ through the matrix proposed in Refs. 41 and 70 and is given below:

$$\begin{bmatrix} N & 0 & V_{NC}\sqrt{y} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & N & 0 & V_{NC}\sqrt{y} & 0 & 0 & 0 & 0 & 0 & 0 \\ V_{NC}\sqrt{y} & 0 & C & 0 & -\frac{1}{\sqrt{2}}P_+ & \sqrt{\frac{2}{3}}P_z & \frac{1}{\sqrt{6}}P_- & 0 & \frac{1}{\sqrt{3}}P_z & \frac{1}{\sqrt{3}}P_- \\ 0 & V_{NC}\sqrt{y} & 0 & C & 0 & -\frac{1}{\sqrt{6}}P_+ & \sqrt{\frac{2}{3}}P_z & \frac{1}{\sqrt{2}}P_- & \frac{1}{\sqrt{3}}P_+ & -\frac{1}{\sqrt{3}}P_z \\ 0 & 0 & -\frac{1}{\sqrt{2}}P_+^* & 0 & H & \alpha & \beta & 0 & \frac{\alpha}{\sqrt{2}} & \sqrt{2}\beta \\ 0 & 0 & \sqrt{\frac{2}{3}}P_z & -\frac{1}{\sqrt{6}}P_+^* & \alpha^* & L & 0 & \beta & \left(\frac{D}{\sqrt{2}} - \sqrt{2}\varepsilon\right) & -\sqrt{\frac{3}{2}}\alpha \\ 0 & 0 & \frac{1}{\sqrt{6}}P_-^* & \sqrt{\frac{2}{3}}P_z & \beta^* & 0 & L & -\alpha & -\sqrt{\frac{3}{2}}\alpha^* & -\left(\frac{D}{\sqrt{2}} - \sqrt{2}\varepsilon\right) \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}}P_-^* & 0 & \beta^* & -\alpha^* & H & -\sqrt{2}\beta^* & \frac{\alpha^*}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{3}}P_z & \frac{1}{\sqrt{3}}P_+^* & \frac{\alpha^*}{\sqrt{2}} & \left(\frac{D}{\sqrt{2}} - \sqrt{2}\varepsilon\right) & -\sqrt{\frac{3}{2}}\alpha & -\sqrt{2}\beta & S & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}}P_-^* & -\frac{1}{\sqrt{3}}P_z & \sqrt{2}\beta^* & -\sqrt{\frac{3}{2}}\alpha^* & -\left(\frac{D}{\sqrt{2}} - \sqrt{2}\varepsilon\right) & \frac{\alpha}{\sqrt{2}} & 0 & S \end{bmatrix} \quad (20)$$

* denotes complex conjugate.

where

$$N = E_N + \varepsilon_2(z),$$

$$C = E_G + \varepsilon_1(z) + \frac{\hbar^2}{2m_0} \left[\frac{1}{m_e^*} - \frac{E_P}{3} \left(\frac{2}{E_G} + \frac{1}{E_G + \Delta} \right) \right] \times (k_x^2 + k_y^2 + k_z^2),$$

Chapter 3 Band parameters, band model, and optical gain model

$$\begin{aligned}
H &= -\frac{\hbar^2}{2m_0}[(k_x^2 + k_y^2)(\gamma_1 + \gamma_2) + k_z^2(\gamma_1 - 2\gamma_2)] + \varepsilon_2(z), \\
L &= -\frac{\hbar^2}{2m_0}[(k_x^2 + k_y^2)(\gamma_1 - \gamma_2) + k_z^2(\gamma_1 + 2\gamma_2)] - \varepsilon_2(z), \\
S &= -\frac{\hbar^2}{2m_0}[(k_x^2 + k_y^2 + k_z^2)\gamma_1] - \Delta, \\
P_{\pm} &= P(k_x \pm ik_y) - P(e_{xx}k_x \pm ie_{yy}k_y), \\
P_z &= Pk_z - P(e_{zz}k_z), \\
\alpha &= \frac{\hbar^2}{2m_0}2\sqrt{3}[k_z(k_x - ik_y)\gamma_3], \\
\beta &= \frac{\hbar^2}{2m_0}\sqrt{3}[(k_x^2 - k_y^2)\gamma_2 - 2ik_xk_y\gamma_3], \\
D &= \frac{\hbar^2}{2m_0}[2(k_x^2 + k_y^2)\gamma_2 - 4k_z^2\gamma_2], \\
\varepsilon_1(z) &= \begin{cases} 2(a_c + a_v)(1 - c_{12}/c_{11})e_{xx}, & \text{in the well,} \\ 0, & \text{in the barrier,} \end{cases} \\
\varepsilon_2(z) &= \begin{cases} b(1 + 2c_{12}/c_{11})e_{xx}, & \text{in the well,} \\ 0, & \text{in the barrier.} \end{cases} \tag{21}
\end{aligned}$$

E_G is the unstrained band gap energy of the well layer. E_N is shifted by the amount of energy caused by the shear strain, $\varepsilon_2(z)$, since the origin of the calculation is at the middle of the heavy-hole and light-hole band edge after splitting. Δ is the spin-orbit splitting energy. a_c and a_v are the hydrostatic deformation potential for conduction and valence band, respectively. b is the shear deformation potential. c_{11} and c_{12} are the elastic stiffness constants. $e_{xx} = (a_s - a_w)/a_w$ is the in-plane strain, a_s and a_w are the lattice constants for the substrate material and the well layer, respectively. In the case of quantum well, where the different layers of material are stacked in the z -

Chapter 3 Band parameters, band model, and optical gain model

direction, $e_{yy} = e_{xx}$, whereas $e_{zz} = -2(c_{12}/c_{11})e_{xx}$ is the strain in the perpendicular direction. P is the Kane matrix element and is normally expressed in terms of energy unit as^{45,71}

$$E_P = \frac{2m_0}{\hbar^2} P^2. \quad (22)$$

The valence band parameters $(\gamma_1, \gamma_2, \gamma_3)$ used in the 10-band and 8-band Hamiltonian is not identical to the Luttinger parameters $(\gamma_1^L, \gamma_2^L, \gamma_3^L)$ normally used in 6-band Hamiltonian, since the conduction band is now treated exactly in the 10-band and 8-band Hamiltonian and must be subtracted off the original Luttinger parameters.⁷² These parameters are called modified Luttinger parameters and are related to Luttinger parameters as followed:^{69,72,73}

$$\begin{aligned} \gamma_1 &= \gamma_1^L - \frac{1}{3} \frac{E_P}{E_G}, \\ \gamma_2 &= \gamma_2^L - \frac{1}{6} \frac{E_P}{E_G}, \\ \gamma_3 &= \gamma_3^L - \frac{1}{6} \frac{E_P}{E_G}. \end{aligned} \quad (23)$$

The Bloch wave functions for the 10-band Hamiltonian are:⁶⁹

$$\begin{aligned} \phi_N(+) &= |S_N \uparrow\rangle, \\ \phi_N(-) &= |S_N \downarrow\rangle, \\ \phi_c(+) &= |S \uparrow\rangle, \\ \phi_c(-) &= |S \downarrow\rangle, \\ \phi_v\left(\frac{3}{2}, \frac{3}{2}\right) &= -\frac{i}{\sqrt{2}} |(X + iY) \uparrow\rangle, \end{aligned}$$

Chapter 3 Band parameters, band model, and optical gain model

$$\begin{aligned}
\phi_v\left(\frac{3}{2}, \frac{1}{2}\right) &= -\frac{i}{\sqrt{6}} \left| [(X + iY) \downarrow - 2Z \uparrow] \right\rangle, \\
\phi_v\left(\frac{3}{2}, -\frac{1}{2}\right) &= \frac{i}{\sqrt{6}} \left| [(X - iY) \uparrow + 2Z \downarrow] \right\rangle, \\
\phi_v\left(\frac{3}{2}, -\frac{3}{2}\right) &= \frac{i}{\sqrt{2}} \left| (X - iY) \downarrow \right\rangle, \\
\phi_v\left(\frac{1}{2}, \frac{1}{2}\right) &= \frac{i}{\sqrt{3}} \left| [(X + iY) \downarrow + Z \uparrow] \right\rangle, \\
\phi_v\left(\frac{1}{2}, -\frac{1}{2}\right) &= \frac{i}{\sqrt{3}} \left| [(X - iY) \uparrow - Z \downarrow] \right\rangle,
\end{aligned} \tag{24}$$

where, $|X\rangle$, $|Y\rangle$, $|Z\rangle$, and $|S\rangle$ are the orbital wave functions of the top of the valence band and the bottom of the conduction band, respectively. $\uparrow$ and $\downarrow$ denote spin-up and spin-down components, respectively.

The total Hamiltonian for strained QW is given by

$$H = H_k + H_s + V(z), \tag{25}$$

where, $V(z)$ describes the conduction and valence band offset. We have neglected the interaction between E_N and the valence subbands in Eq. (20),⁷⁴ which is consistent with the assumption of the BAC model that the influence of E_N on the valence band energy is minimal and negligible.³⁵

3.6 Envelope wave function and identification of band components

The 10-dimensional electron and hole envelope wave function for the QW can be expressed as

$$\Phi_n = \{\Phi_n^j\}, \quad (j = 1, 2, \dots, 10), \tag{26}$$

Chapter 3 Band parameters, band model, and optical gain model

where

$$\Phi_n^j = \exp[i(k_x x + k_y y)] \sum_m a_{n,m}^j \frac{1}{\sqrt{L}} \exp\left[i\left(k_z + m \frac{2\pi}{L}\right)z\right], \quad (27)$$

and $L = l + d$ is the period of the QW structure, l and d are the width of the well and barrier layer, respectively. k_x , k_y , and k_z are the wave vectors. n is the index for the energy subbands and $a_{n,m}^j$ is the expansion coefficient.

In order to identify the nitrogen-related (N), conduction (e), heavy hole (hh), light hole (lh), and spin-orbit split-off (so) band components in the energy states of the QW, the following probability functions were introduced:

$$\begin{aligned} P_n^N &= \sum_{j=1,2} \sum_m a_{n,m}^{j*} a_{n,m}^j, \\ P_n^e &= \sum_{j=3,4} \sum_m a_{n,m}^{j*} a_{n,m}^j, \\ P_n^{hh} &= \sum_{j=5,8} \sum_m a_{n,m}^{j*} a_{n,m}^j, \\ P_n^{lh} &= \sum_{j=6,7} \sum_m a_{n,m}^{j*} a_{n,m}^j, \\ P_n^{so} &= \sum_{j=9,10} \sum_m a_{n,m}^{j*} a_{n,m}^j. \end{aligned} \quad (28)$$

By calculating P_n^N , P_n^e , P_n^{hh} , P_n^{lh} , and P_n^{so} , the constituting components of the nitrogen-related, electron, heavy hole, light hole, and spin-orbit split-off states in the QW state Φ_n can be known. These probability functions are particularly useful in identifying the dominant character in a particular energy state and assist in the study of polarization of radiative transition in the calculation of optical gain. However, the following sum rule is valid:

$$\sum_i P_n^i = 1, \quad i = N, e, hh, lh, so. \quad (29)$$

Chapter 3 Band parameters, band model, and optical gain model

The wave function Φ_n can be classified into two categories, Φ_{n_c} and Φ_{n_v} , which belongs to conduction band and valence band, respectively. The classification is determined according to the position of the energy subband and also the magnitude of each component calculated using the probability function mentioned above.

