Gallium nitride based optoelectronic devices on silicon-on-insulator substrates

Lin, Kaixin

2012

Lin, K.X. (2012). Gallium nitride based optoelectronic devices on silicon-on-insulator substrates. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/50478>

<https://doi.org/10.32657/10356/50478>

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A thesis submitted to the Nanyang Technological University
in fulfillment of the requirement for the degree of
Doctor of Philosophy

2012

ACKNOWLEDGEMENTS

In the course of my study, many people have helped and supported me. I would like to acknowledge and express my greatest gratitude to the following persons.

First and foremost, I would like to express my heartiest gratitude to my main supervisor Dr. Ramam Akkipeddi and co-supervisor Dr. Tripathy Sudhiranjan for their timeless guidance, fruitful suggestions and constant encouragement. Despite their busy schedules, they have always made time to have regular discussions on my work. It is through their knowledge and guidance that I have managed to complete this research work.

I would like to extend my gratitude to my co-supervisor Assoc. Prof. Subodh Mhaisalkar at School of Materials Science and Engineering @ NTU for his constant support and encouragement. I am thankful to him for believing in me and helping me to resolve the difficulties I faced during the course of study.

I would like to specially thank Assoc. Prof. Ng Geok Ing and Dr. Arulkumaran Subramaniam of Temasek Laboratories @ NTU for the useful discussions in the initial phase of my research project.

I would like to heartily thank Dr. Armin Dadgar and Prof. Alois Krost from Otto-von Guericke Universität Magdeburg for their advices in epitaxy and the useful discussions in the publications.

I would like to sincerely thank my research team mates in IMRE: Siew Lang for training me on all the fabrication tools. It is through her selfless guidance that I acquired all the skills for device fabrication. Special thanks to

Esther for all the fruitful discussions on micro-Raman measurements and Surani for the optical and electrical measurements.

I would like to thank the people in my capability group. Chum, Cheong, Yi Fan, Deng Jie, Neo, Xiaosong, Vincent, Poh Chong, Hui Kim, Shen Lu, Zhang Zheng, Doreen, for their kind support and the valuable discussions I had with them to resolve the technical problems I faced. Special thanks to Hui Kim for the samples preparation for TEM and also image collection. I would also like to thank my IMRE colleague Bee Keen for her kind assistance in the responsivity setup.

I would like to thank the SERC Nano-Fabrication, Processing and Characterization (SnFPC) Cluster in Institute of Materials Research and Engineering (IMRE) for the facilities and use of the necessary equipment needed for this research work and the equipment specialists for the effort they put in for the trainings and technical support in my work.

Lastly and most importantly, I would like to thank my family and my best friends, Siew Lang, Vicknesh and Janis for their constant encouragement and blessings in my research work. I would like to express utmost gratitude to my father who always believed in me and supported me in all my pursuits. My loving thanks to my husband, Lawrence and my son Edward, whose tremendous support and understanding had allowed me to pursue my dreams.

It is to them that this thesis is dedicated.

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Journal Articles:

- (1) **Vivian Kaixin Lin**, Surani-bin Dolmanan, Siew Lang Teo, Hui Hui Kim, Esther Alarcon-Llado, Armin Dadgar, Alois Krost, and Sudhiranjan Tripathy. (2011). $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures on a thin silicon-on-insulator substrate for metal-semiconductor-metal photodetectors. *Journal of Physics D: Applied Physics*, 44, 365102-1-7.
- (2) **Vivian K. X. Lin**, S. Tripathy, S. L. Teo, S. B. Dolmanan, A. Dadgar, M. Noltemeyer, A. Franke, F. Bertram, J. Christen, and A. Krost. (2010). Luminescence Properties of Photonic Crystal InGaN/GaN Light Emitting Layers on Silicon-on-Insulator. *Electrochemical and Solid-State Letters*, 13, H343-H345.
- (3) **Vivian K. X. Lin**, Esther Alarcon-Llado, Hui Hui Kim, S. Arulkumaran, G. I. Ng, A. Ramam, and S. Tripathy. (2010). Structural and electrical characterization of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ Interfaces for UV Photodetectors. *Electrochemical and Solid-State Letters*, 13, H301-304.
- (4) S. Tripathy, S. L. Teo, **V. K. X. Lin**, M. F. Chen, A. Dadgar, J. Christen, and A. Krost. (2010). Light extraction from GaN-based LED structures on silicon-on-insulator substrates. *Physica Status Solidi C*, 7, 88-91.
- (5) S. Tripathy, A. Dadgar, A. Krost, S. L. Teo, and **V. K. X. Lin**. (2009). Reflecting layer boosts LEDs brightness. *Compound Semiconductor*, 15, 25-27.
- (6) S. Tripathy, T. E. Sale, A. Dadgar, **V. K. X. Lin**, K. Y. Zang, S. L. Teo, S. J. Chua, J. Blasing, and A. Krost. (2008). GaN-based microdisk light emitting diodes on (111)-oriented nanosilicon-on-insulator templates. *Journal of Applied Physics*, 104, 053103-1-7.
- (7) S. Tripathy, **V. K. X. Lin**, S. L. Teo, A. Dadgar, A. Diez, J. Blasing, and A. Krost. (2007). InGaN/GaN light emitting diodes on nanoscale silicon on insulator. *Applied Physics Letters*, 91, 231109-1-3.

Conference Presentations:

- (1) **Vivian K. X. Lin**, S. Tripathy, S. Arulkumaran, G. I. Ng, and A. Ramam, “Structural properties of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ 2DEG heterostructure for UV photodetector application”, E-MRS 2009 Spring Meeting, Strasbourg, France, 8 - 12 June, 2009.
- (2) **Vivian K. X. Lin**, Esther Alarcon-Llado, S. B. Dolmanan, Hui Hui Kim, S. L. Teo, A. Ramam, A. Krost, A. Dadgar, and S. Tripathy “ $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ UV Metal-Semiconductor-Metal Photodetectors on Silicon-on-Insulator Substrate”, International workshop on Nitride Semiconductors, Tampa, Florida, 19 – 24 Sept, 2010.

ABSTRACT

The III-Nitride material system finds applications in many optoelectronic and power electronic devices and is of utmost importance to address the performance gaps in current silicon and conventional III-V compound semiconductors. However, the performance of the III-Nitride devices on silicon substrate has been limited by the material quality due to the lack of an ideal substrate.

This thesis seeks to address the material quality issues by providing an alternative solution, the silicon-on-insulator (SOI) platform. The demonstration of III-Nitride devices on large area 6-inch (111)-oriented SOI substrates, namely InGaN/GaN-based light-emitting diodes (LEDs) and $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based photodetectors (PDs) are also reported for the first time. Structural characterization carried out with high resolution X-ray diffraction (HRXRD) and micro-Raman spectroscopy shows nearly stress-free epilayers and equivalent crystalline quality for the III-Nitride structures grown on SOI(111) substrates as compared to structures grown on bulk Si(111) substrates. The thicknesses of the respective epilayers on such engineered substrates were determined from cross-sectional transmission electron microscopy (XTEM). The improvements in device performance brought about by the utilization of such engineered substrates were studied in relation to the optical and electrical properties.

For the InGaN/GaN-based LED structures on SOI(111) substrates, an enhancement in the electroluminescence integrated intensity was brought about by the Fabry-Perot effects. Efficient emission in the green-gap spectral

range were also achieved due to the lower surface temperature of the SOI wafer which led to high In content in the multi-quantum wells. The small spectral shift in the EL peak at high currents demonstrated devices that are beneficial for wavelength stabilization. Additionally, an enhancement in the light extraction was observed with the incorporation of photonic crystals.

For the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ structures grown on SOI(111) substrates for UV PDs, the Al content in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer was found to be ~29% with HRXRD, TEM and micro-photoluminescence techniques. The dislocation densities were found to be in the range of $1.2 \times 10^9 \text{ cm}^{-2}$ to $5.2 \times 10^9 \text{ cm}^{-2}$ from HRXRD, along with hot H_3PO_4 etching followed by atomic force microscopy studies. Voltage-dependent Raman measurements with 325 nm excitation show optical phonon modes at 608, 702 and 720 cm^{-1} which were attributed to be an interface mode, a disordered activated phonon mode, and the $\text{A}_1(\text{LO})$ phonon mode of GaN which is shifted due to the screening effects of the two-dimensional electron gas (2DEG), respectively. Despite a low photocurrent-to-dark current contrast ratio of 3 (5V, 325 nm illumination), strong detector responsivity varying from 1500 A/W (-3V) to 7800 A/W (-5V) at 250 nm illumination was observed. Moreover, photocurrent was detectable even at very low excitation intensity of 0.1 mW/cm^2 at 325 nm.

In summary, III-Nitride devices on large area 6-inch (111)-oriented SOI substrates were demonstrated. With the benefits offered by the SOI substrate together with combination of PhCs, bright electroluminescent InGaN/GaN-based LEDs could be realized. The high sensitivity observed from the 2DEG AlGaN/GaN-based heterostructures in the UV spectral range shows that such PDs could be useful for highly sensitivity photo sensors.

CHAPTER 1

Introduction

As of today, the semiconductor market has been dominated by the silicon (Si) material, with its well-established complementary metal-oxide-semiconductor (CMOS) process. Almost all integrated circuits and chips are built with Si as the base material. However, specific applications such as optoelectronics, radio-frequency (RF) and high power electronics required material properties that cannot be offered by silicon. An equally important semiconductor market is the compound semiconductor industries [1-2]. The III-V materials that are based on GaAs, AlAs, GaP, InP and its related materials have addressed the applications but have limitations in high power, high frequency, high temperature and short wavelength optical devices . In contrast, the III-Nitride materials are of great interest for such applications [3]. The (Al, Ga, In)N-based material system are direct bandgap semiconductors with bandgap ranging from 0.7 eV (InN) to 3.4 eV (GaN) and 6.2 eV (AlN) and forms a continuous solid solution across the alloy system [4-5]. This material property allows bandgap to be engineered for short wavelength optical devices targeting applications in the visible to deep ultraviolet (UV) wavelength spectral regions [6]. Besides their superior optical properties, the III-Nitride materials also show good thermal conductivity, high breakdown electric fields, high maximum electron velocities, high electron mobility and high sheet carrier concentration at heterojunction interfaces which make them well-suited for high power and high temperature applications [7-8]. In

summary, the III-Nitride material system finds applications in many optoelectronic and power electronic devices and is of utmost importance to address the performance gaps in current silicon and conventional III-V compound semiconductors. As such, the III-Nitride material system forms the main basis of this thesis.