3.7 Various $\mathbf{k} \cdot \mathbf{p}$ formalisms considered

From the 10-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian in Eq. (20), it is possible to derive 5 more formalisms based on the common simplifications adopted among the literature. The 8-band Hamiltonian can be obtained by removing E_N and using band parameters of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$. Together with different predictions of m_e^* , this results in 8-band model with BAC's m_e^* and 8-band with “heavy” m_e^* (using the phenomenological relationship).

In many cases, the interaction between CB and VB has been neglected (by setting the matrix elements P to zero). The 10-band Hamiltonians are then decoupled into 6+4-band model, whereas the 8-band models will be decoupled into 6+2-band with BAC's m_e^* , and 6+2-band with “heavy” m_e^* . Under such condition, the modified Luttinger parameters are identical to the original Luttinger parameters. The details for the six $\mathbf{k} \cdot \mathbf{p}$ models used in this thesis are summarized in Table II.

Chapter 3 Band parameters, band model, and optical gain model

Table II. Details of various $\mathbf{k} \cdot \mathbf{p}$ models used in this thesis

Model	CB and VB interaction	Presence of E_N	Electron effective mass	Valence band parameters
10-band	Yes	Yes	InGaAs's	InGaAs's
8-band	Yes	No	InGaAsN's by BAC model	InGaAsN's
8-band with heavy m_e^*	Yes	No	InGaAsN's by phenomenological relationship	InGaAsN's
6+2-band	No	No	InGaAsN's by BAC model	InGaAsN's
6+2-band with heavy m_e^*	No	No	InGaAsN's by phenomenological relationship	InGaAsN's
6+4-band	No	Yes	InGaAs's	InGaAsN's

3.8 Density of states and carrier density

In order to investigate the maximum optical gain obtainable at certain carrier density, the corresponding quasi-Fermi levels must be determined from the integration of the two-dimensional density of states in the QW over all k_x and k_y . The carrier density as calculated for the parabolic energy subbands is not used in this thesis because the interaction between CB and VB has caused the energy dispersion curves to be highly nonparabolic. Therefore, a determination of carrier density by numerically integrating over k -space is more accurate and appropriate,⁷⁵

$$N = \sum_{n_c} \int \frac{1}{4\pi^2 l} f_c[E_{en_c}(k_x, k_y)] dk_x dk_y, \quad (30)$$

$$P = \sum_{n_v} \int \frac{1}{4\pi^2 l} f_v[E_{vn_v}(k_x, k_y)] dk_x dk_y, \quad (31)$$

Chapter 3 Band parameters, band model, and optical gain model

where N and P are the electron and hole density, respectively. E_{en_c} is the electron energy in the conduction subband while E_{hn_v} is the hole energy (not the electron energy) in the valence subband. f_c and f_v are the Fermi-Dirac distributions for electrons in the conduction band and holes (not for electron) in the valence band, respectively.⁷⁵ They are given by

$$f_c = \frac{1}{1 + \exp[(E_{en_c} - E_{f_c})/k_B T]}, \quad (32)$$

$$f_v = \frac{1}{1 + \exp[(E_{hn_v} - E_{f_v})/k_B T]}, \quad (33)$$

where E_{f_c} and E_{f_v} are the electron and hole quasi-Fermi level, respectively, and are dependent on the carrier density. k_B is the Boltzmann's constant and T is the temperature, which is 300 K in this thesis, unless otherwise stated.

3.9 Optical transition matrix elements

The squared optical transition matrix elements, which measure the momentum of the transitions between the hole subbands and the electron subbands, are given by⁷⁶

$$Q_i^{n_c n_v} = \frac{2}{m_0} \left| \langle \Psi_{n_c} | \hat{\mathbf{e}} \cdot \mathbf{p}_i | \Psi_{n_v} \rangle \right|^2, \quad i = x, y, z, \quad (34)$$

where $\hat{\mathbf{e}}$ is the unit vector in the direction of the electric field, $\mathbf{p}_i$ is the momentum operator. Ψ_{n_c} and Ψ_{n_v} are the real electron and hole wave functions, respectively. The real wave function is the product of the envelope wave functions in Eq. (26) and the Bloch wave functions as listed in Eq. (24). The final expressions for squared optical transition matrix elements in the X , Y , and Z directions are given below.⁷⁷

Chapter 3 Band parameters, band model, and optical gain model

$$\begin{aligned}
Q_{x\uparrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(-\frac{i}{\sqrt{2}} a_{n_v, m}^3 + \frac{i}{\sqrt{6}} a_{n_v, m}^5 + \frac{i}{\sqrt{3}} a_{n_v, m}^8 \right) a_{n_c, m}^{1*} \right|^2, \\
Q_{x\downarrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(-\frac{i}{\sqrt{6}} a_{n_v, m}^4 + \frac{i}{\sqrt{2}} a_{n_v, m}^6 + \frac{i}{\sqrt{3}} a_{n_v, m}^7 \right) a_{n_c, m}^{2*} \right|^2, \\
Q_{y\uparrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{2}} a_{n_v, m}^3 + \frac{1}{\sqrt{6}} a_{n_v, m}^5 + \frac{1}{\sqrt{3}} a_{n_v, m}^8 \right) a_{n_c, m}^{1*} \right|^2, \\
Q_{y\downarrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{6}} a_{n_v, m}^4 + \frac{1}{\sqrt{2}} a_{n_v, m}^6 - \frac{1}{\sqrt{3}} a_{n_v, m}^7 \right) a_{n_c, m}^{2*} \right|^2, \\
Q_{z\uparrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(i\sqrt{\frac{2}{3}} a_{n_v, m}^4 + \frac{i}{\sqrt{3}} a_{n_v, m}^7 \right) a_{n_c, m}^{1*} \right|^2, \\
Q_{z\downarrow}^{n_c n_v} &= \frac{2P_0^2}{m_0} \left| \sum_m \left(i\sqrt{\frac{2}{3}} a_{n_v, m}^5 - \frac{i}{\sqrt{3}} a_{n_v, m}^8 \right) a_{n_c, m}^{2*} \right|^2,
\end{aligned} \tag{35}$$

and

$$Q_i^{n_c n_v} = Q_{i\uparrow}^{n_c n_v} + Q_{i\downarrow}^{n_c n_v}, \quad i = x, y, z, \tag{36}$$

where $P_0 = \langle S | p_x | X \rangle = \langle S | p_y | Y \rangle = \langle S | p_z | Z \rangle$. To obtain $Q_{xy}^{n_c n_v}$ for the TE model, $Q_x^{n_c n_v}$ and $Q_y^{n_c n_v}$ are averaged in the calculation. $Q_z^{n_c n_v}$ alone indicates the TM model.

Due to the interaction between CB and VB, Φ_{n_c} is not fully a conduction band state but will have some components contributed by the valence band and vice versa. Therefore, if more accurate results are required, the contribution from the non-conduction band component in Φ_{n_c} and the non-valence band components in Φ_{n_v} must be considered in the derivation of $Q_i^{n_c n_v}$. However, the contribution of these non-conventional transitions will be very small as compared to the stronger transitions as depicted in Eq. (35).

Chapter 3 Band parameters, band model, and optical gain model

3.10 Optical gain model

The optical gain spectra are calculated using⁷⁸

$$G(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\pi^2 c^2 \hbar^2}{n^2 E^2} R_{sp}(E), \quad (37)$$

$$R_{sp}(E) = \frac{ne^2 E}{\pi m_0^2 \epsilon_0 \hbar^2 c^3} \sum_{n_c} \sum_{n_v} \iint \frac{Q^{n_c n_v}}{4\pi^2 l} f_c f_v \times \frac{1}{\pi} \frac{\hbar/\pi}{(E_{eh} - E)^2 + (\hbar/\tau)^2} dk_x dk_y, \quad (38)$$

where $R_{sp}(E)$ is the spontaneous emission rate, $\Delta F = E_{fc} - E_{fv}$ is the separation between quasi-Fermi levels and is dependent in the carrier density, E is the photon energy, e is the electron charge, ϵ_0 is the free-space dielectric constant, n is the refractive index, c is the speed of light, $Q^{n_c n_v}$ is the squared optical transition matrix element as given in Eqs. (35) and (36), E_{eh} is the transition energy, and τ is the intraband relaxation time. $\tau = 0.1$ ps is used in all calculations in this thesis, which are performed at $T = 300$ K, as it is the value widely used for the ideal case of QW simulations.^{41,79,80} Although smaller value of τ was proven to better fit the experimental measured spontaneous emission spectrum at room temperature, it will only reduce the peak gain and differential gain linearly.⁴¹ We believe that the fitting of τ depends very much on the quality of samples under study, and our conclusion should not be affected by the value of τ chosen. The radiative current density (J_{rad}), which is related to the spontaneous emission spectrum, is given by

$$J_{rad} = el \int R_{sp}(E) dE. \quad (39)$$

This is different from injection current density, which includes not only J_{rad} , but also contributions from monomolecular, Auger recombinations, etc.

Chapter 3 Band parameters, band model, and optical gain model

3.11 Summary

In this chapter, the band parameters, the $\mathbf{k} \cdot \mathbf{p}$ band model, and the optical gain model are presented. E_G and m_e^* of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ as predicted by the BAC model are used in the calculations in this thesis. A new equation for Q_C of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ is also presented, which shows reasonable good agreement with experimental data. Finally, the 10-band realistic $\mathbf{k} \cdot \mathbf{p}$ model was discussed and the relationship between this model and other simplified models is also discussed. The results calculated using the $\mathbf{k} \cdot \mathbf{p}$ models and the optical model presented in this chapter will form the basis for the discussion in subsequent chapters.

Chapter 4 Band structure

4.1 Comparison of band structure with published literatures

In this thesis, the results were calculated using an $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW, with well width (l) of 7 nm and barrier width (d) of 20 nm at room temperature, $T = 300$ K. The main focus of the calculation is in the range of $x = 35\%$ and $y = 0$ to 4%. These should cover the range of composition of reported laser structures emitting at 1.3 and near 1.55 μm in the literatures.²⁻¹⁸ Comparison between the band structure formalism presented in Chapter 3 and the published literatures was performed using a strained 3 nm $\text{InAs}/\text{In}_{0.4}\text{Ga}_{0.6}\text{Sb}$ superlattice⁸¹ and an unstrained 5 nm $\text{GaAs}/\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ QW⁸². The results agree reasonably well.

4.2 Comparison of E_{eh} calculated by 10-band $\mathbf{k} \cdot \mathbf{p}$ with published emission wavelength

In order to verify the accuracy of the 10-band $\mathbf{k} \cdot \mathbf{p}$ model presented in Chapter 3, the calculated transition energies (E_{eh}), from ground state $e1$ to $hh1$, have been compared with emission wavelengths reported in the literature for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs lasing in the region of 1.3 and 1.55 μm (Table III). As can be seen, E_{eh} predicted by the 10-band model agrees reasonable well with the experimental values. Better agreement is expected if many-body effects, which include band gap renormalization (BGR) and Coulomb enhancement (CE), are being considered in the optical gain calculation. The typical shift caused by BGR in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QW has been shown to be around 40 to 50 meV.⁸³

Chapter 4 Band structure

Table III. Comparison of theoretical transition energies of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs by 10-band $\mathbf{k} \cdot \mathbf{p}$ model with experimental values.