1.1 Background and Motivation

Extensive research efforts globally have been devoted to obtaining high quality Gallium Nitride (GaN) and related nitrides because of their promising applications in many optoelectronic and microelectronic devices such as blue lasers [9], blue-green, UV light emitting diodes (LEDs) [10], UV photodetectors (PDs) [11], heterostructure field effect transistors (HFETs) [12] and high electron mobility transistors (HEMTs) [13]. However, the performance of these devices has been limited by the material quality due to the lack of an ideal substrate. Presently, these devices are commonly grown on sapphire and silicon carbide (SiC) substrates. However, for the realization of large scale wafer processing, these substrates pose some disadvantages such as higher costs, wafer bowing issues and limited size. A cost effective solution will be to use Si substrates for the nitrides growth. The availability of Si substrates in large diameters at a relatively low cost ($\sim 1/10$ of sapphire, $< 1/100$ of SiC) [14] makes scale-up possible. In addition, the higher thermal and electrical conductivity also makes Si a better substrate compared to insulating sapphire [15]. With the use of suitable buffers, interlayer and substrate engineering, the growth of high quality and crack-free GaN epilayers on Si substrates has been recently reported [16-30]. Despite these advantages,

Si poses the same disadvantages as sapphire and SiC, that is, high lattice and thermal mismatch to GaN [31-32]. Table 1.1 summaries the material properties of GaN, AlN, Si, SiC and sapphire. The large differences in lattice constants, crystal structure, and thermal expansion coefficients between GaN and silicon led to tensile stress, resulting in cracking and high density of misfit and threading dislocations (TDs). Several research groups have also reported on the growth of GaN on bulk GaN native substrates as it is believed that this is the ultimate solution to achieving high performance devices [33-34]. With the use of bulk GaN native substrates, the problems of heteroepitaxy of GaN on foreign substrates can be overcome. Furthermore, growth process can be simplified since the use of buffer layers, interlayer or epitaxial lateral overgrown techniques can be avoided. However, the development of growth of GaN on bulk GaN native substrates is still at an early stage and the cost of commercial available GaN native substrates is still very high [35]. Alternatively, a low cost approach exists which is to use compliant substrates such as the silicon-on-insulator (SOI) substrate for the growth of high quality and crack-free GaN epilayers [32, 36-40]. With the use of SOI substrates for the growth of GaN layers, strain can be released and absorbed in the thin Si overlayer of the SOI substrate according to the compliant substrate principle [41-43]. This leads to improvement in the material, structural, optical and electrical properties and thus, devices built on such layers would be able to take full advantage of the intrinsic properties of III nitrides. In addition, the availability of large size SOI substrates up to 12 inch makes scale-up possible. The growth of GaN on SOI substrates is also promising from the viewpoint of integration with current SOI photonics, micro-opto-electromechanical systems

(MOEMS) and sensors [44-46]. In this thesis, the growth and fabrication of GaN and related devices on the SOI substrate have been explored. The thesis also presents a detailed study of these devices for their applicability in light emitters and UV sensors.

Table 1.1: Material properties of GaN, AlN, Si, SiC and sapphire. [32]

Material	a (Å)	c (Å)	Thermal conductivity (W/cmK)	Thermal expansion coefficient in-plane ($10^{-6}/K$)	Lattice mismatch between GaN & substrate (%)	Thermal mismatch between GaN & substrate (%)
GaN	3.189	5.185	1.3	5.59	-	-
AlN	3.11	4.98	2.85	4.2	2.4	25
Si(111)	5.430	-	1-1.5	2.59	-16.9	54
6H-SiC	3.080	15.12	3.0-3.8	4.2	3.5	25
sapphire	4.758	12.991	0.5	7.5	16	-34

1.2 Research objectives and scope

To demonstrate the feasibility of the SOI substrate for GaN and related devices, material study of InGaN/GaN-based LED structures on SOI substrate and $Al_xGa_{1-x}N$ /GaN-based heterostructures on SOI substrate for UV PDs has been investigated. The drive for the use of the SOI substrates for the growth of InGaN/GaN-based LED structures and $Al_xGa_{1-x}N$ /GaN-based PD structures are summarized as follows:

1.2.1 InGaN/GaN-based LED structures on SOI substrates

In the context of InGaN/GaN-based LEDs when Si is used as the substrate, a significant amount of blue and green light emitted from the active layers of the multi-quantum wells (MQWs) is absorbed in the Si substrate

[38,47], leading to a decrease in the light extraction efficiency. Therefore, additional processing steps such as the removal of the Si substrate become essential in order to achieve high brightness LEDs. In contrast, when SOI is used as the substrate, absorption of visible light from LEDs is much lower on very thin SOI due to the Fabry-Perot effects arising as a result of the high refractive index contrast at the AlN/Si/SiO₂/Si substrate-interfaces [48], leading to an increase in the light extraction efficiency. In addition, the Si/SiO₂ interface also acts as a back-side reflector such that light emanating from the active region can be reflected back and escape from the semiconductor through the top surface [47], increasing the light extraction efficiency even further. Since strain can be released and absorbed in the thin Si overlayer according to the compliant substrate principle [41-43], a reduction in the dislocations will lead to improved material quality and hence, an improvement in the device performance.

Conventional InGaN/GaN-based LEDs suffered from poor light extraction efficiency due to the total internal refraction (TIR) of the generated light in the active region, at the LEDs surfaces (GaN/air interface) [49-51]. Due to the large differences in the refractive index (n) between GaN ($n_{GaN} = 2.5$) and air ($n_{air} = 1$), the critical angle [$\theta_c = \sin^{-1}(n_{air}/n_{GaN})$] for the light generated in the active region to escape is about 23°, leading to a low extraction efficiency of about 4% ($1/4 n^2$) per surface. Light extraction efficiency can be further improved when there is surface roughening of the top LED surface [49-51], geometrical shaping of the LED die [52-54], utilization of the flip-chip approach [55-57], patterning of the substrate [58-60], or incorporation of photonic crystal (PhC) structure [61-70]. Among these

methods, the incorporation of PhC structure proves to be the best method [65]. With PhCs, the photons generated within the active region are able to escape by multi-scattering from rough surfaces, thus enabling a more effective out coupling of visible light in PhC-structured LEDs. Hence, in this thesis, the PhCs technique is used for light extraction enhancement in the LEDs on SOI substrates. With the combination of the benefits offered by the SOI substrate and the incorporation of PhCs on the LED surfaces, an increase in the light extraction efficiency is expected.

In order to study the influence of the SOI substrate on LEDs performance, structural characterization of as-grown InGaN/GaN-based LED structures on SOI substrates as well as fabrication of the LED devices were carried out. Techniques such as high resolution X-ray diffraction (HRXRD) and Micro-Raman spectroscopy were used for material characterization, and cross-sectional transmission electron microscopy (XTEM) for the determination of the thickness of respective layers. In order to check on device characteristics, LED devices were fabricated by multiple-mask photolithography, inductively coupled plasma (ICP) etching, p- and n- contact metallization and annealing of the p- and n- contacts. Following these, device characterization was carried out with micro-electroluminescence (EL) measurements. For comparative studies, InGaN/GaN-based LED structures on were also grown on bulk Si substrates and LEDs were fabricated. Additionally, light extraction studies with the incorporation of PhCs on LEDs on SOI substrates were discussed. Different 2-dimensional (2D) PhCs patterns were created by electron beam lithography (EBL) and transferred onto the surface of the LEDs via ICP etching. The morphology of the ICP-etched PhCs

on the LED surfaces were investigated by performing plane-view and cross-sectional imaging with a field emission secondary electron microscope (FESEM). For light emission studies, micro-photoluminescence (PL) measurements were performed. It is well known that PL is not equivalent to EL. That is, a wafer with high PL efficiency may or may not exhibit high EL efficiency and hence good LEDs. Hence, in order to demonstrate electrically simulated light emission from PhC-patterned LEDs, full LED device processing has been carried out. After which, the micro-EL spectra were recorded from LEDs with and without PhC structures as a function of different injection currents.

1.2.2 $Al_xGa_{1-x}N/GaN$ -based heterostructures on SOI substrate for UV PDs

UV PDs based on wide bandgap III-nitride semiconductors have been extensively studied and various types of detector structures have been demonstrated. The different types of detector structures included photoconductors [71-72], Schottky barrier PDs [73-74], p-i-n PDs [75-76], avalanche PDs [77-78], and Schottky metal-semiconductor-metal (MSM) PDs [79-85]. Among them, Schottky MSM PDs offered specific advantages over the rest in terms of easier growth and fabrication simplicity [79-85]. Schottky MSM PDs are based on two rectifying contacts connected back-to-back and the fabrication of such devices involved the deposition of two interdigitated Schottky metal contacts on top of the active layer. Light is received at the gap between the interdigitated Schottky metal contacts which get absorbed in the semiconductor. Since the contacts are of a Schottky nature, the growth of the epilayers for such devices do not require p-type or n-type doping to form p+

and n+ layers for ohmic contacts formation as in photoconductors, Schottky barrier PDs, p-i-n PDs and avalanche PDs, as high resistive and unintentionally doped layers can be used as the device layer structure which simplified the growth process. In addition, the planar configuration of Schottky MSM PDs enabled such devices to be used in optoelectronic-integrated-circuits (OEICs) due to its ease of integration and compatibility with FET process technologies. The lateral, planar structure of Schottky MSM PDs also resulted in extremely low capacitances, which matched well with the requirements of large bandwidth and low-noise performance. In terms of device performance, Schottky MSM PD offered a large active area that enabled high operation speed (high bandwidth), high response speed, low dark current (high dark current in photoconductors) and superior responsivity to be achieved [79-85].

In order to extend detection to deep UV spectral range, wide direct bandgap $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ternary alloy with a bandgap energy that can be tuned from 6.2 eV to 3.4 eV, corresponding to a photon wavelength range of 200 nm (at $x = 1$, absorption edge of AlN) to 365 nm (at $x = 0$, absorption edge of GaN), is the most promising material system [86]. This tunability of the detection edge by varying the Al concentration makes detectors fabricated from $\text{Al}_x\text{Ga}_{1-x}\text{N}$ materials intrinsically blind to photons with energies higher than that of the bandgap of the active layer. In addition, when the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ternary alloy is coupled to the GaN material, a two dimensional electron gas (2DEG) is formed due to the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface and the existence of polarization effects in the (0001) direction. When $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based Schottky MSM PDs are fabricated, the electric field distribution below the

electrodes is modified due to the presence of the 2DEG in the layer structure. As a result of this vertical electric field, photogenerated electrons will be compelled to move towards the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface while photogenerated holes will be repelled towards the substrate, which reduces the probability of recombination of the photogenerated carriers leading to an improved detector responsivity [87-88]. It was reported that when ohmic contacts are used as electrodes, dark current was high as a result of the polarization fields due to the high density of 2DEG at the interface [89]. Thus, to reduce the dark current, Schottky contacts were used and it has been reported that the use of a GaN capping layer also helped in reducing the dark current [90]. Hence, in this thesis, Schottky MSM PD detector structure is fabricated on an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructure to take advantage of the various benefits offered by the Schottky MSM PD detector structure and the 2DEG in an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructure. With improved material quality provided by the use of the SOI substrate for the growth of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based PDs according to the compliant substrate principle, such 2DEG-based $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ MSM UV PDs on low cost silicon-based platform with low dark current and fast response, may lead to widespread applications due to the compatible device processing with FETs. The demonstration of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures as UV PDs on a SOI-based platform is desirable for the integration with current SOI photonics and MOEMS.

In order to study the influence of the 2DEG and SOI substrate on PDs performance, structural characterization of as-grown $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures on SOI substrates as well as fabrication of the MSM PDs

were carried out. Techniques such as HRXRD were used for material characterization and XTEM for the determination of the thickness of respective layers. The Al content in the AlGaN layer was determined using a combination of techniques, namely, HRXRD, TEM and micro-PL. Since dislocation densities will affect the electrical and optical properties of the material, the determination of the dislocation densities was carried out using HRXRD and hot phosphoric acid (H_3PO_4) etching followed by atomic-force microscopy (AFM) studies. To understand the 2DEG interface vibrational properties, UV micro-Raman spectroscopy was used to probe the as-grown layer structure as well as MSM PDs under electrical simulation.

To demonstrate the applicability of the thin AlGaN layer grown on GaN template for UV detection, device processing of the Schottky MSM PDs were carried out by photolithography and contact metallization. Device characterization was carried out by performing current-voltage (I - V) under dark and illumination conditions and spectral response measurements. The I - V characteristics of the devices under illumination are correlated to the responsivity results.

1.3 Thesis organization

Chapter 1 gives a brief introduction on the importance of the III-Nitrides material system followed by the background and motivation of this thesis. The research objectives and scope of the thesis work are also defined in this chapter.

Chapter 2 gives an overview of the growth challenges of the GaN-on-Si approach and the methods used to overcome them. The GaN-on-SOI

approach, which is the approach used in this thesis, is discussed in more detail. To address the need for improvement in light extraction efficiency in LEDs, a brief literature review of the different light extraction methods employed to enhance light extraction is presented. An introduction on the operation of MSM and 2DEG-MSM PD followed by the layer structure required to achieve the formation of the 2DEG and the advantages of using the 2DEG layer structure is also discussed.

Chapter 3 describes the details of the experimental techniques used to achieve GaN-on-SOI devices. The details of the epitaxial layers of the as-grown heterostructures are presented. The materials characterization techniques, device fabrication procedures and device characterization techniques are also presented. Techniques such as HRXRD and Micro-Raman spectroscopy were used to characterize the structural properties of the as-grown heterostructures and the thicknesses of the respective epitaxial layers were determined from XTEM. For the determination of the Al content in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer, a combination of techniques such as HRXRD, TEM and micro-PL was used. For dislocation densities studies, HRXRD and hot H_3PO_4 etching followed by AFM studies were performed. Micro-PL was used for light emission studies. Techniques such as micro-EL, IV and responsivity measurements were used for device characterization.

Chapter 4 presents the experimental results and discussions on the study of InGaN/GaN-based LED structures grown on SOI substrates. The structural properties of the as-grown heterostructures were characterized with HRXRD and Micro-Raman spectroscopy. The thicknesses of the respective epitaxial layers of the as-grown heterostructures were determined from XTEM.

In order to check on device characteristics, LED devices were fabricated by multiple-mask photolithography, ICP etching, p- and n- contact metallization and annealing of the p- and n- contacts. Following these, device characterization was carried out with micro-EL measurements. For comparative studies, InGaN/GaN-based LED structures were also grown on bulk Si substrates and LEDs were fabricated. Additionally, light extraction studies with the incorporation of PhCs on LEDs on SOI substrates are discussed. Different 2D PhCs patterns were created by EBL and transferred onto the surface of the LEDs via ICP etching. FESEM was used for the plane-view and cross-sectional imaging of the morphology of the ICP-etched PhCs on the LED surfaces. For light emission studies, micro-PL measurements were performed. In order to demonstrate electrically simulated light emission from PhC-patterned LEDs, fabrication of LEDs with PhCs was carried out and micro-EL spectra as a function of different injection currents were recorded from the devices.

Chapter 5 presents the experimental results and discussions on the study of the applicability of the thin AlGaN layer grown on GaN template for UV detection. The thicknesses of the respective epitaxial layers of the as-grown heterostructures were determined from XTEM and the structural properties of the as-grown heterostructures were characterized with HRXRD. The Al content in the AlGaN layer was determined using a combination of techniques, namely, HRXRD, TEM and micro-PL. Since dislocation densities will affect the electrical and optical properties of the material, the determination of the dislocation densities were carried out using HRXRD and hot H_3PO_4 etching followed by AFM studies. To understand the 2DEG

interface vibrational properties, UV micro-Raman spectroscopy was used to probe the as-grown layer structure as well as MSM PDs under electrical simulation. Device processing of the Schottky MSM PDs were carried out by photolithography and contact metallization to demonstrate the applicability of the thin AlGa_N layer grown on GaN template for UV detection. Device characterization was carried out by performing I - V under dark and illumination conditions and spectral response measurements. The I - V characteristics of the devices under illumination are correlated to the responsivity results.

Chapter 6 presents the summary of the experimental results and concluding remarks.

Chapter 7 presents the recommendations for future work.

CHAPTER 2

Literature Review

This chapter is divided into three sections. The growth of GaN via two approaches: the GaN-on-Si and GaN-on-SOI approach are discussed in section one. An overview of the growth challenges of the GaN-on-Si approach and the methods used to overcome them are discussed. The GaN-on-SOI approach, which is the approach used in this thesis, is discussed in more detail. To address the need for improvement in light extraction efficiency in LEDs, a brief literature review of the different light extraction methods employed to enhance light extraction is presented in section two. In the last section, an introduction on the operation of MSM and 2DEG-MSM PD followed by the layer structure required to achieve the formation of the 2DEG and the advantages of using the 2DEG layer structure are discussed.

2.1 Growth of GaN

2.1.1 GaN-on-Silicon – the different approaches

In summary, the growth of GaN on Si substrates suffers from 3 main problems [32,36]. The high lattice mismatch between GaN and Si (~17%) which leads to high dislocation densities in the GaN layer; the high thermal mismatch between GaN and Si (~54%) which leads to cracking at thickness below the desired device layer thickness; and the meltback etching effect which is induced by surface nitridation (formation of Si_xN_y) as a result of the strong chemical reactivity of GaN and Si at elevated temperatures which leads

to a destruction of the layers and substrate. Despite these problems, the growth of high quality and crack-free GaN epilayers on Si substrates has been reported with the use of suitable buffers, interlayer and substrate engineering. Some of the buffer layers schemes that have been investigated include AlN, AlAs, GaAs, SiC, Al(Ga)N/GaN superlattices, or even a combination of them [16-27]. The purpose of the buffer layer is to accommodate most of the dislocations generated as a result of the lattice mismatch such that the propagation of the dislocations into the active layer is prohibited. From the work reported by various authors, it seems that different buffer layer schemes had their own benefits (some are chosen and summarized in Table 2.1) and are not directly comparable due to different buffer layer thickness, different buffer layer combination and the different growth parameters used.

Among the various buffer schemes, the AlN buffer layer is the most widely studied and high quality GaN film has been successfully grown on Si(111) substrates using the AlN buffer layer [91-93]. The growth of the GaN film is strongly dependent on the growth conditions of the AlN buffer which include the growth temperature and the thickness of the AlN buffer layer.

Depending on the growth temperature of the AlN buffer layer, the growth mode of the GaN films can either be two- or three-dimensional (2D or 3D) which will lead to changes in the structural, electronic and optical properties of the GaN layers. In a study carried out by Lu et al [94], it was found that the optimum growth temperature of the AlN buffer lay within a narrow window of several tens of degrees. When the temperature was lower than the minimum temperature required, a complete coalescence of the AlN islands nucleating on the Si substrate did not take place leaving holes on the Si

surfaces which were not covered by the AlN islands. As a consequence, surface nitridation took place when the growth of GaN film initiated leading to the formation of the Si_xN_y films which deteriorated the quality of GaN films. Therefore, in order to obtain high quality GaN films, the growth temperature of the AlN buffer must be carefully controlled to be within the narrow window.

An optimum thickness of the AlN buffer existed such that two-dimensional growth of the AlN buffer took place to cover the Si substrate completely in order to prevent the formation of the Si_xN_y films [95]. When the AlN buffer was thinner than the optimum value, 2D growth did not take place because islands nucleating on Si substrate have not completely coalesced leaving some of the Si substrate not covered by the AlN islands. When the growth of GaN film initiates, surface nitridation took place which led to the formation of the Si_xN_y films and deteriorated the quality of GaN films.

Table 2.1: Benefits offered by the different buffer layer scheme.

Buffer layer	Advantages	Ref.
AlN	<ul style="list-style-type: none"> • Small lattice mismatch to GaN (~2.5%) • No meltback etching effect due to good wetting properties and high Al-N bonding energy (no rearrangement of the AlN layers) 	[23,94-97]
AlAs	<ul style="list-style-type: none"> • Thermally stable even at high temperature (~1050°C) as compared to GaN or AlN buffer layers, preventing the formation of Si_xN_y, that is, no meltback etching effect 	[19]

SiC	<ul style="list-style-type: none"> • Small lattice mismatch to GaN (~3%) • 3C-SiC(111) surface formed has the same atom arrangement as 6H-SiC(0001) plane which is the common plane for GaN growth on SiC substrates, enabling the growth of high quality GaN layers • No meltback etching effect due to formation of 3C-SiC(111) surface by the conversion of Si to 3C-SiC by carbonization at high temperatures • Good wetting properties between Ga and SiC(111) leads to 2D growth 	[20,98-99]
AlGaN/AlN	<ul style="list-style-type: none"> • No meltback etching effect due to high thermal stability of AlGaN and AlN • To enhance the series resistance and compressive stress 	[18,23,32,]
Al(Ga)N/GaN Superlattices	<ul style="list-style-type: none"> • At the interfaces of superlattices, dislocations tend to bend, increasing the probability of recombination and annihilation with other dislocations with opposite burgers vector. As a result, the dislocation densities reduced. • Compressive stress induced by such superlattices compensate for the tensile stress built-up in the GaN layers during growth on Si(111) substrate reduces cracking 	[21,32]

Other than buffer layers, the introduction of interlayers at regular intervals during the growth of the GaN layer as stress migration layers was also investigated by various authors with the more successful ones being the

Si_xN_y [27,100] and AlN interlayer [26,101-102]. The thickness of the Si_xN_y interlayer is usually in the range of one to few monolayers while the thickness of the AlN interlayer is usually in the range of 10 – 20 nm. The insertion of Si_xN_y interlayer in the GaN layer led to the formation of a nanoporous Si_xN_y network, changing the growth mode of GaN from 2D to 3D or island growth. This island growth led to the bending and annihilation of dislocations enabling a smooth layer to be achieved after a certain GaN thickness when growth returns to 2D mode [32, 100]. For the AlN interlayer, it was reported that the deposition temperature of the AlN interlayer is a very important parameter for the control of the interlayer to act as a stress compensating layer as shown in Figure 2.1. When the AlN interlayer is deposited at high temperatures, the AlN interlayer grows pseudomorphically on GaN such that the subsequent growth of GaN layer on top of the AlN interlayer is fully strained. That is, the subsequent GaN layer has the same lattice parameter a as the AlN interlayer. In contrast, when the AlN interlayer is deposited at low temperatures, the coherence of the layers is destroyed and the AlN interlayer behaved like a seed layer. As a result of the smaller lattice constant of the AlN, the subsequent GaN layer grown on top of this AlN interlayer is compressively stressed and able to counteract the tensile stress build up during the GaN growth [26].

Figure 2.1: Average tensile stress of 1.3 mm thick GaN layers on Si(111) substrates at room temperature as determined from the a -lattice constant by HRXRD measurements. One LT-AlN interlayer was introduced at different deposition temperatures after 500 nm of GaN was grown [26].

While the buffer layers and the interlayers approach is an in-situ process, the substrate engineering approach is mostly an ex-situ process like patterning of the substrate by masking or by etching trenches followed by a lateral overgrowth process [28-29], ion-implantation of the substrate to create an amorphous surface prior to growth [30], or the use of compliant substrates such as SOI [39-40]. By patterning the substrate prior to growth, the tensile stress built-up in the GaN layer can be confined to small-area films defined by the patterns and crack-free films can be grown in the patterned areas [103-104], as shown in the schematic in Figure 2.2.

Figure 2.2: Schematic of substrate masking and guiding cracks in masked areas (top). Due to the high tensile stress (bottom) cracks preferentially form in the masked regions and thus only in the Si substrate leading to a partial reduction of strain in the GaN layer for small masked regions. “C” denotes compressively strained regions, “T” tensily strained regions [32].

The mechanism for the reduction of tensile stress built-up in the GaN layers during subsequent growth by performing ion-implantation of the substrate is the same as the strain relieving mechanism provided by the compliant substrates [105]. The idea is to create a defective or amorphous layer below the substrate surface such that the subsequent growth layer is separated from the bulk substrate crystallographically. Thus, through this rearrangement process of the AlN islands on the disordered layer, a higher quality of GaN is obtained upon regrowth [32]. The main purpose of these approaches is strain management to relieve the tensile stress built-up in the

GaN layer during growth to reduce cracking, as well as to reduce the dislocation density. Another substrate engineering approach, which is the compliant substrate approach and also the approach used in this thesis, will be discussed next.

2.1.2 GaN-on-SOI – the compliant substrate approach

The main obstacles towards the integration of dissimilar materials are the lattice and thermal mismatches between such materials. As a result, devices built on such layers are unable to take full advantage of the intrinsic properties of such materials, inhibiting the optimum performance of devices to be achieved. In order to solve these problems, schemes such as the introduction of buffer layers, interlayers and substrate engineering has been proposed and investigated by various material scientists and engineers all over the world. The compliant substrate approach which is discussed in more detail is also one of the substrate engineering approaches.