Well layer composition		Well	Theoretical	Experimental	Difference
Indium, x	Nitrogen, y	width	value (1)	value (2)	(1)–(2)
(%)	(%)	(nm)	(eV)	(eV)	(meV)
36	1.9	6.8	0.946	0.954 ^a	–8
32	1.5	7.0	1.002	0.943 ^b	59
36	1.6	6.0	0.978	0.942 ^c	36
32	1.0	9.0	1.020	0.954 ^d	66
37	0.5	7.7	1.028	0.961 ^e	67
32	0.9	10.0	1.025	0.969 ^f	56
40	0.5	6.0	1.020	0.958 ^g	62
35	1.5	6.0	0.993	0.959 ^h	34
35	1.8	6.5	0.964	0.965 ⁱ	–1
35.5	3.6	9.2	0.828	0.795 ^j	33
38	5.0	7.6	0.759	0.832 ^k	–73
38	5.3	8.2	0.739	0.800 ^l	–61
38	5.0	7.6	0.759	0.817 ^m	–58
34	5.3	6.5	0.786	0.795 ⁿ	–9
38	3.3	8.0	0.836	0.785 ^o	51
20.4	5.5	7.2	0.852	0.800 ^p	52
26	3.0	9.0	0.932	0.821 ^q	111

^aReference 2.^jReference 11.^bReference 3.^kReference 12.^cReference 4.^lReference 13.^dReference 5.^mReference 14.^eReference 6.ⁿReference 15.^fReference 7.^oReference 16.^gReference 8.^pReference 17.^hReference 9.^qReference 18.ⁱReference 10.

4.3 Comparison of band structure calculated by different $\mathbf{k} \cdot \mathbf{p}$ models

The 10-band model is the most realistic model because it includes the nitrogen-related energy levels, E_N , and the CB and VB interaction. 8-band models do not consider E_N but retain the interaction between CB and VB. When the CB and VB interaction is reduced to zero (by setting matrix elements P to zero), 10-band model and 8-band model will become 6+4 band model and 6+2 band model, respectively.

We have calculated the energy dispersion curves along [100] and [110] (where $k_x = k_y$) crystal directions for conduction and valence subbands for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW using the six models described in Table II. These two crystal directions are chosen to show the model-dependent nonparabolicity of the band structures. The results for nitrogen composition of 2% and indium composition of 35% and 15% are shown in Figure 4 and Figure 5, respectively. The solid lines are the results calculated by the 10-band model, and are being compared with the remaining five models.

In Figure 4(a) and Figure 5(a), where only the energy dispersion curves calculated by the 10-band model are shown, the conduction subbands are far from parabolic. The conduction subbands exhibits m_e^* predicted by the BAC model at small k , and flattened at larger k due to the increased interaction between the localized E_N and the extended E_C of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ host matrix. This is a typical characteristic of the band structure calculated by the BAC model.

Chapter 4 Band structure

Figure 4. Energy dispersion curves for conduction and valence subbands along $[100]$ and $[110]$ crystal directions for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW. (a) is the result calculated by 10-band $\mathbf{k} \cdot \mathbf{p}$ model and is duplicated in (b) to (f) as solid lines for ease of comparison. The dashed lines in every graph are the results calculated by (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

From Figure 4(b), the 8-band's results agree very well with that of the 10-band at high indium composition (35%). This confirmed the initial assumption that by using m_e^* predicted by the BAC model in the 8-band model, we should be able to obtain identical conduction band structure with the 10-band model, at least for the first two conduction subbands ($e1$ and $e2$). However, at low indium composition (15%), the agreement deteriorates; see Figure 5(b). In this case, the second and the third conduction subbands

Chapter 4 Band structure

are very close to one another in the 10-band's results. This is due to the fact that in the 10-band model, the conduction band structures of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}/\text{GaAs}$ calculated by the 8-band model will interact with the two nitrogen-related resonant states, E_N . At low indium composition, the conduction band barrier height in the $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}/\text{GaAs}$ QW is very low, this causes only the first conduction subband is confined in the well, and the subsequent two subbands with higher energy are unbound. After interacting with E_N , the second and third energy subbands remain very near to one another as in the 10-band's results. On the other hand, in the 8-band calculation, the conduction band barrier height used is that of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW, which is definitely larger than that of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}/\text{GaAs}$ QW. In addition, m_e^* used in the 8-band model is that of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}_{0.98}\text{N}_{0.02}$, which again is heavier than that of $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$. This explains why the first three energy subbands in the 8-band model are still confined in the potential well.

Figure 5. Continued on next page.

Chapter 4 Band structure

Figure 5. Energy dispersion curves for conduction and valence subbands along $[100]$ and $[110]$ crystal directions for a 7 nm $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.

Solid lines in every graph are the results calculated by 10-band $\mathbf{k} \cdot \mathbf{p}$ model.

Comparison is made with dashed lines in (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

When comparing the results calculated by the 6+2-band model with those of the 10-band model in Figure 4(c) and Figure 5(c), we can observe that with the interaction of CB and VB taken into account, and further flattening of the band structure by E_N , the 10-band results is highly nonparabolic. Another effect of the CB and VB interaction as in the 8-band model is to bring down the second conduction subband and this reduces the energy separation between the first two conduction subbands. This will definitely increase the density of states near the band edge, and may have detrimental effect on the optical differential gain. However, when the heavier m_e^* predicted by the phenomenological relationship is being used in the 6+2-band model, as being shown in Figure 4(d), the energy separation is the same as that of the 10-band model despite the CB and VB interaction being neglected in the model. Upon closer examination, the first conduction subband is flatter than that of the 10-band's results, which implies that if the band structure calculated by the 10-band model is the correct one, then the real

Chapter 4 Band structure

bulk m_e^* of the $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ material may not be that heavy as predicted by the phenomenological relationship as given in Eq. (6).

From the comparison of the energy dispersion curves calculated by 6+4-band and 10-band models (see Figure 4(e) and Figure 5(e)), it can be observed that agreement between the calculated transition energy is reasonably good although the CB and VB interaction was neglected in the former model. This has something to do with the strain band parameters, such as a_c , a_v , and b , used in the calculation. As can be observed from Table II, the strain band parameters for 6+4-band and 10-band models are that of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ and $\text{In}_x\text{Ga}_{1-x}\text{As}$, respectively. While the CB and VB interaction was not considered, the calculated E_{eh} should be higher for the 6+4-band's results, as in the comparison between 6+2-band and 8-band models. However, the strained band gap energy calculated for the 6+4-band model is actually lower than that calculated for the 10-band model and thus compensating for the increase in E_{eh} due to the lack of CB and VB interaction.

Although the results from 8-band model with BAC's m_e^* agree very well with the 10-band model's results at both indium compositions of 15% and 35%, attempt to use m_e^* as predicted by the phenomenological relationship results in conduction subbands that are overly flattened compared to the 10-band models, see Figure 4(f) and Figure 5(f). While the $e2 - e1$ energy separation is much better at 15% indium with the heavier m_e^* , the 8-band model with heavy m_e^* predicted $e2 - e1$ that is 80 meV less than that predicted by the 10-band model at indium of 35%. This has surely cast a doubt on the validity of a large m_e^* at high indium range.

Chapter 4 Band structure

As observed from Figure 4 and Figure 5, the interaction between CB and VB and the inclusion of the BAC model in the conduction band has very little effect on the energy dispersion curves of valence subbands, even though some of the models used $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$'s band parameters and others used $\text{In}_x\text{Ga}_{1-x}\text{As}$'s band parameters. This is due to the fact that although $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$'s band parameters are dependent on the nitrogen composition, which is less than 4% in our calculations, the differences between the two sets of band parameters are not great enough to effect any significant modification to the band structure in the valence band, as shown in Table IV.

Table IV. Comparison of band parameters for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.96}\text{N}_{0.04}$ and $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}$.

Quantity	Unit	$\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.96}\text{N}_{0.04}$	$\text{In}_{0.35}\text{Ga}_{0.65}\text{As}$
Δ	eV	0.344	0.358
a_c	eV	-6.26	-6.44
a_v	eV	-1.22	-1.10
b	eV	-1.93	-1.93
c_{11}	GPa	114.41	108.52
c_{12}	GPa	56.41	52.63
γ_1^L	--	11.20	11.54
γ_2^L	--	4.18	4.31
γ_3^L	--	4.97	5.12
E_p	eV	26.20	26.25

4.4 Dependence of E_{eh} and energy separation on nitrogen and indium composition

In this section, the dependence of transition energy (E_{eh}) and energy separation between the first two conduction subband ($e_2 - e_1$) on nitrogen composition will be

Chapter 4 Band structure

compared, for results predicted by the 10-band model and other models, as plotted in Figure 6 and Figure 7. Graph (a) of both figures is the results calculated by the 10-band model. Graph (b) and (c) show the difference in results calculated by other models than those of the 10-band model, at indium equals 15% and 35%. In these graphs, ΔE_{eh} is the difference between E_{eh} calculated by the individual models and E_{eh} calculated by the 10-band model. Positive ΔE_{eh} implies that E_{eh} calculated by that particular model is larger than that calculated by the 10-band model and vice versa.

Figure 6. (a) Dependence of transition energy E_{eh} for a 7 nm $In_xGa_{1-x}As_{1-y}N_y/GaAs$ quantum well on nitrogen composition for $In_w = 15\%$ and 35% as calculated by the 10-band model. (b) and (c) are differences of E_{eh} calculated by other models from that calculated by the 10-band model at $In_w = 15\%$ and 35% , respectively. ($\square$) denotes results of 10-band model, ($\circ$) denotes results of 8-band, ($\triangle$) denotes results of 6+2-band, (∇) denotes results of 6+2-band model with heavy m_e^* , ($\diamond$) denotes results of 6+4-band, and ($\triangleleft$) denotes results of 8-band with heavy m_e^* .

As pointed out in the previous section, at indium composition equal 35%, E_{eh} predicted by the 6+2 band model with BAC's m_e^* is consistently about 20 meV higher than that predicted by the 8-band model due to the neglecting of interaction between

Chapter 4 Band structure

CB and VB, although both models used the same set of band parameters for the calculation. This confirms that CB and VB interaction must be included in the simulation of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW for a more realistic representation of the band structure, especially when the band gap energy for the well layer is lower than 1 eV. However, this is not totally observed in the case of 6+4-band and 10-band, since the band parameters used in these two models are not the same (please refer to Table II).

Figure 7. (a) Dependence of energy separation between the first two conduction subbands ($e2-e1$) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for $\text{In}_w = 15\%$ and 35% as calculated by the 10-band model. (b) and (c) are differences of ($e2-e1$) calculated by other models from that calculated by the 10-band model at $\text{In}_w = 35\%$ and $\text{In}_w = 15\%$, respectively. Same legend from Figure 6 applies.

From Figure 6(c) and Figure 7(b), it can be observed that at indium composition of 35%, E_{eh} and ($e2-e1$) calculated by the 8-band model with BAC's m_e^* is in good agreement with the results calculated by the 10-band model for the range of nitrogen composition considered. This suggests that the 8-band model with BAC's m_e^* is a good enough alternative for the 10-band model from the aspect of band structure calculation in the high indium region. However, as shown in Figure 6(b) and Figure 7(c), 6+4-

Chapter 4 Band structure

band model and 8-band model with heavy m_e^* are able to match the E_{eh} and $(e2 - e1)$ calculated by 10-band at lower indium composition (15%). This further suggests that the heavy enhancement of m_e^* can only be observed at low indium compositions but not at high indium compositions.