In conventional epitaxial growth between lattice-mismatched materials where the substrate is much thicker than the epilayer, all the strain resides in the grown epilayer. Figure 2.3 illustrates the differences between an ideal and non-ideal growth of lattice-mismatched materials.

Figure 2.3: (a) Schematic of ideal lattice-mismatched growth where strain is relieved as edge dislocations; and (b) non-ideal case where strain is relieved as edge and threading dislocations [40].

In order for an ideal lattice-mismatched growth to take place, two conditions need to be met which are (i) growth proceeds layer-by-layer such that there is only a single island which is 1 monolayer high on the substrate at any point of substrate coverage; (ii) growth rate is slow enough such that the layer is able to reach its minimum energy state. If these two conditions are met, growth is accompanied by strain relief through edge dislocations formed at the

epilayer-substrate interface and the layer grows as a free-standing unstrained layer, that is, the layer has the same lattice constant as the bulk substrate. In non-ideal lattice-mismatched growth which is the more realistic situation, growth proceeds by nucleation of several islands occurring at the same time instead of single island growth as in an ideal growth situation. In addition, accumulation of strain energy at the edge dislocation sites as a result of the lattice mismatch leads to the destabilization of chemical bonds and atoms are unable to stack perfectly. As a result, TDs are formed in addition to edge dislocations. These TDs which are formed at the epilayer-substrate interface and propagate through the epilayer are highly detrimental to device performance.

In the compliant substrate (SOI) approach, the substrate [Si(111) thin overlay] is much thinner than the epilayer (GaN) and thus, strain in the lattice-mismatched epilayer (GaN) can be reduced via partial accommodation of the total strain in the substrate [Si(111) thin overlay] so that the total energy is reduced. A schematic of the compliant substrate (SOI) used for the growth of the lattice-mismatched epilayer (GaN) is shown in Figure 2.4.

Figure 2.4: Schematic of the compliant substrate (SOI) / GaN layer structure.

In order for equilibrium to be attained in the material system, the net force on the material system must be zero. That is,

$$\sigma_f h_f - \sigma_s h_s = 0 \quad (2.1)$$

where σ_f is the biaxial stress in the film, σ_s is the biaxial stress in the substrate, h_f is the thickness of the epilayer, and h_s is the thickness of the substrate.

The strain that is produced during the growth is distributed between the substrate and the lattice-mismatched epilayer according to the following relation:

$$\epsilon_0 \equiv \epsilon_s + \epsilon_f = \frac{a_s - a_f}{a_f} \quad (2.2)$$

$$\epsilon_s = -\epsilon_0 \frac{h_f}{h_s + h_f}, \epsilon_f = \epsilon_0 \frac{h_s}{h_s + h_f}, h_s \ll h_f \quad (2.3)$$

where ϵ_0 is the total strain of the system due to the lattice mismatch, ϵ_s is the biaxial strain in the substrate, ϵ_f is the biaxial strain in the film, a_s is the in-plane lattice constant of the substrate and a_f is the in-plane lattice constant of the epilayer.

Neglecting the bending stresses, the strain energy per unit area in the system can be represented as:

$$E = K\epsilon_0 \left(\frac{h_f h_s}{h_f + h_s} \right) \quad (2.4)$$

where K is the elastic constant of the system.

Misfit dislocations will be generated when the strain energy in the system reached the critical energy, E_c . By defining h_f as the effective critical thickness t_{eff} when the strain energy in the system reaches E_c , the dependence of the t_{eff} on h_s is:

$$\frac{1}{t_{\text{eff}}} = \frac{1}{t_c} - \frac{1}{h_s} \quad (2.5)$$

The plot on the dependence of the effective critical thickness on the substrate thickness is shown in Figure 2.5.

Figure 2.5: Dependence of effective critical thickness on the substrate thickness. Both axes are normalized to the critical thickness for infinitely thick substrate [41].

From the plot, if the substrate is thinner than the conventional critical thickness, then the effective critical thickness is infinite. Thus, infinitely thick structures can be grown on top of the thin substrate without the generation of misfit dislocations.

Apart from misfit dislocations, the generation of TDs at the epilayer-substrate interface which propagated through the epilayer is another critical problem for device performance. In conventional epitaxial growth where the substrate is much thicker than the epilayer, an image force [106] existed which pulled the misfit dislocations situated at the interface towards the surface of

the epilayer. As a result of this image force, misfit dislocations tended to move to the surface by climbing or slipping [106] and led to the generation of TDs which are detrimental to device performance. In the compliant substrate approach where the substrate is much thinner than the epilayer, the image force will pull the misfit dislocations situated at the interface away from the epilayer and into the thin substrate; an effect known as dislocation gettering. Therefore, with the proper design of the compliant substrate ($h_s < t_c$), infinitely thick structures can be grown on such substrates.

2.2 *Light extraction methods*

The LED efficiency can be improved by (i) improving the internal quantum efficiency (η_i) which is related to the crystal quality of the epitaxial layers, and (ii) improving the external quantum efficiency (η_{ext}) which is related to chip processing, die geometry and LED packaging. The external quantum efficiency is the key performance indicator for high efficiency LEDs and is defined as the number of photons generated per injected electron. The external quantum efficiency is related to the internal quantum efficiency and light extraction efficiency (η_{extr}) in the following manner [51,107]:

$$\eta_{ext} = \eta_i \times \eta_{extr} \quad (2.6)$$

where η_i is defined as the number of photons generated from radiative recombination of injected electron-hole pairs in the active region and η_{extr} is defined as the number of photons generated in the active region that escape from the device.

Approaches such as the use of suitable buffers, interlayer and substrate engineering discussed earlier are some methods which can be used to improve

the crystal quality and hence, the internal quantum efficiency. In this thesis, the compliant substrate approach is used to improve the internal quantum efficiency. However, even if the internal quantum efficiency of LEDs were to reach ~100%, the external quantum efficiency of conventional LEDs is still limited to a few percent due to the TIR of the emitted light at the LEDs surfaces. For conventional InGaN/GaN-based LEDs, the critical angle $[\theta_c = \sin^{-1}(n_{air}/n_{GaN})]$ for the light generated in the active region to escape is about 23° , leading to a low extraction efficiency of about 4% ($1/4n^2$) per surface. Thus, in order to improve the external quantum efficiency, the light extraction efficiency needs to improve first.

To address the need for improvement in light extraction efficiency, various light extraction methods have been investigated and demonstrated by researchers globally. The methods that have been investigated include surface roughening of the top LED surface [49-51], geometrical shaping of the LED die [52-54], utilization of the flip-chip approach [55-57], patterning of the substrate [58-60], or incorporation of PhC [61-70]. Among these methods, the incorporation of PhC structure proves to be the best method [65]. Therefore, in this thesis, the PhC approach is used as the light enhancement approach together with the compliant substrate approach for the growth of InGaN/GaN-heterostructures for LEDs. An increase in the light extraction efficiency is expected with the combination of the benefits offered by the SOI substrate and the incorporation of PhCs on the LED surfaces. Nevertheless, a short overview of the different light extraction methods will be given in this section.

2.2.1 Surface roughening of the top LED surface

The light emission from the active region of a conventional LED is directionally isotropic and thus, light is only able to escape from the LED if the angle of incidence to the chip wall is less than the critical angle [49]. Figure 2.6 shows the possible photon paths inside the structures of a conventional LED with and without surface roughening. With surface roughening of the top LED surface, TIR of the emitted light is reduced and the scattering of photons emitted in the active layer was much enhanced due to the angular randomization of photons inside the LED structure. Thus, a roughened surface structure can help to improve the probability of the photons escaping from the LED, which will lead to an improvement in the light-out power [49].

Figure 2.6: Possible photon paths inside the structures of (a) conventional LED and (b) LED with a roughened top surface [108].

Some reported methods to create the surface roughening of the top LED surface include wet etching or dry etching process with different materials [eg. Pt or Ni metal clusters, ITO] serving as the etch mask [49,108-113]. Table 2.2 shows a comparison between the output power @ 20 mA of LEDs with and without surface roughening of the top surface extracted from literature.

Table 2.2: A comparison between the output power @ 20 mA of LEDs with and without surface roughening of the top surface extracted from literature.

Without surface roughening	With surface roughening	% increase in output power	Ref.
0.05mW	0.075mW	52.0	49
4.5mW	6.3mW	40.0	109
5.3mW	8.3mW	55.0	110
6.1mW	7.1mW	16.0	111
9.1mW	7mW	30.0	112
11.7mW	13.3mW	12.0	113

From the results shown in Table 2.2, an enhancement in the output power is indeed observed with surface roughening of the top p-GaN surface. The enhancement was due to a lower forward voltage (V_f) and series resistance obtained with surface roughening. However, this method provides little control over how the roughened surface extracts the light out of the LED chip [56]. In addition, as the p-GaN layer in conventional LEDs is very thin, a tight control of the etching process and etch depth is required so as not to destroy the p-n junction or cause any plasma damage to the p-GaN layer such that the electrical properties are deteriorated [112-113].

2.2.2 Geometrical shaping of the LED die

The mechanism of light extraction enhancement with geometrical shaping of the LED die works by reducing the range of incident angle (θ_i) for TIR to occur inside the chip [114-115]. In a study carried out by Wang et al [54], the conventional LED with a rectangular shape was the most inefficient geometrical shape for light extraction among the various polygons investigated. On the other hand, the triangular shape was the most efficient geometrical shape for light extraction.

An illustration of the light paths inside a conventional rectangular LED chip and a triangular LED chip is shown in Figure 2.7(a) and (b), respectively.

Figure 2.7: Light paths inside a (a) conventional rectangular LED and (b) triangular LED. θ_i is the incident angle of the photon emitted from the point-like light source (P) and θ_r is the incident angle of the photon reflected from the 2nd sidewall back to the 1st sidewall. For conventional InGaN/GaN-based LEDs, the light escape cone critical angle [$\theta_c = \sin^{-1}(n_{air}/n_{GaN})$] for the light generated in the active region to escape is about 23.5° [114].

In the conventional rectangular LED, photons will be able to escape from the LED if $\theta_i < \theta_c$ and reflected back at the 1st sidewall $\theta_i > \theta_c$. For the case where $\theta_i > \theta_c$, another incident angle $\theta_r = 90^\circ - \theta_i$ will be created at

the second sidewall as shown in the Figure 2.7(a). If $\theta_r > \theta_c$, TIR will take place and the photons will be trapped inside the LED chip. Therefore, the range of θ_i for TIR to take place in a conventional rectangular LED is given by:

$$23.5^\circ < \theta_i < 66.5^\circ \quad (2.7)$$

For a triangular LED, photons will be able to escape from the LED if $\theta_i < \theta_c$ and reflected back at the 1st sidewall $\theta_i > \theta_c$. For the case where $\theta_i > \theta_c$, another incident angle $\theta_r = 60^\circ - \theta_i$ will be created at the second sidewall as shown in the Figure 2.7(b). If $\theta_r > \theta_c$, TIR will take place and the photons will be trapped inside the LED chip. Therefore, the range of θ_i for TIR to take place in a triangular LED is given by:

$$23.5^\circ < \theta_i < 36.5^\circ \quad (2.8)$$

From the illustration and calculations shown, the range of θ_i for TIR to take place in a triangular LED is much smaller than that of a conventional rectangular LED. This meant that the probability of photons escaping from the triangular LED is very much enhanced leading to an enhancement in the light extraction as compared to a conventional rectangular LED chip.

Table 2.3 shows a comparison of the output power with and without geometrical shaping of the LED chip @ 20 mA. With geometrical shaping of the LED chip, an enhancement in the output power is observed. However, the standard processing steps associated with conventional rectangular chips which are invariably adopted in most LED commercial products needs to be modified extensively and care has to be taken when dicing the LEDs into the required geometrical shapes to avoid cracking or damage to the chips in order

to get the highest yield. Thus, the practical utility of such method has not been realized due to the cost associated with shaping the chips.

Table 2.3: A comparison of the output power with and without geometrical shaping of the LED chip @ 20 mA.

Type of chip shaping	Without chip shaping	With chip shaping	% increase in output power	Ref.
Pyramid reflector incorporated	-	-	13.9	53
Triangular	8.9mW	13.2mW	48.0	114
Lozenge	23.8mW	21.2mW	12.0	115

2.2.3 The flip-chip approach

In conventional LEDs, light extraction is limited due to the absorbing metal contacts, bonding pads and wire bonds. The major source of absorption comes from the p-ohmic metal contact which is required to facilitate current spreading across the active region area (resistive p-GaN) and covers a majority of the LED surface. Ideally, a thick p-ohmic contact is required to reduce the series resistance and improve current spreading. However, to minimize light absorption, the p-ohmic contact needs to be thin. Hence, a compromise between light extraction and spreading resistance needs to be made, creating a compromised LED design that limits both power conversion efficiency and operation voltage of the LED [55,116].

In a flip-chip LED design, the LED chip is “flipped-over” or inverted compared to conventional LEDs and mounted to a conductive sub-mount. Light is now extracted through the transparent sapphire substrate avoiding

absorption from the metal contacts, bond pads and wire bonds. In addition, the p-ohmic contact which is located at the bottom act as a reflector to direct the light upwards through the transparent sapphire substrate, increasing light extraction. Since now absorption from the metal contacts are avoided, the p-ohmic metal can be thick to reduce series resistance such that better current spreading and lower operating voltage can be achieved. Furthermore, heat generated in a flip chip LED can be removed more quickly and more efficiently due to a shorter thermal path between the p-n junction and the conductive submount as compared to a longer thermal path and thermally resistive sapphire substrate in a conventional LED [55,57].

Figure 2.8: Schematic diagrams of a (a) conventional LED and (b) flip-chip LEDs [117].

A comparison of the output power @ 350 mA, the maximum output intensity and the operating voltage of a conventional LED with a flip-chip

LED is shown in Table 2.4. As expected, a lower operating voltage is observed in the flip-chip LED which is attributed to the better current spreading. Also, the enhancement in the output power is a consequence of the improved light extraction through the transparent sapphire substrate in the flip-chip LED. The injection current at which the maximum output intensity is achieved is related to the heat dissipation. A better heat dissipation will allow the maximum output intensity to saturate at a higher injection current. From the results, the maximum output intensity occurred at a higher injection current for the flip-chip LED. This is due to the better thermal conductivity of the sub-mount used in the flip-chip LEDs compared to the thermally resistive sapphire substrate.

Table 2.4: A comparison of the output power @ 350 mA, the maximum output intensity and the operating voltage of a conventional LED with a flip-chip LED.

	Conventional LED	Flip-chip LED	Ref.
Output power @ 350 mA	185.1 mW	271.8 mW	57
Current which maximum output intensity occur	700 mA	1400 mA	
Operating voltage	3.41 V	3.23 V	
Output power @ 350 mA	185.1 mW	366.2 mW	116
Current which maximum output intensity occur	700 mA	1450 mA	
Operating voltage	3.41 V	3.22 V	

2.2.4 The substrate patterning approach

By patterning the substrate prior to growth, the tensile stress built-up in the GaN layer can be confined to small-area films defined by the patterns and crack-free films can be grown in the patterned areas [103-104]. This led to a decrease in the dislocation densities and hence an improvement in the internal quantum efficiency. In addition, light scattering at the patterned substrate/GaN interface led to an increase in the photon escaping probability and hence, an increase in the light extraction efficiency. The possible photon path for a conventional LED and for patterned substrate LED is shown in Figure 2.9. Since the external quantum efficiency is related to the internal quantum efficiency and light extraction efficiency by the relation: $\eta_{ext} = \eta_i \times \eta_{extr}$, an increase in the external quantum efficiency is expected.

Figure 2.9: The possible photon paths for (a) conventional LED and (b) patterned substrate LED [59].

The substrate patterning approach has attracted much attention and different geometrical shapes of the patterned sapphire have been reported in the literature with the same aim of increasing the light output. A comparison

of the output power @ 20 mA of a conventional LED and patterned substrate LED adopting different geometrical shapes is shown in Table 2.5.

Table 2.5: A comparison of the output power @ 20 mA of a conventional LED and patterned substrate LED adopting different geometrical shapes.

Without substrate patterning	With substrate patterning	% increase in output power	Pattern	Ref.
12.2mW	16.5mW	35		59
5.4mW	6.5mW	20		118
8.6mW	10.4mW	21		119
7.8mW	9mW	15		120
9.3mW	12mW	29		121
4.05mW	5.86mW	44		122

The difference in the enhancement of the light output is attributed to (1) the different growth modes encountered by using different geometrical shapes which led to different dislocation densities reduction and hence different internal quantum efficiency; (2) the inclined angle the patterned surface made with the (0001) c-axis which led to different light scattering pattern and hence different light extraction efficiency.

2.2.5 *The photonic crystals approach*

In LEDs, spontaneous emission that is not extracted from the device leads to losses. Spontaneous emission is the process by which a light source such as an atom undergoes a transition from an excited state to a lower energy state and emits a photon. The rate of spontaneous emission is given by Fermi's golden rule [123] and is determined by the number of optical modes. Therefore, in order to control spontaneous emission, the optical modes must first be manipulated. There are two approaches of manipulating the optical modes using PhCs; (1) the photonic bandgap approach [61,70,124-125], and (2) the diffraction grating approach [62-69,126]. In the photonic bandgap approach, the lattice dimension of the PhC is tuned near a photonic bandgap such that spontaneous emission into guided modes is inhibited. In this case, light extraction is increased since light generated in the bandgap region can only coupled to radiation modes and radiated out of the LED [124]. However, this approach is limited due to strong non-radiative recombinations at room temperature, hindering its use in real devices [127]. In the diffraction grating approach, spontaneous emission into guided modes is allowed and these modes are subsequently diffracted into air by the PhCs, increasing light

extraction efficiency. The diffraction grating approach is the more popular approach as it offers the advantage of being compatible with present technologies which can be implemented in real devices. Figure 2.10 shows how PhCs are used to diffract the guided modes into air which each guided mode is represented by an in-plane wavevector ($k_{||m}$) which is related to the angle of propagation within the active layer (θ_m) by

$$k_{||m} = k_0 n_s \sin(\theta_m) \quad (2.9)$$

where m is the mode number (1, 2, 3...), k_0 is the original in-plane wavevector, and n_s is the refractive index of the active layer.

Equation (2.8) can be further derived to

$$k_{||m} = (2\pi/\lambda)n_{GaN} \sin(\theta_m) \approx \sqrt{\left[\left((2\pi/\lambda)n_{GaN}\right)^2 - (m\pi/L)^2\right]} \quad (2.10)$$

where λ is the wavelength of light, n_{GaN} is the refractive index of the GaN layer, and L is the thickness of the GaN layer.

Figure 2.10: Guided modes in an InGaN/GaN LED structure with PhCs incorporated. Each guided mode possesses a wavefactor $k_{||m}$ that can be coupled to a harmonic $k_{||m} + G$ [69].

In the presence of a periodic structure which is characterized by a reciprocal lattice whose vectors $\{G\}$ coupled to harmonics of a light wave propagating in the PhC, the guided modes become Bloch modes and the wavevectors $k_{||m}$ are coupled to other harmonics $\{k_{||m} + G\}$ by the reciprocal lattice vectors $\{G\}$. In order to diffract the guided modes into air, the following diffraction condition needs to be satisfied:

$$|k_{||m} + G| < k_0 < \frac{2\pi}{\lambda} \quad (2.11)$$

Therefore, a harmonic propagates into air when the diffraction condition is met and diffracts the Bloch mode's power into air. This is the reason why the Bloch mode is sometimes referred to a leaky mode because its power leaks into air as it propagates.

After propagation into air, the radiated harmonic behaves like a plane wave with an angle,

$$\theta_{m,air} = \sin^{-1} \left((\lambda/2\pi) |k_{||m} + G| \right) \quad (2.12)$$

It can be seen from the above relations that the diffraction condition is dependent on the wavelength, lattice constant of the PhC and the angle of propagation. That is, in order to achieve high extraction efficiency, it is necessary to extract guided light propagating in all azimuthal directions. Hence, a 2D PhC is required which acts as a 2D diffraction grating and high light extraction efficiency can be achieved when the lattice constants of the PhC corresponds to the wavelength of the light generated from the active layer.

In the literature, extensive work has been carried out by researchers using 2D PhCs as diffraction gratings to improve the light extraction efficiency. Techniques such as EBL, nanoimprinting, nanosphere lithography

had been used for fabrication of the PhCs. From the massive data available, it is found that there are many other parameters which need to be taken into consideration when designing the PhCs such as the depth of holes, size of holes, filling factor, different crystal lattices, and thickness of the material of interest [127-128]. It is also found that other than these parameters, the material of interest will affect the trends and optimal design [127]. The wide range of parameters makes the optimization of the PhCs design rather challenging and till now, no documentation of an optimal design is available in the literature. However, despite the tedious process of optimizing the PhCs, the advantage of using PhCs is that with an optimized design, the issue of trapped light can be addressed directly by tailoring the light emission and hence, light emission can be increased significantly [65].

2.3 The 2DEG $Al_xGa_{1-x}N/GaN$ -based Schottky MSM PD

2.3.1 Operation of a Schottky MSM PD

Figure 2.11: Schematic of a MSM PD [81].

A schematic of a MSM PD is shown in Figure 2.11. Schottky MSM PDs are based on two rectifying contacts connected back-to-back and the fabrication of such devices involved the deposition of two interdigitated Schottky metal contacts on top of the active layer. When light with an energy that is greater than the bandgap ($h\nu > E_g$) of the semiconductor is shone onto the detector, electron-hole pairs will be generated by the photons that get absorbed in the semiconductor layer. At zero bias, the energy band diagram is symmetrical and no electric field is present. By biasing the MSM PD with an appropriate bias, the generated electron-hole pairs get separated by the built-in electric field between the biased Schottky contacts and get collected at the electrodes, resulting in a light-induced photocurrent.

The speed of the MSM PD is limited by the device capacitance and the transit time of the photogenerated electron-hole pairs through the semiconductor layer, where the transit time is related to the spacing between the interdigitated Schottky contact electrodes.

Figure 2.12: (a) Energy band diagram of the MSM PD under illumination, at zero bias. (b) Energy band diagram of the MSM PD under illumination, bias applied [81].

2.3.2 A conventional MSM PD versus 2DEG-MSM PD

Figure 2.13: Potential distribution of a conventional MSM PD and a 2DEG-MSM PD without applied bias. The electric field is perpendicular to the equipotential lines [129-131].

In a conventional MSM PD, an applied voltage between the two Schottky contact electrodes led to a built-in electric field which is directed mainly parallel to the surface in the region between the two Schottky contact electrodes. With the presence of a 2DEG in the layer structure, that is, a 2DEG-MSM PD, the electric field distribution below the interdigitated Schottky contact electrodes is modified. Figure 2.13 shows the potential distribution of a conventional MSM PD and a 2DEG-MSM PD without applied bias. From the figure, the density of the equipotential lines under the electrodes of the 2DEG-MSM PD is much larger than in the conventional MSM PD. The 2DEG in the 2DEG-MSM PD acted as an equipotential plane and forced the electric field into the region below the Schottky contact electrodes leading to a strong electric field perpendicular to the surface, between the electrodes and the 2DEG. This is in contrast to a conventional MSM PD where the electric field extended between the Schottky contact electrodes, parallel to the surface, giving low electric field strength under the

electrodes. With this vertical electric field, photogenerated electrons will be compelled to move towards the 2DEG interface while photogenerated holes will be compelled to move towards the substrate which reduced the probability of recombination of the photogenerated carriers and hence an improved detector responsivity. The active length of a conventional MSM PD is given by the distance between the two Schottky contact electrodes whereas the active length of the 2DEG-MSM PD is given by the distance between the Schottky contact electrodes and the 2DEG. The shorter transit distances in a 2DEG-MSM PD led to a faster transit time and hence, an improved bandwidth (faster response speed).