To further examine this, the dependence of E_{eh} and $(e2 - e1)$ on indium composition from 25% to 40% using all the six models are plotted in Figure 8 and Figure 9, respectively. As can be observed in Figure 8(b), Figure 8(c), Figure 9(b), and Figure 9(c), the agreement between the results calculated by the 10-band model and the 8-band model with heavy m_e^* assumption deteriorates with increasing indium composition, which supports the view that great enhancement of m_e^* is only observable at low indium compositions.

Figure 8. (a) Dependence of transition energy E_{eh} for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on indium composition for $N_w = 0\%$, 2% and 4% as calculated by the 10-band model. (b) and (c) are differences of E_{eh} calculated by other models from that calculated by the 10-band model at $N_w = 2\%$ and 4%, respectively.

Chapter 4 Band structure

(□) denotes results of 10-band model, (○) denotes results of 8-band, (△) denotes results of 6+2-band, (▽) denotes results of 6+2-band model with heavy m_e^* , (◇) denotes results of 6+4-band, and (◁) denotes results of 8-band with heavy m_e^* .

Another observation is that the 6+2-band model with heavy m_e^* is able to achieve good agreement in its prediction with the 10-band model across the range of indium composition considered but only at nitrogen composition equal 2%. This shows that the phenomenological relationship for m_e^* may work well only when CB and VB are not considered in the $\mathbf{k} \cdot \mathbf{p}$ simulations.

Figure 9. (a) Dependence of energy separation between the first two conduction subbands ($e2-e1$) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on indium composition for $N_w = 0\%$, 2% and 4% as calculated by the 10-band model. (b) and (c) are differences of ($e2-e1$) calculated by other models from that calculated by the 10-band model at $N_w = 4\%$ and 2% , respectively. Same legend from Figure 8 applies.

4.5 Dependence of energy dispersion curves on indium and nitrogen composition

In this section, the curvature of the first conduction subband ($e1$) and first valence subband ($hh1$) are compared for all the models to determine if they exhibit the same trend when the composition of the well layer are changed. The energy levels for $e1$ and $hh1$ at $k = 0$ are intentionally set to zero to facilitate the pure comparison of the curvature.

In Figure 10, the dependence of curvature of $e1$ and $hh1$ on indium composition is examined, for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW. The $hh1$ dispersion curve of all models are quite similar and the effective mass for $hh1$ reduces with an increase in compressive strain in the well layer with the indium composition. Of particular interest is the curvature of $e1$ subband by the 8-band model with heavy m_e^* , see Figure 10(f1). While other models, whether with or without the consideration of CB and VB interaction, predicted an increase in curvature of $e1$ with increasing indium composition in accordance with the trend of m_e^* in Figure 1, the 8-band model with heavy m_e^* shows otherwise. This could be due to the exceptionally heavy m_e^* predicted by the phenomenological relationship which does not match the conduction band parameters (E_p and the inverse electron mass in Eq. 21) obtained using the light or normal m_e^* condition. This may pose a serious problem to using the heavy m_e^* together with CB and VB interaction, which may result in a wrong prediction of electronic band structure for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$.

Chapter 4 Band structure

Figure 10. Comparison of curvatures of $e1$ and $hh1$ for $In_xGa_{1-x}As_{0.98}N_{0.02}/GaAs$ QW with indium composition from 25% to 40%, in steps of 5%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* . Arrow pointing in the direction of increasing indium composition.

In Figure 11, the dependence of the curvature of $e1$ and $hh1$ on nitrogen composition is studied, for $In_{0.35}Ga_{0.65}As_{1-y}N_y/GaAs$ QW. The $hh1$ dispersion curve directly depends on the decreasing compressive strain in the well layer as the nitrogen composition increased. However, both the models using the phenomenological relations for their m_e^* prediction show exceptional changes in the curvature of $e1$ subband with respect to other models. As previously mentioned, this will cause the tremendous increase in density of state near the conduction band edge in the active

Chapter 4 Band structure

layer, the effect of which will be examined in the next few chapters. Although the $e1$ subband calculated by the 10-band model is in the order that is different from the others, the changes are too small to effect any significant changes.

Figure 11. Comparison of curvatures of $e1$ and $hh1$ for $In_{0.35}Ga_{0.65}As_{1-y}N_y/GaAs$ QW with nitrogen composition from 0% to 4%, in steps of 1%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* . Arrow pointing in the direction of increasing nitrogen composition, unless nitrogen composition is stated in the figure.

4.6 Summary

In this chapter, transition energies (E_{eh}) calculated by the 10-band model were compared with emission wavelengths reported in literature and reasonably well agreement was shown. Comparison for energy dispersion curves calculated by different models yields almost identical results for the valence band but vastly different curves for conduction band due to the flattening of energy subbands by band-anticrossing or the unusually large electron effective mass predicted by the phenomenological relationship. For prediction of E_{eh} across nitrogen range, the results calculated by the 8-band model yields smallest deviation from results calculated by the 10-band model (ΔE_{eh}) for high indium composition, which made the 8-band model a simpler alternative for prediction of compositional dependence of E_{eh} . The curvature of first energy subband in the conduction band ($e1$) was also compared across different models. The exceptional changes in the curvature of $e1$ shown by the models using m_e^* predicted by the phenomenological relationship were not observed in the results calculated by other models, including the 10-band model.

Chapter 5 Density of states for quantum well

In this chapter, the density of states (DOS) in quantum well calculated by numerical integration of energy dispersion curves using various $\mathbf{k} \cdot \mathbf{p}$ formalisms are shown. The dependency of carrier density (N_c), calculated using DOS and quasi-Fermi levels, on nitrogen and indium composition in the well are calculated and compared between the different $\mathbf{k} \cdot \mathbf{p}$ models.

5.1 Relationship of energy dispersion curves and QW's DOS

In Figure 12, the energy dispersion curves and the corresponding DOS in both conduction band and valence band for $\text{In}_{0.32}\text{Ga}_{0.68}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QWs using 10-band $\mathbf{k} \cdot \mathbf{p}$ are shown. Dashed lines in Figure 12(a) denote the boundary of the band gap energy for the GaAs barrier. Only those energy levels within the two dashed lines are considered as bound or confined states. In the example shown, there are seven bound conduction band states and three bound valence band states.

Figure 12. (a) Energy dispersion curves for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW using 10-band $\mathbf{k} \cdot \mathbf{p}$ model. (b) Corresponding density of states in conduction band and valence band.

Chapter 5 Density of states for quantum well

The corresponding energy levels at $k = 0$ for the bound states are indicated with arrow in Figure 12(b), together with the conduction subband index (n_c) and valence subband index (n_v). Of particular interest is the step-like characteristic of the density of states with each introduction of the confined state, which is typical of a two-dimensional structure. The DOS is higher in valence band than in conduction band, even over a smaller interval of energy, due to the closely spaced valence subband and the heavier effective mass of hole than electron. The DOS is obtained by performing numerical integration over k -space for all the energy levels. To further identify the dominating band component (N , e , hh , lh , or so) of each subband, the probability functions according to Eq. (28) are calculated. Figure 13 and Figure 14 illustrate the results for the first three conduction subbands and first four valence subbands, respectively.

Figure 13. Constituting band components for the first three conduction subbands as calculated by the 10-band $\mathbf{k} \cdot \mathbf{p}$ model for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW.

P_n^N , P_n^e , P_n^{hh} , P_n^{lh} , and P_n^{so} are denoted by thin solid, thin dashed, thick solid, thick dashed, and thick dashed-dotted lines, respectively.

Due to the existence of band intermixing, P_n^N , P_n^e , P_n^{hh} , P_n^{lh} , and P_n^{so} are probability functions required to identify the constituting components in particular energy subband. These probability functions are essential in the study of polarization of radiative transition in the simulation of optical gain. As can be seen from Figure 13, in the conduction subbands, the results calculated by the 10-band model consist mainly of

Chapter 5 Density of states for quantum well

P_n^N and P_n^e due to the interaction between E_N and E_C . The value of P_n^N overtakes that of P_n^e at larger k due to the stronger interaction away from the Brillouin zone centre, in agreement with the flattened energy dispersion curves observed for the 10-band model. This increased interaction is absent in the 8-band model, where E_N is not included, and will be proven crucial in the studies of optical radiative transition of QW in the later chapter. The very small contributions from hh , lh , and so band are due to their interaction with the conduction band states only through the off-diagonal elements in the 10-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian.

Figure 14. Constituting band components for the first four valence subbands as calculated by the 10-band $\mathbf{k} \cdot \mathbf{p}$ model for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW. Same legend from Figure 13 applies.

In the valence subbands as shown in Figure 14, the energy states are predominantly occupied by the hh or lh , as indicated by P_n^{hh} and P_n^{lh} in the graphs. The dominant characters at the zone center are used to denote each of the energy subbands on the top-left corner of each figure. In this example, the three confined valence band states

Chapter 5 Density of states for quantum well

are $hh1$, $hh2$, and $hh3$, while the first unbound state is the $lh1 + so$. This may give the impression that lh -related energy states will always be unbound, which is not true. The number of bound energy states in the valence band depends on the height of the valence band offset. In the case of compressive strain, valence band edge for hh is higher than that of lh , coupled with the heavy effective mass from the hh , hh -related energy states is usually on top of lh -related energy states. lh -related energy states can also be bound if the height of the valence band offset is large enough and the compressive strain is small, which results in smaller split between the valence band edges of hh and lh . It is worth mentioning that the narrower spike in P_n^{lh} in Figure 14(d) compared to the rest of the graphs in Figure 14 is due to the stronger intermixing between the unbound hh and lh states.

5.2 Dependence of DOS and carrier density on nitrogen composition

In Figure 15 and Figure 16, the conduction band DOS and carrier density of $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW, with nitrogen composition varying from 0% to 4%, are compared using different $\mathbf{k} \cdot \mathbf{p}$ models. The intention here is to compare the possible different prediction of DOS by either the neglecting of CB and VB interaction, the E_N and E_C interaction, or the choice of electron effective mass in the models. The origin of all the curves are intentionally shifted with their zero reference at the energy level of $e1$ at $k = 0$.

Chapter 5 Density of states for quantum well

Figure 15. Comparison of density of states (DOS) in conduction band versus energy for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%. (a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

A comparison of Figure 15(a) and (b) for the 10-band and 8-band models, respectively, show that at the conduction band edge, the DOS calculated by the 10-band model and the 8-band model with BAC-predicted m_e^* are almost identical. The obvious difference is only observable at higher energy in the conduction band. While the results of the 8-band model continue to exhibit the step-like characteristic, the DOS calculated by the 10-band model starts to increase significantly due to the increased flattening of the energy dispersion curves. However, neglecting the interaction of CB and VB results in significantly lower DOS being predicted, as in the case of 10-band and 6+4-band model (Figure 15(a) and Figure 15(e)), and 8-band and 6+2-band model (Figure 15(b) and Figure 15(c)). The ideal step-like DOS is shown by both the 6+2-band model in Figure 15(c) and Figure 15(d), whether using the m_e^* predicted by the BAC model or the phenomenological relationship. This is due to the fact that by neglecting the CB and VB interaction, the conduction band is simply a potential well without influence

Chapter 5 Density of states for quantum well

from the energy states in the valence band. The progressively significant increase in DOS with the increase in nitrogen composition is only observable in the 6+2-band model with heavy m_e^* . However, when the CB and VB interaction are taken into consideration, as in the case of 8-band model with heavy m_e^* (in Figure 15(f)), the resultant DOS is extremely high when compared to other models.