2.3.3 Formation of the 2DEG in an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure

Figure 2.14: Energy band diagram of an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure.

A heterojunction is a junction formed between two dissimilar semiconductors [132]. For a 2DEG to form at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface in an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, the conduction band of the larger bandgap semiconductor layer, that is, $\text{Al}_x\text{Ga}_{1-x}\text{N}$ must be located at a higher energy

level than the conduction band of the smaller bandgap semiconductor layer, that is, GaN. The larger bandgap semiconductor layer $\text{Al}_x\text{Ga}_{1-x}\text{N}$, played the role of a potential barrier while the smaller bandgap semiconductor layer GaN, played the role of a quantum well confining the electrons to the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface as shown in Figure 2.14. It is important to note that as the Al content increase in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer, the bandgap of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer will increase and the potential barrier between the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and the GaN layer as well as the potential barrier between the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and the Schottky contact will increase.

In the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ material system, another phenomenon existed which constituted to the formation of the 2DEG, that is, the influence of the piezoelectric and spontaneous polarization effects.

In strained $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure with the wurtzite crystal structure grown in the (0001) orientation on sapphire (lattice mismatch between GaN and sapphire is approximately 14% [133]), which is the most commonly growth orientation, piezoelectric polarization effects existed which can exert a substantial influence on the concentration and distribution of free carriers in the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure [134].

Piezoelectric polarization refers to the presence of a polarization field resulting from the distortion of the crystal lattice. In an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer that is grown on top of the GaN layer is strained due to the differences in the lattice constants of AlN and GaN. The parameters that characterized the strength of the piezoelectric polarization electric field are the piezoelectric polarization coefficients and the differences in the lattice constants that caused the strain which are illustrated in Figure

2.15. From Figure 2.15, it can be seen that with increasing Al content, the piezoelectric polarization in the strained $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer increases.

Figure 2.15: The piezoelectric polarization coefficients versus the lattice constants of the AlN, GaN and InN material systems [13].

Further contributing to the polarization induced effects in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures is the spontaneous polarization, that is, the built-in polarization field presented in unstrained crystals owing to their wurzite structures. Wurzite structure is the structure with the highest symmetry compatible with the existence of spontaneous polarization [135]. The wurzite group III-nitrides InN, GaN and AlN are tetrahedral coordinated direct bandgap semiconductor having a hexagonal Bravais lattice with four atoms per unit cell. As a consequence of the noncentrosymmetry of the wurzite structure and the large ionicity factor of the covalent metal-nitrogen bond, there existed a large spontaneous polarization oriented along the hexagonal c-axis [(0001) orientation], which is the most commonly growth orientation for

nitride semiconductors. The parameter that characterized the strength of the spontaneous polarization electric field is the spontaneous polarization coefficient which increased with the increase in the Al content in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer [136].

The sheet carrier concentration and the confinement of the 2DEG located close to the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface induced by the polarization effects are dependent on the polarity of the growth material.

Figure 2.16: Schematic of the wurtzite Ga-face and N-face GaN crystal structure [137].

GaN belonged to the group of noncentrosymmetric compound crystals which exhibited two different sequences of atomic layering in two opposing directions parallel to certain crystallographic axes in which crystallography polarity along the axes can consequently be observed [137-138]. For GaN with a wurtzite crystal structure grown in the (0001) orientation, the sequence of the atomic layers of the constituents Ga and N is reversed along the [0001] and $[000\bar{1}]$ directions leading to the formation of Ga-faced which corresponded to

the $[0001]$ polarity and N-faced which corresponded to the $[000\bar{1}]$ polarity. It is important to note that the (0001) and $(000\bar{1})$ surfaces of GaN are nonequivalent and differed in their chemical and physical properties [137-138]. Ga-faced is preferred as it has been reported that the structural quality of Ga-faced heterostructures is much higher as compared to N-faced heterostructures. Ga-faced heterostructures have smoother morphologies and lower defect densities [139] as compared to N-faced heterostructures.

The polarity of materials played an important role in the polarization induced sheet charge density and directions of the spontaneous and piezoelectric polarization as illustrated in Figure 2.17. The piezoelectric polarization is negative for tensile and positive for compressive strained GaN or $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers, respectively. The sign of the spontaneous polarization of wurzite group III-nitrides InN, GaN and AlN was found to be negative [135]. The orientation directions of the spontaneous and piezoelectric polarization are defined by assuming that the positive direction goes from the cation (Ga) to the nearest anion neighbor (N) along the c axis [124,137]. Hence, for a Ga-faced strained $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, the tensile strain in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer will contribute to a negative piezoelectric polarization, pointing towards the substrate. Since the spontaneous polarization in wurzite GaN and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers is negative; the negative spontaneous polarization will also point towards the substrate. The spontaneous and piezoelectric polarization changes its signs and directions when the polarity of the material changes from Ga-faced to N-faced.

Figure 2.17: Polarization induced sheet charge density and directions of the spontaneous and piezoelectric polarization in Ga- and N-faced $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures [137].

The polarization induced sheet charge density (σ) at an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface is defined as:

$$\begin{aligned}\sigma &= P(\text{top}) - P(\text{bottom}) \\ &= \{P_{sp}(\text{top}) + P_{pe}(\text{top})\} - \{P_{sp}(\text{bottom}) + P_{pe}(\text{bottom})\}\end{aligned}\quad (2.13)$$

where P_{sp} is the spontaneous polarization and P_{pe} is the piezoelectric polarization.

From this, it can be seen that the polarization induced sheet charge density is positive in Ga-faced $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures ($+\sigma$). To compensate the net polarization induced positive charge, free electrons are formed resulting in the formation of the 2DEG with a sheet carrier concentration n_{sc} , assuming that the quantum well at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface falls below the Fermi level, (E_F). In contrast, for N-faced $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, the spontaneous and piezoelectric polarizations have opposite directions in comparison to Ga-faced $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure. The net total polarization resulted in a net negative sheet charge density at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface. This net negative sheet charge density resulted in

the accumulation of holes instead of electrons at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface and no 2DEG is formed. Hence, it is essential to have a Ga-faced $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure such that a net positive polarization charge is induced at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ interface for the formation of a 2DEG which will be confined in the quantum well formed by the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure.

2.3.4 A 2DEG $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based MSM PD

Figure 2.18: The electric field distribution in an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ MSM PD under 5 V bias [140].

The potential distribution of a conventional MSM PD and a 2DEG-MSM PD without applied bias is shown in Figure 2.13. At 0 V, the presence of a 2DEG in the 2DEG-MSM PD led to a strong electric field perpendicular to the surface, between the electrodes and the 2DEG. When a bias is applied to the MSM structure as shown in Figure 2.17, the electric field is concentrated

in the vicinity of the cathode. When the material system is an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure, the polarization electric field induced by the spontaneous and piezoelectric polarization further enhanced the electric field along the vertical direction. With this vertical electric field, photogenerated electrons will be compelled to move towards the 2DEG interface while photogenerated holes will be compelled to move towards the substrate which reduced the probability of recombination of the photogenerated carriers and hence an improved detector responsivity. In a conventional MSM PD with a laterally internal electric field, photogenerated electrons moved laterally across the contacts and upward to the contacts. That is, the transit distance of the photogenerated electrons is the horizontal distance between the two Schottky contact electrodes. In a 2DEG MSM PD with a vertical electric field, photogenerated electrons moved towards the 2DEG interface while photogenerated holes moved towards the substrate. That is, the transit distance of the photogenerated electrons is the vertical distance between the 2DEG and the Schottky contact. In conclusion, the change in the transport path of the photogenerated electrons as the result of the vertical electric field induced in a 2DEG MSM PD led to a shorter transit distance and hence a faster response time.

CHAPTER 3

Experimental Procedures

This chapter presents details of the experimental techniques used to achieve GaN-on-SOI devices and is divided into three sections. The first section shows details of the epitaxial layers of the InGaN/GaN-based LED structures grown on SOI and bulk Si substrate, as well as the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /GaN-heterostructures grown on SOI substrate for UV PDs. The techniques used to characterize the structural, electrical and optical properties of the as-grown heterostructures, as well as the techniques used for device characterization are discussed in section two. The details of the device fabrication are discussed in the last section.

3.1 Epitaxial layer details

3.1.1 InGaN/GaN-based LED structures on SOI and Si substrate

Figure 3.1: Schematic of InGaN/GaN-based LED structures on (a) SOI(111) and (b) bulk Si(111) templates.

InGaN/GaN-based LED structures were grown on *n*-type Si(111) and SOI(111) substrates by metal-organic chemical vapor deposition (MOCVD). The 6-inch (111)-oriented SOI substrates used in this study were prepared using the separation by implantation of oxygen (SIMOX) method [141]. Such SIMOX SOI substrates with SOI overlay thickness of 45 nm with a buried oxide (BOX) of thickness 150 nm was chosen for GaN epitaxy. The full LED layer structure consisted of a high-temperature (HT) AlN buffer layer grown at $\sim 1050^\circ\text{C}$, an Al-rich graded AlGa_xN_{1-x} buffer with Al composition around 15% towards the GaN overgrown layer, $\sim 2.7\ \mu\text{m}$ thick *n*-type Si-doped GaN template, five periods of InGa_xN_{1-x}/GaN multi-quantum wells (MQWs), and a 100 nm *p*-type Mg-doped GaN layer. The thickness of the HT-AlN buffer was designed based on the optimum thickness for 2D growth to occur to prevent nitridation (formation of Si_xN_y films) and at the same time avoid the growth of thick AlN epilayer [94-96]. To avoid cracking and tensile stress during the growth of the *n*-type GaN template, strain-compensating low-temperature (LT) AlN interlayers of around 10 nm grown at $\sim 650^\circ\text{C}$ were introduced. The thickness of the LT-AlN interlayers was designed to counterbalance the growth-induced tensile stress and the thermally induced tensile stress during cooling. With increasing thickness of LT-AlN, an increase of compressive stress that is induced in the subsequently grown GaN layer is expected until a saturation thickness is reached which is around 10-20 nm of LT-AlN layer thickness. This meant that LT-AlN layers thicker than the saturation thickness have no effect of further inducing compressive stress or reducing tensile stress [26,32]. Five periods of InGa_xN_{1-x}/GaN multi-quantum wells (MQWs) was chosen on the basis of reducing the strain-induced piezoelectric field or

quantum confined Stark effect (QCSE) and to improve the light output intensity from LEDs [142-144].

For comparative studies on LED performance, the same LED layer structure was grown on SOI(111) and bulk Si(111) substrate. Despite similar layer structures and growth conditions, a difference in the emission wavelength from the LED structures was due to a difference in the In incorporation in the MQWs giving a green emission ~ 525 nm and a blue emission ~ 485 nm from the LED structures grown on SOI(111) and bulk Si(111) substrate, respectively. For the LED structure on SOI(111) substrate, the lower surface temperature for the SOI(111) wafer during MQW growth led to wafer bowing which resulted in an increased In-incorporation.

For light extraction studies, the LED structure grown on SOI(111) substrates were used.

3.1.2 $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures on SOI substrate for UV PDs

Figure 3.2: Schematic of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructure structure on SOI(111) substrate.

For the growth of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures, 6-inch SOI(111) wafers were prepared by the SIMOX process. The thickness of the SOI(111) overlayer was about 90 nm with a buried oxide thickness of 140-150 nm. The $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures were then grown on such composite substrates by MOCVD. The schematic of the 2DEG layer structure on SOI(111) substrate is shown in Figure 3.2. About 250 nm of HT-AlN and ~90–100 nm AlGa_N buffer are first grown on top of the thin SOI overlayer followed by ~2.65 μm of thick crack-free semi-insulating (S.I.) Fe-doped GaN with several strain-compensating LT thin AlN interlayers (9-10 nm). Fe doping has been shown to produce high resistive GaN layers such that high quality HEMT structures can be grown on such Fe-doped GaN buffers [145]. The active layers consisted of about 1.0 nm AlN spacer, 17 nm unintentionally doped (UID) $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer and a thin ~2.0 nm GaN cap layer.