Figure 16. Comparison of carrier density (N_c) in conduction band versus quasi-Fermi level (E_{fc}) for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Same legend from Figure 15(c) applies.

In Figure 16, it is observed that N_c in the conduction band is generally higher with the increase in nitrogen composition in the well. However, the adoption of heavy m_e^* in the $\mathbf{k} \cdot \mathbf{p}$ model increases the N_c significantly, and results in the neat trend in Figure 16(d) for the 6+2-band model with heavy m_e^* which is not being observed in other models.

Chapter 5 Density of states for quantum well

In Figure 17 and Figure 18, the valence band DOS and carrier density of $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW, with nitrogen composition varying from 0% to 4%, are compared using different $\mathbf{k} \cdot \mathbf{p}$ models. As pointed out in Chapter 4, the energy dispersion curves for the valence subband as calculated by the different $\mathbf{k} \cdot \mathbf{p}$ models are quite similar, even when either $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ band parameters are being used in the calculation. Therefore, there is no major difference in the resultant DOS calculated from the energy dispersion curves for the different models. This presents us with the opportunity to study the optical gain calculated by the various models in the next chapter knowing that the major difference lies in the conduction band.

Figure 17. Comparison of density of states (DOS) in valence band versus energy for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Same legend from Figure 15(c) applies.

The calculated DOS of the QW increases with the nitrogen composition as the hole effective mass increases and the compressive strain reduces. Compressive strain is

Chapter 5 Density of states for quantum well

known to reduce the hole effective mass by increasing the separation between the hh band edge and the lh and thus smaller repulsion between them. The result is an energy dispersion curve that exhibit “lighter” mass and thus small DOS.

Figure 18. Comparison of carrier density (N_c) in valence band versus quasi-Fermi level (E_{f_v}) for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QW with nitrogen composition from 0% to 4%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Same legend from Figure 15(c) applies.

In Figure 18, it is confirmed that the N_c in the valence band calculated by the various $\mathbf{k} \cdot \mathbf{p}$ formalisms do not vary very much from one another. However, one thing to note is that as the nitrogen increases, the quasi-Fermi level for the valence band (E_{f_v}) moves closer to the $hh1$ level at $k = 0$. This will reduce the separation between the quasi-Fermi levels (ΔF) significantly.

5.3 Dependence of DOS and carrier density on indium composition

In Figure 19 and Figure 20, the conduction band DOS and carrier density of $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW, with indium composition varying from 25% to 40%, are compared using various $\mathbf{k} \cdot \mathbf{p}$ models. As can be observed, except for the 8-band model with heavy m_e^* , all the models predicted lower DOS as indium composition increases because of lower m_e^* (see Figure 19(f)). However, those models with the inclusion of CB and VB interaction (10-band and 8-band models) still predicted higher DOS than those without (6+4-band and 6+2-band models), which means that CB and VB interaction has to be included to obtain accurate prediction of DOS and N_c . Of particular interest is the 8-band model with heavy m_e^* . As can be seen from Figure 19(f), the trend of prediction is opposite to other models, with higher DOS predicted for higher indium composition, in accordance with what was observed in the energy dispersion curves. It is of a strong concern that these may give an incorrect prediction of material properties when this formalism is used.

Chapter 5 Density of states for quantum well

Figure 19. Comparison of density of states (DOS) in conduction band versus energy for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%. (a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Figure 20. Comparison of carrier density (N_c) in conduction band versus quasi-Fermi level (E_{fc}) for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.

(a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Chapter 5 Density of states for quantum well

As shown in Figure 20, the opposite DOS trend calculated by the 8-band model with heavy m_e^* is also reflected in the conduction band N_c . The implication is that while other models predict an increase in quasi-Fermi level (E_{f_c}) in conduction band with increase in indium composition in the well layer, the 8-band model with heavy m_e^* predicted otherwise. This may result in an opposite trend being observed in the optical gain calculation, where E_{f_c} is a contributing factor through ΔF .

From the discussion of energy dispersion curves and also seen in previous section, the dependence of DOS and carrier density on different models is minimal. However, for the sake of a thorough investigation, the valence band DOS and carrier density of $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW, with indium composition varying from 25% to 40%, are compared using various $\mathbf{k} \cdot \mathbf{p}$ models in Figure 21 and Figure 22. It can be observed that with the increase in indium composition, the DOS in the valence band decreases, due to the lower hole effective mass and increase in compressive strain. The end result is that the quasi-Fermi level in the valence band (E_{f_v}) is increased with a higher indium composition in the well layer, as observed in Figure 22.

Chapter 5 Density of states for quantum well

Figure 21. Comparison of density of states (DOS) in valence band versus energy for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.
 (a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

Figure 22. Comparison of carrier density (N_c) in valence band versus quasi-Fermi level (E_{f_v}) for $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ QW with indium composition from 25% to 40%.
 (a) 10-band, (b) 8-band, (c) 6+2-band, (d) 6+2-band with heavy m_e^* , (e) 6+4-band, and (f) 8-band with heavy m_e^* .

5.4 Summary

In this chapter, the density of states (DOS) for quantum well as calculated by numerical integration of energy dispersion curves was shown. The relationship between energy subbands and the increase in DOS was also shown. The DOS for quantum well was far from step-like when the interaction of conduction band and valence band was considered. The DOS and carrier density in valence band as predicted by different models were almost similar since the *hh*, *lh*, and *so* bands are considered in all models. However, DOS and carrier density in conduction band calculated by different models were very different from one another and may affect the calculation of optical gain in the next chapter.

Chapter 6 Optical gain

Optical gain is the material properties directly impacted by the changes in well composition, other than the transition energies. Although there have been studies being done to investigate the optical gain obtained for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs in the literature, this chapter will give a complete study of carrier density, radiative current density at transparency, and differential gain when the nitrogen or indium composition changes in the well layer. Comparison of results obtained using the six formalisms highlighted in the previous chapter will also be carried out in this chapter to assess the impact of various simplifications in the formalisms on the prediction of these optical properties.

6.1 Dependence of N_{tr} and $J_{rad(tr)}$ of QWs on nitrogen composition

After comparing the band structure calculated by different models, it is important to assess their impact on the prediction of optical properties at transparency condition since that is the focus of most studies. The quasi-Fermi energy levels (E_{fc} and E_{fv}) for the preselected interval of carrier density have been determined, because they will be the input to the optical gain calculation instead of the carrier density. Subsequently, the dependence of material optical gain of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs on carrier density and radiative current density is being determined.

Figure 23. Dependence of (a) transparency carrier density (N_{tr}) and (b) transparency radiative current density ($J_{rad(tr)}$) for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for various $\mathbf{k} \cdot \mathbf{p}$ models considered. (□) denotes results of 10-band model, (○) denotes results of 8-band, (△) denotes results of 6+2-band, (▽) denotes results of 6+2-band model with heavy m_e^* , (◇) denotes results of 6+4-band, and (◁) denotes results of 8-band with heavy m_e^* .

The point of interest is where the optical gain transits from the negative (loss) to the positive (amplification) region. The results are being plotted in Figure 23. Figure 23(a) and 22(b) show the dependence of carrier density (N_{tr}) and radiative current density ($J_{rad(tr)}$) at transparency on nitrogen composition in the well layer. As anticipated, since the valence subbands for all models are almost similar, even for the 10-band model which uses InGaAs's parameters or the 8-band and 6-band model which uses InGaAsN's band parameters, N_{tr} can be concluded to be mainly dependent on the m_e^* in the conduction band structure and the interaction of CB and VB. The relationship is consistent with the m_e^* plotted in Figure 1. The increase in N_{tr} from 0% to 4% of nitrogen is greater than that from 2% to 4% of nitrogen and can be easily understood since the increase in m_e^* is greater for 0% to 2% of nitrogen. Of greater importance is

Chapter 6 Optical gain

that the 6+2-band and 8-band models with heavy m_e^* predicts N_{tr} which is almost double that of other models. Therefore, the value of m_e^* does affect N_{tr} very much. In Figure 23(b), however, only the 6+2-band model with heavy m_e^* shows a monotonous increase in $J_{rad(tr)}$. These may at first glance seem to be contrary to the results calculated by the 10-band model, which observed weak dependence of $J_{rad(tr)}$ on nitrogen composition.⁷⁹ Upon closer comparison, it was observed that in Ref. 79, both indium and nitrogen composition were varied while maintaining the emission wavelength at 1.3 μm , as opposed to ours, which only varied nitrogen or indium composition and results in different emission wavelengths. Therefore, the weak dependence observed is partly due to the decrease in indium composition and compressive strain that could result in higher $J_{rad(tr)}$ in the QWs. The reduction in $J_{rad(tr)}$ with increasing nitrogen composition, in Figure 23(b), can be attributed to two factors, (1) the reduction in transition energy which directly affects the $J_{rad(tr)}$, according to Eqs. (38) and (39), (2) the stronger interaction between the conduction subbands with either the nitrogen resonant energy level (for the 10-band and the 6+4-band models) or valence subbands (for the 10-band and the 8-band models) thus causing lower strength of $Q_{xy}^{n_c n_v}$ at $k = 0$. Since in the 10-band model, $J_{rad(tr)}$ is under the influence of both the factors mentioned above, its reduction with nitrogen composition is the greatest as observed in Figure 23(b). However, in the case of the 6+2-band model with heavy m_e^* , the heavier electron effective mass not only causes the QW to achieve transparency at higher carrier density, but it also produces a greater J_{rad} with its much flatter conduction band structure and better overlapping of Φ_{n_c} and Φ_{n_v} , and thus higher $Q_{xy}^{n_c n_v}$ at $k \neq 0$.

Figure 24. Dependence of (a) P_n^e for the first conduction subband, e1 and (b) TE-mode squared transition matrix elements for e1 to hh1 transition for various $\mathbf{k} \cdot \mathbf{p}$ models on nitrogen composition at $k = 0$ in a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well.

Same legend from Figure 23 applies.

The probability function P_n^e for the first conduction subband is given in Figure 24(a) to show the degree of band intermixing mentioned above. Figure 24(b) shows the $Q_{xy}^{n_e n_v}$ at $k = 0$, for $n_e = 1$ and $n_v = 1$, which clearly shows the declining of momentum for optical transition with increasing nitrogen composition. In Figure 23(a) and Figure 23(b), the N_{tr} and $J_{rad(tr)}$ for the 8-band model with heavy m_e^* seems to peak at nitrogen composition of 2%. This is caused by the variation of $e2 - e1$ energy separation with increased nitrogen composition which flattened at nitrogen composition of 2%, as observed in Figure 7(b). By referring to Figure 15(f), we can see that the resultant density of states in the conduction band for the 8-band model with heavy m_e^* is less than predictable. While m_e^* increases linearly with nitrogen composition, the $e2 - e1$ energy separation is the lowest at nitrogen composition of 2%. The resultant carrier density in the conduction band at fixed energy level with

Chapter 6 Optical gain

respect to conduction band edge peaks at the same nitrogen composition, see Figure 16(f). With Q_{xy} for $e1$ to $hh1$ decreasing with increased nitrogen composition, we see that the $J_{rad(tr)}$ for nitrogen composition of 4% is actually lower than nitrogen composition at 2% in Figure 23(b).

Our $J_{rad(tr)}$ is comparatively lower than other published values. However, recent experimental determination of $J_{rad(tr)}$ for $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}_{0.995}\text{N}_{0.005}/\text{GaAs}/\text{GaAs}_{0.85}\text{P}_{0.15}$ and $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}/\text{GaAs}/\text{GaAs}_{0.85}\text{P}_{0.15}$ single QWs with well width of 6 nm agree with our calculation results,⁸⁴ especially with the prediction of lower $J_{rad(tr)}$ with increasing nitrogen composition by the 10-band and 6+4 band models. Their measured $J_{rad(tr)}$ of about $15 \pm 2 \text{ A/cm}^2$ and $19 \pm 2 \text{ A/cm}^2$, for structure with and without nitrogen, have demonstrated the ability of achieving low current density at both transparency and threshold for InGaAsN-based QWs. It also reveals the possibility of achieving a lower $J_{rad(tr)}$ with InGaAsN active layer than with InGaAs layer of the same indium composition.

6.2 Dependence of N_{tr} and $J_{rad(tr)}$ of QWs on indium composition

Other than nitrogen composition, the studies on the influence of indium composition in the well layer cannot be neglected if optimum laser design were to be achieved. Figure 25(a) and 25(b) show the dependence of carrier density (N_{tr}) and radiative current density ($J_{rad(tr)}$) at transparency on indium composition in the well layer. It can be observed that for all the models, $J_{rad(tr)}$ reduces with increasing indium composition, which is the much desired effect. This is understood to be the effect of lower E_{eh} and

Chapter 6 Optical gain

the introduction of higher compressive strain in the well later when more indium is added. The N_{tr} is also decreasing sublinearly with increasing indium composition in accordance with the smaller m_e^* with increasing indium composition, with the exception of the results from 8-band model with heavy m_e^* . Both reduction in N_{tr} and $J_{rad(tr)}$ are the results of higher compressive strain in the well layer that causes the hole effective mass to become lighter in band structure, as observed in Figure 10.

Figure 25. Dependence of (a) transparency carrier density (N_{tr}) and (b) transparency radiative current density ($J_{rad(tr)}$) for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well on indium composition for various $\mathbf{k} \cdot \mathbf{p}$ models considered. Same legend from Figure 23 applies.

The probability function P_n^e for the first conduction subband is given in Figure 26(a) to show the degree of band intermixing. Figure 26(b) shows the $Q_{xy}^{n_c n_v}$ at $k = 0$, for $n_c = 1$ and $n_v = 1$. There is a distinct difference between the results calculated by 8-band and 10-band models. While the 8-band models, with or without heavy m_e^* , show that P_n^e is decreasing with more indium content due to the lower E_{eh} and increased interaction, the 10-band model predicted otherwise. As the indium composition

Chapter 6 Optical gain

increases, the energy separation between E_N and E_C increases, thus reducing the interaction between the two energy levels. Consequently, the stronger and dominating band intermixing between the two energy levels, compared to CB and VB interaction, decreases with increasing indium composition, resulted in a small overall increase in both P_n^e and $Q_{xy}^{n_e n_v}$ at $k = 0$ for the 10-band and 6+4-band models, see Figure 26(b).

Figure 26. Dependence of (a) P_n^e for the first conduction subband, e1 and (b) TE-mode squared transition matrix elements for e1 to hh1 transition for various $\mathbf{k} \cdot \mathbf{p}$ models on indium composition at $k = 0$ in a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well.

Same legend from Figure 23 applies.

6.3 Importance of m_e^* on the calculation of band structure and optical gain

It is now obvious that the prediction of m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ at indium of around 30% to 40% by the phenomenological relationship or simple BAC model [see Figure 1(b)] does affect the results greatly, especially in the prediction of E_{eh} , N_{tr} and

Chapter 6 Optical gain

$J_{rad(tr)}$. While the measurements have shown that $\text{GaAs}_{1-y}\text{N}_y$ and lattice matched $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ layers exhibit large enhancement of m_e^* , the measurement of m_e^* in the high indium range involves great difficulties since the growth of thick free standing epilayer for accurate measurements, typically 1 to 3 μm thick,^{85,86} is inherently challenging. Currently, the only direct determination of m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ is reported in Ref. 85. However, the m_e^* of $0.4m_0$ for $\text{In}_{0.08}\text{Ga}_{0.92}\text{As}_{0.967}\text{N}_{0.033}$ is determined from reflectivity spectra, at an electron concentration of $6 \times 10^{19} \text{ cm}^{-3}$, when the Fermi level is high up in the conduction band where the energy dispersion curves is flattened due to the presence of E_N according to the BAC model. The same author admits that reflectivity measurements are unable to determine accurately m_e^* at the bottom of the conduction band.⁴⁶

Other measurements are being performed on $\text{GaAs}_{1-y}\text{N}_y$ material.⁸⁶⁻⁸⁸ Using optically detected cyclotron resonance (ODCR) technique, m_e^* of $0.12m_0$ and $0.19m_0$ were obtained for $\text{GaAs}_{0.988}\text{N}_{0.012}/\text{GaAs}$ and $\text{GaAs}_{0.98}\text{N}_{0.02}/\text{GaAs}$ multiple quantum wells, respectively.^{87,88} The larger measured m_e^* in $\text{GaAs}_{1-y}\text{N}_y$ than that predicted by the BAC model has been attributed to the possible strong interaction between the CB edge of the host matrix and the nitrogen cluster states resulting in hybridization that can further increase m_e^* .^{89,90} Note the measurements performed using the method of four coefficients on $\text{GaAs}_{1-y}\text{N}_y$ thin film yield different results, with m_e^* decreasing from $0.084m_0$ to $0.029m_0$ as the nitrogen composition increases from 0 to 0.4%.⁸⁶ Although there is another independent report that gives the same finding, by inferring m_e^* for $\text{GaAs}_{1-y}\text{N}_y$ of $0.55m_0$ for 1% of nitrogen and $0.15m_0$ for 4% nitrogen from their own

Chapter 6 Optical gain

measurements,⁹¹ these results are controversial because of their fitting by parabolic CB using a simple quantum well model.⁴⁶ The widely accepted understanding is still that m_e^* will increase with nitrogen composition in $\text{GaAs}_{1-y}\text{N}_y$ material.⁹⁰

However, many reports [including Eq. (6)] have tried to assume the large enhancement of m_e^* observed in $\text{GaAs}_{1-y}\text{N}_y$ will not be affected by the addition of indium into $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ layer. The initial samples for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ QWs showed high threshold current density (J_{th}) of above 1 kA/cm^2 when more nitrogen is being added into the well layer,^{3,5} especially for those that are emitting near $1.55 \text{ }\mu\text{m}$, thus lending support to the view that m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ is heavy according to the phenomenological relationship, especially according to the results shown in Figure 23(b) for the 6+2-band model with heavy m_e^* . However, it has been shown recently that the major part that contributed to the large J_{th} is due to the nonradiative monomolecular recombination that can be reduced using better processing techniques during the fabrication of the laser.⁹² Therefore, it is believed that the lower enhancement of m_e^* for $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ as predicted by the BAC model is more reasonable since it has been shown to agree very well with the measured J_{rad} (through 10-band $\mathbf{k} \cdot \mathbf{p}$ model) (Ref. 92) and the assignment of energy levels in photomodulated reflectance measurements.⁷⁰

In summary, according to the BAC model, with statistical local nitrogen environment taken into consideration as in Eqs. (10) and (11), it is believed that the enhancement of m_e^* in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ will be weakened as more indium is added into the well layer

Chapter 6 Optical gain

since the downward shift of E_C with respect to valence band maximum is greater than that of E_N , resulting in reduced interaction between E_C and E_N .

6.4 Dependence of dG/dN and dG/dJ_{rad} on nitrogen composition

Another important property for the design of semiconductor laser is the differential gain, which determines the modulation speed for the device. The maximum obtainable TE-mode differential gain with respect to carrier density (dG/dN) and radiative current density (dG/dJ_{rad}) are plotted in Figure 27(a) and Figure 27(b), respectively.

Figure 27. Dependence of maximum TE-mode differential gain (a) dG/dN and (b) dG/dJ_{rad} for a 7 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well on nitrogen composition for various $\mathbf{k} \cdot \mathbf{p}$ models. Same legend from Figure 23 applies.

Our dG/dN of $0.7 \times 10^{-15} \text{ cm}^2$ for $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}/\text{GaAs}$ QW is comparable to the values published in other literature. In Ref. 80, dG/dN between 0.8×10^{-15} and $1.4 \times 10^{-15} \text{ cm}^2$ were obtained for $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QWs emitting at $0.98 \mu\text{m}$ with indium

Chapter 6 Optical gain

composition varied from 15% to 30%. At a well width of 8.5 nm, dG/dN of $0.7 \times 10^{-15} \text{ cm}^2$ was obtained for $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}/\text{In}_{0.86}\text{Ga}_{0.14}\text{As}_{0.3}\text{P}_{0.7}$, although without strain.⁹³ However, higher dG/dN were also reported, with about $2 \times 10^{-15} \text{ cm}^2$ for 8 nm $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}/\text{Al}_{0.20}\text{Ga}_{0.80}\text{As}$ QW,⁹⁴ and $2.5 \times 10^{-15} \text{ cm}^2$ for 7 nm $\text{In}_{0.55}\text{Ga}_{0.45}\text{As}/\text{GaAs}$ QW.^{41,79} It is believed that the higher dG/dN were obtained when smaller strained conduction band offset ratio (Q_C) were used. In Refs. 41, 79, and 94, Q_C of about 0.62 was used. Ref. 80 used Q_C of 0.65, while Q_C of 0.70 was used in our calculations. Although the corresponding valence band discontinuity has very little effect on the hh energy states, the lh energy will be moved further towards the barrier's valence band maximum. Consequently, the hh and lh band mixing that is detrimental to the TE-mode transition is reduced and the valence band DOS will be reduced as well, causing a larger ΔF as in Eq. (37). These will definitely result in higher TE-mode dG/dN in the calculation of gain characteristics.

One of the important observations is that dG/dN for the 10-band model decreases with an increase in nitrogen composition while the opposite was observed in the prediction by the 8-band model. The reduction of dG/dN in 10-band model was also observed in Ref. 79. The presence of E_N actually reduces the magnitude of P_n^e [as shown in Figure 24(a)] with increasing nitrogen composition due to stronger interaction between nitrogen and conduction bands. Since the orbital wave function $|S_N\rangle$ for the nitrogen-induced level is different from $|S\rangle$ for the conduction band and it is not involved in the radiative transition, the decrease in P_n^e is detrimental to dG/dN . Looking at Figure 27(a) again, dG/dN actually decreases with CB and VB

Chapter 6 Optical gain

interaction. This is due to the reduction in energy separation between $e1$ and $e2$ in the conduction band, which results in lowering of separation between quasi-Fermi levels, ΔF , as the density of states increases near the bottom of the conduction band. However, the 6+2-band model with heavy m_e^* yields the highest dG/dN even when its N_{tr} is the highest among that predicted by other models. As mentioned above, with larger m_e^* , the overlapping between Φ_{n_c} and Φ_{n_v} is improved, which increases optical gain and radiative current density through the increase in $Q_{xy}^{n_c n_v}$. Therefore, the dG/dJ_{rad} is almost the same as calculated by others. The monotonous increase in dG/dJ_{rad} with nitrogen composition in Figure 27(b) is related to the lowering of transition energy with the addition of nitrogen atoms. The lower E_{eh} restricts the increment in J_{rad} while the increase in optical gain continues to outpace that of J_{rad} . In Figure 27(a), we observe that dG/dN for the 8-band model with heavy m_e^* is deflected with a minimum at nitrogen composition of 2%. Since there is not much difference between the valence band energy dispersion curve of 8-band model with heavy m_e^* and the rest of the models, the deflection is mainly due to the density of states and the resultant N_c in the conduction band which are maximum at nitrogen composition of 2%, see Figure 15(f) and Figure 16(f). ΔF is in turn affected and peaks at the same nitrogen composition. Consequently, dG/dN is the lowest at nitrogen composition of 2% and slowly recovers at higher nitrogen compositions, see Figure 27(a).