3.2 *Material and Device Characterization*

- ***Transmission Electron Microscopy (TEM)***

The TEM consisted of a high voltage electron source which consisted of a cathode and an anode, electromagnetic lenses, apertures, sample stage and an image recording system, all of which operated in high vacuum mode. An electron beam is formed when the tungsten filament at the cathode gets heated up which is then accelerated down the column by the anode, focused by the electromagnetic lenses and apertures to filter out scattered electrons such that a monochromatic beam is produced to interact with the sample. The transmitted light through the sample is used to produce the image in normal imaging

conditions. An imaging system which consists of an electromagnetic lens system and a screen is used to focus the electrons that emerged through the sample into an image which gets projected onto a phosphor coated screen.

The TEM sample was prepared using Dual Beam Focused Ion Beam (FIB) Helios 600 Nanolab. It was first milled into a lamella using 30 kV at various currents and then transferred to the Cu grid using an in-situ liftout probe where the lamella was further thinned down to less than 100 nm. Finally 5 kV and 2 kV were used for low kV cleaning to reduce the FIB induced damage. A Philips FEI CSM 300 TEM was used for the imaging. XTEM was performed to determine the thickness of the individual epitaxial layers of the as-grown structures. The imaging was performed at all interfaces from the bottom of the substrate to the top surface. The propagation of the dislocations can be clearly seen from the XTEM images.

- ***High resolution X-Ray diffraction (HRXRD)***

HRXRD is a powerful tool which is widely used in the assessment of epitaxial grown wafers. Information such as alloy composition, thickness, lattice constants, lattice mismatch, tilts, relaxation, curvature, dislocations, mosaicity and homogeneity can be determined from the diffraction patterns. In this work, the HRXRD measurements were performed with a PANalytical X'Pert PRO diffractometer. The incident X-ray beam was produced at 40 mA and 40 kV of the generator and

passed through a 4-bounce hybrid mirror which consisted of a combination of an x-ray mirror and a 4-crystal Ge(220) channel cut monochromator to obtain a monochromatized Cu $K\alpha_1$ radiation ($\lambda = 1.5406\text{\AA}$). The divergence slit that was placed in front of the optics is 0.5° . To improve the experimental resolution, another divergence slit of 1° (1 mm) was inserted in front of the detector. An open detector was used to collect the signals for the omega (ω) and omega-2theta (ω - 2θ) scans.

- ***Micro-Raman Spectroscopy***

When light interacts with matter, it can either be absorbed, reflected, transmitted or scattered. When the interaction of light with matter is in such a way that energy is either gained or lost and causes a shift in the frequency, inelastic scattering occurs which is also called Raman scattering. Micro-Raman spectroscopy is a non-destructive technique that is based on the inelastic scattering of monochromatic light, usually from a laser source where the frequency of the scattered light is changed by the gain or loss of energy corresponding to the vibrational modes of the material. Therefore, this technique provides information on the vibrational, rotational and low-frequency modes of a material system and is sensitive to the crystalline quality, stress, free carrier concentration, alloy composition and temperature [146].

For the structural studies of as-grown InGaN/GaN-based LED structures on SOI(111) and bulk Si(111) substrates, the 514.5 nm line

of an argon ion laser was used for the Raman scattering measurement. The scattered light was dispersed through the Jobin Yvon T64000 triple monochromator system attached to a liquid nitrogen cooled charge coupled device detector. The spectral accuracy of the Raman measurements was kept at 0.2 cm^{-1} with a lateral spatial resolution less than $1.0 \text{ }\mu\text{m}$. The Raman spectra from the as-grown LED structures were recorded using the $z(xx)\bar{z}$ backscattering configuration. In this geometry with the laser beam incident on the (0001) surface, only the $E_2(\text{low, high})$ and $A_1(\text{LO})$ phonon modes are allowed [146-147]. The excitation power was kept very low ($<0.4 \text{ mW}$ on the sample surface) during measurement to avoid any thermal red-shift of the E_2 -high optical phonon mode.

To understand the interface properties of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures on SOI(111) substrate, UV micro-Raman (Horiba LabRam HR spectrometer equipped with a thermoelectrically cooled coupled charged detector, spot size of $2 \text{ }\mu\text{m}$) with 325 nm excitation from a He-Cd laser was used for the measurements. With 325 nm excitation, the optical penetration depth is less than 40 nm in GaN [147-148] and hence, UV micro-Raman spectroscopy can be used to probe the surface properties of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures. The UV micro-Raman experiments were performed with a micro-Raman set-up in a backscattering geometry along the (0001) axis of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures. To study the 2DEG interface vibrational properties, UV-micro Raman spectroscopy

was used to probe the as-grown layer structure as well as MSM PDs under electrical simulation. An Agilent 4156B parameter analyzer was used to apply electrical bias onto the MSM PDs through micro-manipulator probes.

- **Atomic Force Microscopy (AFM)**

The surface morphology of the as-grown and etched surfaces was analyzed by carrying out AFM measurements (Multi-mode IV, Veeco Instruments Inc) in tapping mode. The probe consists of a silicon tip on the end of a cantilever which bends in response to the force between the tip and the sample. Under tapping mode, the cantilever is oscillated at its resonant frequency and positioned above the sample surface such that it only tapped the surface for a very small fraction of its oscillation period. The advantages of the tapping mode are the elimination of a large part of permanent shearing forces and the causing of less damage to the sample surface. The short contact time also implies that the lateral force is very much reduced as the tip scanned over the region. The AFM measurements were performed in ambient conditions with a typical scan area of $2\text{ }\mu\text{m} \times 2\text{ }\mu\text{m}$ and at a scan rate of 1.5 Hz. Prior to the AFM measurements of the etched surface morphology, the samples were subjected to H_3PO_4 etching at 180°C for 10 minutes.

- **Field emission secondary electron microscope (FESEM)**

In FESEM, a thermal field emission electron source is used to form an electron beam which is then accelerated down the column by the anode,

focused into a beam using electromagnetic lenses, and raster over the sample surface by deflection coils, all of which operated in high vacuum mode. As a result of the interaction of the electron beam with the sample, the incident beam loses energy in a variety of signals. These signals included secondary electrons, backscattered electrons, characteristic X-rays, cathodoluminescence and heat. Depending on the type of imaging, secondary electrons imaging (SEI) or backscattered electron imaging (BSE), the emitted secondary electrons or backscattered electrons are collected by different detectors, respectively. The intensity of the emitted electron signal collected by the detectors is then displayed on a cathode ray tube for image formation. The SEI mode is used for high resolution imaging of the surface topography while BSE mode is used for compositional analysis. An ultra high resolution thermal FESEM (ESM-9000) was used for the plane-view and cross-sectional imaging of the photonic crystals for light extraction studies. An acceleration voltage of 5 kV was used for the imaging. The samples were coated with a thin layer of Pt (~3 nm) to avoid charging effects during imaging.

- **Micro-Photoluminescence (PL) / Micro-Electroluminescence (EL)**

It is well known that PL is not equivalent to EL. That is, high PL measured from MQWs from as-grown samples does not necessarily mean high EL from finished devices. PL is normally measured on a bare sample and hence is dependent on the optical properties of the material. Whereas, EL is measured on a finished device and is not only

dependent on the optical properties of the material but also on the electrical contacts through which electrical current is injected. The fabrication process and the metals used in the contacts will play a role in the measured EL from the finished device.

PL spectroscopy is a contactless and non-destructive technique providing information on the electrical and optical properties of semiconductor materials, such as bandgap, emission wavelength, crystal quality, impurity levels, etc. Typically, light from a laser beam is impinged onto the sample, where it is absorbed. The excess energy is imparted into the material in a process called photo-excitation, which is the mechanism of electron excitation by photon absorption. As a consequence of the photo-excitation process, electrons are excited into a higher energy state and return to a lower energy state accompanied by the emission of a photon. Since the excitation of the sample is performed by light, this luminescence is called PL. PL is thus the spontaneous emission of light from a material under optical excitation. A micro-PL experiment is simply a PL experiment with spatial resolution which is determined by the objective of the microscope used.

EL is similar to PL except that in EL, the photo-excitation process is due to current injection and it is usually measured on a finished device.

The micro-PL and micro-EL measurements were performed at room temperature with the same Jobin Yvon LABRAM setup equipped with a thermoelectrically cooled coupled charged detector. For the

collection of the micro-PL and micro-EL spectra from the LEDs with and without PhCs, a He-Cd laser source with 325 nm excitation is used. The LEDs were held onto the sample stage with vacuum and an Agilent 4156B parameter analyzer was used to apply electrical bias onto the LEDs through micro-manipulator probes during measurements. All the experiments were carried out at room temperature. For the micro-PL measurements of the as-grown $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures, a 266 nm UV laser line was used to excite the as-grown sample.

- **Current-Voltage (I - V) measurements under dark and illuminated conditions**

The I - V characteristics of the fabricated MSM PDs under dark and illuminated conditions were recorded with the help of An Agilent 4156B parameter analyzer. The fabricated MSM PDs were held onto the sample stage with vacuum and electrical bias was supplied to the device through micro-manipulator probes. A 325 nm He-Cd laser line with a laser line with an excitation intensity of 16 mW/cm^2 was used to illuminate the MSM PDs.

- **Responsivity measurements**

A PD operates by converting optical signals into electrical signals (voltage or current). The responsivity of a PD is defined as the ratio of photocurrent generated per unit of incident power. That is, the responsivity of a PD is essentially a measure of its effectiveness to

convert electromagnetic radiation to electrical current or voltage. The spectral responsivity of an optical detector is a measure of its response to radiation at a specified wavelength. A spectral response plot is obtained by plotting the absolute responsivity as a function of wavelength.

The spectral responsivities of the MSM PDs were measured with the Bentham Instruments setup where light from a Xenon lamp was filtered by two monochromators. A Keithley current-voltage source unit was used to supply the electrical bias. The incident power on the device surface was about 8 mW/cm^2 measured with a calibrated broadband power meter. The responsivity measurements were conducted in the wavelength range of 250 to 500 nm and the absolute values of responsivity were determined with a calibrated Si detector.

3.3 Device fabrication

3.3.1 InGaN/GaN-based LEDs

The lateral LED devices were fabricated using multiple-mask photolithography, ICP etching, and contact metallization. The as-grown samples were first dipped in concentrated hydrochloric (HCl) acid for 5 mins to remove the native oxide on the surface. Organic cleaning was carried out using acetone and methanol for a duration of 5 mins each. Samples were then rinsed in deionized (DI) water and blown dry with nitrogen (N_2) gun. Structural etching of the top p-GaN to expose the underlying n-type Si-doped GaN was carried out using the boron trichloride/chlorine (BCl_3/Cl_2) gas

chemistry to expose the underlying n-type Si-doped GaN for n-contact metallization. The samples were etched in a load-locked Unaxis SLR 770 high-density plasma etch system consisting of an ICP chamber (operating at 2 MHz) and an additional RF bias (13.56 MHz) for the sample chuck. Helium backside cooling was incorporated to allow the temperature of the substrate to be more effectively controlled. The ICP etching parameters are as follows: 20 sccm of BCl_3 , 10 sccm of Cl_2 , reactive-ion-etching (RIE) power of 300 W, ICP power of 500 W, pressure of 5 mTorr and temperature of 6°C . The Ti/Al/Ti/Au(10/150/15/500 nm)-based n-contact, Ni/Au(5/5 nm)-based p-contact, Au(500 nm) p-bond metallization were carried out by lithography using the respective masks followed by electron-beam evaporation and lift-off. Thermal annealing steps were performed after the n-contact metallization (750°C for 30 s in N_2 ambient) and after the p-bond metallization (575°C for 40 s in air).