It is now known that the choice of orbital function for the nitrogen resonant level affects the prediction of optical properties greatly, especially for dG/dN . The

Chapter 6 Optical gain

reduction in optical transition matrix elements when considering E_N in the $\mathbf{k} \cdot \mathbf{p}$ model was first reported in Ref. 40, in which, the InGaAsN/GaAs QW was compared with a nitrogen-free InGaAs/GaAs QW with transition energy artificially lowered. The optical gain obtained by the former is smaller than the latter. The reason given was due to the increases in m_e^* caused by the band anticrossing. Other reports while presenting the same finding with decrease in TE-mode optical gain with increase in nitrogen composition offers little detailed explanation.⁹⁵ However, as being discussed earlier, greater m_e^* actually resulted in a better overlapping of wave functions from conduction and valence subbands and higher dG/dN . The weakening of optical transition matrix elements even at $k = 0$ is actually due to the stronger interaction between nitrogen and conduction band. The finding by pseudopotential supercell calculation on $\text{GaAs}_{1-y}\text{N}_y$ reveals that interband transition elements are strongly dependent on composition, which is large for small nitrogen composition and very small for large nitrogen composition.⁹⁶ Therefore, our assumption that the nitrogen-like states are not contributing to the radiative is appropriate. Consequently, the intermixing of E_C and E_N results in the reduction of $Q_{xy}^{n_c n_v}$ as illustrated in the 10-band and the 6+4-band models and predicted degrading of dG/dN with the addition of nitrogen atoms.

6.5 Dependence of dG/dN and dG/dJ_{rad} on indium composition

After examined the dependence of dG/dN and dG/dJ_{rad} on nitrogen composition in previous section, the same properties are being examined for their dependence on indium composition to complete the study. Except the 8-band model with heavy m_e^* , all models predicted an increase in dG/dN and dG/dJ_{rad} with increasing indium

Chapter 6 Optical gain

composition. The higher indium composition not only reduces m_e^* , but also reduces effective mass of heavy hole. Both will result in the increase of ΔF , the separation between quasi-Fermi levels in the conduction band and valence band. As with the case when nitrogen was increased, increasing indium composition in the well layer reduces the E_{eh} and thus J_{rad} . However, with the increase of ΔF and thus the optical gain obtainable at fixed carrier density, the monotonous increase in dG/dJ_{rad} in Figure 28(a) is expected. In the case of 8-band model with heavy m_e^* , the curvature of the band structure near the zone centre is flatter for increasing indium composition, which is against the trend predicted by other models. This has caused dG/dN to be rather flat for this case, as E_{fc} is decreasing while E_{fv} is increasing with indium composition, as being reflected in Figure 20(f) and Figure 22(f).

Figure 28. Dependence of maximum TE-mode differential gain (a) dG/dN and (b) dG/dJ_{rad} for a 7 nm $\text{In}_x\text{Ga}_{1-x}\text{As}_{0.98}\text{N}_{0.02}/\text{GaAs}$ quantum well on indium composition for various $\mathbf{k} \cdot \mathbf{p}$ models. Same legend from Figure 23 applies.

6.6 Summary

In this chapter, the dependence of carrier density (N_{tr}) and radiative current density ($J_{rad(tr)}$) at transparency condition on nitrogen and indium composition in the well layer was discussed. It was shown that N_{tr} depends mainly on the m_e^* in the conduction band and the interaction of conduction band and valence band, whereas $J_{rad(tr)}$ depends on the reduction in transition energy, the magnitude of P_n^e , and the TE-mode squared transition matrix elements for $e1$ to $hh1$. It was also concluded that the enhancement of m_e^* in $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ will be weakened as indium composition in the well layer increased. The presence of nitrogen-related energy level (E_N), which reduced the magnitude of P_n^e as nitrogen composition increased, also caused lower differential gain (dG/dN) in the quantum well. Therefore, the optimum method of increasing emission wavelength of quantum well is to increase the indium composition and nitrogen composition at the same time in order that the nitrogen may reduce the compressive strain introduced by the addition of indium while the indium can compensate for the decrease in dG/dN caused by the increase in nitrogen composition.

Chapter 7 Barrier engineering

In previous chapters, the discussions were centred on InGaAsN-based QWs with GaAs barrier. However, recently there have been other material being used in the pursuit of QWs with longer emission wavelength and lower threshold current density (J_{th}). The most prominent candidate being the GaAsN barrier and GaAs/GaAsP/GaAs triple barriers. GaAsN was used because of its tensile strain which was thought to be a better interface or intermediate layer between the InGaAsN well layer and the GaAs substrate. Although the band-gap energy of GaAsN is lower than the GaAs and may increase J_{th} , it was found that the transition energy of InGaAsN/GaAsN is about 50 to 60 meV lower than that of the InGaAsN/GaAs QWs. In GaAs/GaAsP/GaAs triples barrier, it was thought that with the higher band-gap energy of GaAsP was able to provide better carrier confinement, while the tensile strain in the GaAsP layer was seldom considered as strain-mediating layer as in the case of GaAsN layer.

Thus far, Tansu *et al.* has been very successful in reducing J_{th} to 390 A/cm² using direct barriers of GaAsP.²² However, there is still no attempt in using it in a symmetrically structured InGaAsN/GaAs/GaAsP multiple quantum wells (MQW). In this chapter, we used such a structure to investigate the possibility of achieving low J_{th} and investigate the difference between the optical properties obtained using structure with and without the GaAsP layers.

7.1 GaAs/GaAsP/GaAs triple barriers

Instead of a single GaAs layer as the barrier, the structure used two unstrained GaAs layers and one tensile-strained GaAsP layer to form a combined barrier as shown in Figure 29. The wafer sample was grown by IQE (Europe) Ltd. using MOCVD and was part of the research by Qu, Liu and *et al* in Refs. 97 to 100. This structure is believed to have a higher confinement potential than the single GaAs barrier due to the higher band-gap energy of GaAsP and is supposed to reduce the carrier leakage from the QW.

Figure 29. Schematic band diagram for the $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ multiple quantum wells with barrier formed by tensile-strain $\text{GaAs}_{0.82}\text{P}_{0.18}$ and unstrained GaAs layers. d_1 and d_2 are the thickness of the GaAs and GaAsP barriers, respectively. l is the thickness of the compressive strained active layer.

The width of the active layers is 64 Å and total barrier width is 220 Å ($d_1 = 70$ Å, $d_2 = 80$ Å). A sample with such structure was grown by metal organic chemical vapor deposition (MOCVD). Subsequently, ridge laser diodes were fabricated using pulse anodic oxidation technique. In Figure 30, the measured output power versus injection current characteristic was plotted for one of the sample from Refs. 97 to 100, the uncoated $10 \times 1600 \mu\text{m}^2$ broad-area laser, operated in continuous-wave (CW) mode.

Chapter 7 Barrier engineering

As seen, the threshold injection current is about 89 mA, which corresponds to J_{th} of about 556 A/cm^2 . The lasing wavelength is 1295 nm as measured by a spectrometer with Ge detector cooled down to -20°C . The sample has been characterized extensively and reported elsewhere.^{97–100} Here, we intend to address some of the aspects of the low J_{th} achieved by this structure using detailed calculation based on the $\mathbf{k} \cdot \mathbf{p}$ model.

Figure 30. CW light output power versus injection current measured at room temperature (RT) for a $10 \times 1600 \mu\text{m}^2$ ridge waveguide $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ triple quantum wells. The inset shows the lasing spectrum of the MQW at an injection current of 150 mA.

7.2 Derivation of matrix elements for barrier potential and strain in

$\mathbf{k} \cdot \mathbf{p}$ Hamiltonian

The Hamiltonian in Eq. (20) is modified to take into consideration the additional barrier potential and tensile strain in the GaAsP barrier. The Q_c for GaAsP/GaAs was interpolated from the experimental value reported by Zhang *et al.*¹⁰¹ All the other band

Chapter 7 Barrier engineering

parameters were collected from the compilation by Vurgaftman *et al.*⁴⁵ In this section, the derivation of matrix element for barrier potential and strain terms in $\mathbf{k} \cdot \mathbf{p}$ will be presented for normal unstrained GaAs barrier and the GaAs/GaAsP/GaAs barrier.

7.2.1 GaAs barrier

For InGaAsN QW with GaAs barrier, the strain is only present in the well layer. The only barrier height is at the barrier layer due to the higher band-gap energy of GaAs than InGaAsN. Note that the origin for the horizontal axis is at the middle of the active layer to achieve simplest derivation. l is the well width, d is the barrier width, and $L = l + d$ is the period of the quantum well. The schematic band diagram for InGaAsN quantum well with GaAs barrier is shown in Figure 31.

Figure 31. Schematic band diagram for InGaAsN quantum well with unstrained GaAs as barrier.

The derivation for the barrier potential and strain terms is given as follows. Note that

the limit of integration is from $-\frac{l}{2}$ to $L - \frac{l}{2}$.

Chapter 7 Barrier engineering

$$\langle n|V|n\rangle = \frac{d}{L}V \quad (40)$$

$$\langle m|V|n\rangle = -\frac{V}{(n-m)\pi} \sin\left[(n-m)\frac{\pi d}{L}\right] \quad (41)$$

$$\langle n|\varepsilon|n\rangle = \frac{l}{L}\varepsilon_2 \quad (42)$$

$$\langle m|\varepsilon|n\rangle = \frac{\varepsilon_2}{(n-m)\pi} \sin\left[(n-m)\frac{\pi l}{L}\right] \quad (43)$$

7.2.2 GaAs/GaAsP/GaAs barrier

For GaAs/GaAsP/GaAs barrier, compressive strain is present in the well layer and tensile strain in the GaAsP layer sandwiched between two unstrained GaAs layer. The barrier heights from GaAs and GaAsP layers are denoted as V_1 and V_2 , respectively, as depicted in Figure 32. Note that the origin for the horizontal axis is at the middle of the well layer. d_1 is the thickness of the GaAs layer and d_2 is that of the GaAsP layer. $L = l + 2d_1 + d_2$ is the period of the quantum wells.

Chapter 7 Barrier engineering

Figure 32. Schematic band diagram for the InGaAsN quantum well with GaAs/GaAsP/GaAs triple barriers and its origin for the derivation of matrix elements in the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian.

The derivation for the barrier potential and strain terms for the GaAs/GaAsP/GaAs

barrier is given as follows. Note that the limit of integration is from $-\frac{L}{2}$ to $+\frac{L}{2}$.

$$\langle n|V|n \rangle = \frac{2}{L} \left[V_1 d_1 + V_2 \frac{d_2}{2} \right] \quad (44)$$

$$\begin{aligned} \langle m|V|n \rangle &= \frac{1}{(n-m)\pi} \left\{ V_2 \sin \left[(n-m) \frac{2\pi}{L} \left(-\frac{L}{2} + \frac{d_2}{2} \right) \right] \right. \\ &\quad \left. + V_1 \sin \left[(n-m) \frac{2\pi}{L} \left(-\frac{l}{2} \right) \right] + V_1 \sin \left[(n-m) \frac{2\pi}{L} \left(\frac{l}{2} + d_1 \right) \right] \right\} \end{aligned} \quad (45)$$

$$\langle n|\varepsilon|n \rangle = \frac{l}{L} \varepsilon_2^w + \frac{d_2}{L} \varepsilon_2^b \quad (46)$$

$$\begin{aligned} \langle m | \varepsilon | n \rangle &= \frac{\varepsilon_2^w}{(n-m)\pi} \sin \left[(n-m) \frac{\pi l}{L} \right] \\ &+ \frac{\varepsilon_2^b}{(n-m)\pi} \sin \left[(n-m) \frac{2\pi}{L} \left(-\frac{L}{2} + \frac{d_2}{2} \right) \right] \end{aligned} \quad (47)$$

7.3 Comparison of band structure and optical properties of InGaAsN QW with GaAs/GaAsP/GaAs and GaAs barriers

The energy dispersion curves for conduction and valence subbands in the direction of [100] and [110] as calculated by the modified 10-band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian are shown in Figure 33.

Figure 33. The in-plane energy dispersion curves of $\text{In}_{0.35}\text{Ga}_{0.65}\text{As}_{0.985}\text{N}_{0.015}$ quantum wells with GaAs/GaAs_{0.82}P_{0.18}/GaAs barriers (solid line) and GaAs barrier (dashed line). (a) and (b) are the conduction and valence subbands, respectively.

Chapter 7 Barrier engineering

The calculated transition wavelength is 1257 nm (986 meV) for both InGaAsN QWs with GaAs/GaAsP/GaAs and GaAs barriers. As shown in Figure 33, higher barrier height only affects the higher subbands (n_c and n_v greater than 2). We expect a better agreement between the predicted emission wavelength by the 10-band model and the experimental value if the many-body effects are being considered in the optical gain calculation. Typical shift caused by band-gap renormalization in $\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}$ QW has been shown to be around 40 to 50 meV,⁸³ which is just the value that is required to increase the calculated transition wavelength to 1.30 μm .

We have also plotted the maximum TE-mode optical gain obtained at different carrier density for both GaAs/GaAsP/GaAs and GaAs barriers in Figure 34(a). The transparency carrier density (N_{tr}) obtained by GaAs/GaAsP/GaAs barrier is $1.67 \times 10^{18} \text{ cm}^{-3}$, which is slightly lower than N_{tr} of GaAs barrier at $1.69 \times 10^{18} \text{ cm}^{-3}$. In fact, the structure with GaAsP in the barrier actually delivers higher TE-mode optical gain at given carrier density compared to the structure with purely GaAs barrier. This is related to the increase in the confinement potential which not only increases the separation between the energy subbands but also the separation between the quasi-Fermi energy levels (ΔF) in the conduction and valence subbands at fixed carrier density. Moreover, as observed in Figure 34(b), the radiative current density (J_{rad}) for GaAs/GaAsP/GaAs barrier is slightly higher than QWs with GaAs barrier alone. The increase in the barrier potential by the GaAsP layer has very little effect on the ground state energy but has elevated the higher excited states as can be observed from the difference between J_{rad} for structure with or without GaAsP layer, which increases progressively with higher carrier density. From this calculation, we expect that QW

Chapter 7 Barrier engineering

with GaAs/GaAsP/GaAs barrier to achieve the threshold condition with lower N_{th} , and lower total current density if the Auger and monomolecular recombination coefficients remain unchanged for structure with or without GaAsP layer.

Figure 34. (a) Maximum optical gain of the TE-mode as a function of the carrier density and (b) radiative current density as a function of the carrier density for $In_{0.35}Ga_{0.65}As_{0.985}N_{0.015}$ quantum wells.

Solid lines are for GaAs/GaAs_{0.82}P_{0.18}/GaAs barrier and dashed lines are for GaAs barrier.

With the calculated confinement factor of 9.1% for GaAs/GaAsP/GaAs barrier and 9.45% for GaAs barrier, and the experimental determined internal loss α_i of 12 cm^{-1} ,^{98,100} we are able to compute the N_{th} and J_{rad} at threshold condition. By assuming uniform charge injection across the triple quantum wells in Figure 29, we determine that the radiative recombination coefficient B is $6.14 \times 10^{-11} \text{ cm}^3/\text{s}$ for GaAs/GaAsP/GaAs barrier and $5.88 \times 10^{-11} \text{ cm}^3/\text{s}$ for GaAs barrier. As observed the

Chapter 7 Barrier engineering

radiative recombination coefficient calculated by the 10-band model is very close to the $9.5 \times 10^{-11} \text{ cm}^3/\text{s}$ reported by Fehse *et al.*⁹²

We are also interested to estimate the total threshold current density using $J_{tot} = n_w q l (AN + BN^2 + CN^3)$, where n_w is the well number, q is the electron charge, and l is the width of the active layer. A , B , and C are the coefficients characterizing monomolecular, radiative, and Auger recombination, respectively. N is the carrier density in the QWs. By using $A = 2.26 \times 10^8 \text{ 1/s}$ and $C = 4.00 \times 10^{-29} \text{ cm}^6/\text{s}$ from Ref. 92 and our calculated $B = 6.14 \times 10^{-11} \text{ cm}^3/\text{s}$ and $N_{th} = 2.67 \times 10^{18} \text{ cm}^{-3}$, the calculated $J_{th} = 554.5 \text{ A/cm}^2$ agrees very well with the experimental value.

From the above calculation, we would like to attribute the reduction in monomolecular recombination coefficient (A) to better crystal quality and the improved postgrowth preparation of our sample. However, the exact reduction in monomolecular recombination relies on the crystal quality and process, and is beyond the scope of this thesis.

In conclusion, we have calculated the optical properties of the InGaAsN quantum well with both GaAs/GaAsP/GaAs and GaAs barrier and have found that the former structure resulted in a smaller threshold carrier density due to its higher barrier potential.

Chapter 8 Conclusion and recommendations

In conclusion, we have performed calculations on energy dispersion curves and optical emission spectra with different formalism of $\mathbf{k} \cdot \mathbf{p}$ method. We have found that at high indium composition (35%), both E_{eh} and $e2 - e1$ predicted by the 8-band model are the closest to that calculated by the 10-band model, which implies that the 8-band model is a good enough alternative for the 10-band model from the aspect of band structure calculation in the high indium range; at low indium range (15%), the E_{eh} and $e2 - e1$ calculated by the 6+4-band model is the closest to the results predicted by the 10-band model. The m_e^* of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y$ as predicted by the BAC model is more reasonable and the enhancement caused by the addition of nitrogen atom is weakened as the indium composition increases. We have discovered that whenever the interaction between CB and VB is neglected, the differential gain (dG/dN) obtained is higher and the N_{tr} is lower, than the values obtained by those models which considered CB and VB interaction in the calculations due to the effect of interband mixing. In addition, the higher m_e^* predicted by the phenomenological relationship, when used in the 6-band model, monotonously predicted higher dG/dN and also $J_{rad(tr)}$ when the nitrogen content increases. The degrading of dG/dN and even optical gain obtainable at fixed carrier density calculated by the inclusion of the BAC model into the 10-band $\mathbf{k} \cdot \mathbf{p}$ model is due to the fact that more components of the conduction band states are intermixed with the nonradiative nitrogen-like states. The difference in the prediction of dG/dN by the 8-band (predicted an increase) and the 10-band model (predicted a reduction) in this thesis will prompt a more detailed

Chapter 8 Conclusion and recommendations

investigation of the use of the various simplified $\mathbf{k} \cdot \mathbf{p}$ formalisms to predict the various device performances.

The recommendations for future continual research on this topic include the inclusion of many-body effects,⁸³ the investigation of various barrier materials on the transition energy and optical properties of the quantum well structure, and the effects of non-ideal well-barrier interface due to nitrogen interdiffusion.

Many-body effects include carrier scattering, band gap renormalization, and coulomb enhancement.⁸³ They are significant especially when the laser is operating under high current injection and the carrier density is more than $1 \times 10^{19} \text{ cm}^{-3}$, which are the typical operating conditions of quantum well laser.

The studies of various barrier materials will help to find a suitable candidate for the fabrication of quantum well lasers with optimum optical properties, such as low threshold current density, low transparency carrier density, and high differential gain.

Interdiffusion of nitrogen at the well-barrier interface occurs during the physical growth of multi quantum well structure and results in gradual transition of barrier energy potential instead of the abrupt transition in the ideal case. Correct modeling of this gradual transition will help to improve the agreement of results predicted by $\mathbf{k} \cdot \mathbf{p}$ model and the experimental results.

Finally, it is recommended all these future works should be based on the most realistic 10-band $\mathbf{k} \cdot \mathbf{p}$ model.

List of Publications

1. “Comparison of electronic band structure and optical transparency conditions of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum wells calculated by 10-band, 8-band, and 6-band $\mathbf{k} \cdot \mathbf{p}$ models” by **S. T. Ng**, W. J. Fan, Y. X. Dang, and S. F. Yoon, Physical Review B **72**, 115341 (2005).
2. “Influence of $\mathbf{k} \cdot \mathbf{p}$ formalisms on the band structure of $\text{In}_x\text{Ga}_{1-x}\text{As}_{1-y}\text{N}_y/\text{GaAs}$ quantum well: A comparison of 8-band and 10-band models” by **S. T. Ng**, W. J. Fan, Y. X. Dang, and S. F. Yoon, Japanese Journal of Applied Physics **44**, L658 (2005).
3. “Investigation of the optical properties of $\text{InGaAsN}/\text{GaAs}/\text{GaAsP}$ multiple-quantum-well laser with 8-band and 10-band $\mathbf{k} \cdot \mathbf{p}$ model” by **S. T. Ng**, W. J. Fan, S. F. Yoon, S. Z. Wang, Yi Qu, C. Y. Liu, S. G. Ma, and Shu Yuan, Journal of Applied Physics **96**, 4663 (2004).
4. “Effects of tensile strain in barrier on optical gain spectra of $\text{GaInNAs}/\text{GaAsN}$ quantum wells” by W. J. Fan, **S. T. Ng**, S. F. Yoon, M. F. Li, and T. C. Chong, Journal of Applied Physics **93**, 5836 (2003).
5. “Study of interdiffusion in $\text{GaInNAs}/\text{GaAs}$ quantum well structure emitting at 1.3 μm by eight-band $\mathbf{k} \cdot \mathbf{p}$ method” by Y. X. Dang, W. J. Fan, **S. T. Ng**, S. F. Yoon, and D. H. Zhang, Journal of Applied Physics **97**, 103718 (2005).

List of Publications

6. “Study of interdiffusion in GaAsSbN/GaAs quantum well structure by ten-band $\mathbf{k} \cdot \mathbf{p}$ method” by Y. X. Dang, W. J. Fan, **S. T. Ng**, S. Wicaksono, S. F. Yoon, D. H. Zhang, Journal of Applied Physics **98**, 026102 (2005).

7. “Valence band structure of ultrathin silicon and germanium channels in metal-oxide-semiconductor field-effect transistors” by Tony Low, M. F. Li, Y. C. Yeo, W. J. Fan, **S. T. Ng**, and D. L. Kwong, Journal of Applied Physics **98**, 024504 (2005).

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