For light extraction studies, the fabrication of 2D PhC structures on top of the p-GaN surface was carried out by EBL using SiO_2 nanomask. A thin SiO_2 layer (80 nm) was first deposited on the p-GaN surface using plasma enhanced chemical vapor deposition (PECVD). The InGaN/GaN-based heterostructures were then coated with ZEP520A photo resist for the purpose of writing nano-holes using EBL (current 50 pA, dose $190 \mu\text{C}/\text{cm}^2$). Next, the SiO_2 nano-patterns were created using a RIE system using Trifluoromethane/Argon (CHF_3/Ar) gas (25/25 sccm) chemistry. The RIE etching parameters are as follows: 25 sccm of CHF_3 , 25 sccm of Ar, RIE power of 150 W, and pressure of 20 mTorr. Etching was carried out at room temperature. Helium backside cooling was incorporated to regulate substrate

temperature drift and for heat dissipation. After the formation of the SiO₂ nanomask, ICP etching of the p-GaN surface was then carried out using BCl₃/Cl₂ gas chemistry. The samples were etched in a load-locked Unaxis SLR 770 high-density plasma etch system consisting of an ICP chamber (operating at 2 MHz) and an additional RF bias (13.56 MHz) for the sample chuck. Helium backside cooling was incorporated to allow the temperature of the substrate to be more effectively controlled. The ICP etching parameters are as follows: 20 sccm of BCl₃, 10 sccm of Cl₂, RIE power of 300 W, ICP power of 500 W, pressure of 5 mTorr and temperature of 6°C. For light extraction studies between different nano-patterns, the ICP etching time was kept at 90 s. In order to demonstrate electrically simulated light emission from PhC-patterned LEDs, fabrication of LEDs with PhCs was carried out using multiple-mask photolithography, ICP etching, and contact metallization.

3.3.2 $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based MSM PDs

To demonstrate the device properties of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure to be used as an UV detector, interdigitated MSM electrodes with an active area of $625 \times 225 \mu\text{m}^2$, finger width and spacing of $25 \mu\text{m}$ were fabricated. The as-grown samples were first dipped in concentrated HCl acid for 5 mins to remove the native oxide on the surface. Organic cleaning was carried out using acetone and methanol for a duration of 5 mins each. Samples were then rinsed in DI water and blown dry with N₂ gun. Semitransparent Ni/Au (5/5 nm) Schottky electrodes were then defined onto the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer by photolithography, electron-beam evaporation, and lift-off technique.

CHAPTER 4

InGaN/GaN-based Structures on SOI Substrate

The experimental results from InGaN/GaN-based MQW LEDs are presented in this chapter and are divided into two sections. The first section details the results and discussions of the various experiments performed to study the InGaN/GaN-based LED structures grown on SOI substrate and how they led to LED improvement. The structural properties of the as-grown LED structures were characterized with HRXRD and Micro-Raman spectroscopy. The thicknesses of the respective epitaxial layers of the as-grown heterostructures were determined from XTEM. In order to check on device characteristics, LED devices were fabricated by multiple-mask photolithography, ICP etching, p- and n- contact metallization and annealing of the p- and n- contacts. Following these, device characterization was carried out with micro-EL measurements. For comparative studies, InGaN/GaN-based LED structures on were also grown on bulk Si substrates and LEDs were fabricated. Additionally, in section two, light extraction studies with the incorporation of PhCs on LEDs on SOI substrates were discussed. Different 2D PhCs patterns were created by EBL and transferred onto the surface of the LEDs via ICP etching. The morphology of the ICP-etched PhCs on the LED surfaces was investigated by performing plane-view and cross-sectional imaging with a FESEM. For light emission studies, micro-PL measurements were performed. In order to demonstrate electrically simulated light emission from PhC-patterned LEDs, fabrication of LEDs with PhCs was carried out and

micro-EL spectra as a function of different injection currents were recorded from the devices.

4.1 Material Characterization

4.1.1 Cross-sectional Transmission Electron Microscopy (XTEM)

Figure 4.1: (a) Schematic of InGaN/GaN-based LED structures on SOI(111) and bulk Si(111) templates. XTEM image of (b) InGaN/GaN-based LED structures on SOI(111) substrate, (c) SOI(111)/substrate interface, (d) Bulk Si(111) interface, and (e) Five-period of InGaN/GaN MQWs.

The imaging of the epitaxial layers of the as-grown InGaN/GaN-based LED structures was carried out using XTEM and the images are shown in Figure 4.1. From the XTEM images in Figure 4.1 (b) to (e), the interface between AlN and thin Si overlay grown on SOI(111) substrate, the interface

between the AlN and Si(111) interfaces grown on bulk Si(111) substrates, the five-periods of InGaN/GaN MQWs with the top p-GaN capping layer which made up the optically active layers, as well as the strain compensating LT-AlN interlayers within the thick GaN templates can be clearly resolved. The thicknesses of the respective layers were also determined from the XTEM images.

4.1.2 High Resolution X-Ray Diffraction (HRXRD)

Figure 4.2: HRXRD spectra of the as-grown InGaN/GaN-based LED structures grown on SOI(111) and bulk Si(111) substrates. The superlattice fringes are clearly resolved and represented high-crystalline quality GaN material on SOI.

The crystalline and structural properties of the as-grown InGaN/GaN-based LED structures were characterized using HRXRD measurements. Due

to similar growth conditions, the HRXRD spectra of as-grown InGaN/GaN-based heterostructures grown on SOI(111) and bulk Si(111) substrates showed similar patterns. Figure 4.2 shows the ω -2 θ scans of the (0002) diffraction planes of as-grown InGaN/GaN-based LED structures on SOI(111) and bulk Si(111) substrates. From the HRXRD spectra, the GaN (0002), AlN (0002), buffer AlGaIn (0002) reflections and the superlattice fringes caused by the InGaN/GaN MQWs are evident. The full-width-at-half-maximum (FWHM) of the (0002) ω scan rocking curve revealed a value of about 420 arcsec for GaN on 50 nm SOI(111) substrate and this value is almost the same as in the case of layers grown on bulk Si(111) substrate. Tran et al reported a FWHM of 560 arcsec for the (0002) ω scan rocking curve for InGaN/GaN-based LED structure on bulk Si(111) substrate [91]. When comparing the result obtained in this thesis to literature [91], an improvement in the structural quality is achieved. The observation of well-pronounced superlattice peaks up to the sixth order and finite thickness interference fringes in the diffraction pattern indicated that the interface of InGaN/GaN MQWs is sharp and the layers on such SOI(111) substrate possessed good crystal quality. Therefore, SOI substrates can be used for the successful growth of high crystalline quality nitride-based LED structures, as evidenced from the HRXRD spectra.

4.1.3 Micro-Raman Spectroscopy

Micro-Raman measurements were performed to investigate the structural properties of the as-grown InGaN/GaN-based LED structures grown on SOI(111) and bulk Si(111) substrates. Figure 4.3 shows the micro-Raman spectra of the as-grown InGaN/GaN-based LED structures grown on SOI(111)

and bulk Si(111) substrates under 514.5 nm excitation. From the micro-Raman measurements, nearly strain-free LED layers grown on Si(111) and SOI(111) substrates were observed. This is important as stress in the layers will lead to cracking at thickness below the desired device layer thickness. The E_2 -high optical phonon peak measured from a 400 μm thick freestanding strain-free GaN was observed at $567.5 \pm 0.2 \text{ cm}^{-1}$. For the LED samples grown on SOI(111) and bulk Si(111) substrates, the E_2 -high optical phonon peak were observed at $567.3 \pm 0.2 \text{ cm}^{-1}$ and at $567.7 \pm 0.2 \text{ cm}^{-1}$ respectively, which is close to the phonon peak ($567.5 \pm 0.2 \text{ cm}^{-1}$) recorded from the freestanding GaN. The E_2 -high optical phonon mode of the AlN buffer was also observed in the visible Raman spectra.

Figure 4.3: (a) Room temperature micro-Raman spectra of LED structures grown on SOI(111) and bulk Si(111) substrates under 514.5 nm excitation.

The E_2 -high Raman peak can be used to estimate the biaxial stress (σ_{xx}) in these LED structures from the relation: $\Delta\omega = 4.3\sigma_{xx} \text{ cm}^{-1} \text{ GPa}^{-1}$, where ($\Delta\omega$) is the Raman shift [149]. Therefore, the as-grown LED structures films showed an average stress value of $< 0.1 \text{ GPa}$. The accuracy of the stress values in our case is about 50 MPa as it depends on the spectral resolution of the Raman instrument.

From the micro-Raman measurements, no significant difference in the stress values between LED layers grown on bulk Si(111) and SOI(111) substrates were observed. This is due to the identical device structure growth on the two different substrates along with same number of LT-AlN interlayers. From the micro-Raman spectra, the relative intensity of E_2 -high mode for LED on bulk Si(111) substrate is weaker whereas for LED on SOI(111) substrate, the relative intensity of E_2 -high mode is much higher due to the use of scattered green light for visible Raman probing. The improvement of scattered Raman intensity showed a strong visible light outcoupling from the GaN layers on SOI(111) substrate when compared to similar structures on bulk Si(111) substrate. This evidence showed that visible light emission would be stronger from LED structures on SOI(111) substrate and that the absorption of visible light is stronger from LED structures on bulk Si(111) substrate.

4.2 Device Characterization

4.2.1 Micro-EL measurements

In order to check on device characteristics, LED devices are fabricated by multiple-mask photolithography, ICP etching, p- and n- contact metallization and annealing of the p- and n- contacts. Following these, the

micro-EL spectra were recorded from the fabricated LED devices to compare the light output. Figure 4.4 shows the micro-EL spectra of LEDs grown on SOI(111) and bulk Si(111) substrates at 100 mA current injection.

Figure 4.4: The micro-EL spectra of LEDs grown on SOI(111) and bulk Si(111) substrates at 100 mA.

For the case of LEDs on SOI(111) substrate, very strong multiple interference peaks in the micro-EL spectrum with the energetic maxima centered ~ 525 nm were observed. For the case of LEDs on bulk Si(111) substrate, the EL intensity modulation is lower and the EL peak is centered ~ 485 nm. The stronger EL intensity modulation for the LEDs on SOI(111) substrate is due to the lesser visible light absorption by SOI(111) substrate as compared to bulk Si(111) substrate and the cavity effect due to presence of dielectric interfaces [40]. The refractive index contrast at the AlN/SOI/SiO₂/Si interfaces led to an enhancement in the EL intensity and multiple reflections at

Fabry-Perot boundaries led to well-separated interference peaks in the EL spectrum. As a result, the integrated EL intensity is thus higher for the LEDs on SOI(111) substrate when compared to the case of bulk Si(111) substrate due to a significant increase in the out-coupling of visible light.

A difference in the EL peak wavelength is due to the In content in the MQWs in the two LED samples. Due to wafer bowing during MOCVD, the lower surface temperature for the SOI(111) wafer during MQW growth resulted in an increased In-incorporation. This resulted in a red-shifted and relatively broader EL for LEDs on SOI(111) substrate despite similar growth conditions. However, even with this higher In-incorporation the results showed that the LED on SOI(111) substrate is brighter (higher EL integrated intensity) since usually in this spectral range which requires high In-incorporation, a decreasing internal quantum efficiency is expected [150].

In the case of conventional LEDs on sapphire with InGaN/GaN multi-quantum wells as active layers, the piezoelectric effect is dominant and leads to band bending. As a result, at higher drive currents, the EL emission peak usually leads to substantial blue shift. For the case of white LEDs or high-brightness LEDs driven at very high current, the active layer emission blue-shift must be compensated to maintain color chromaticity. In addition, the local heating effect and temperature rise at higher injection current reduced the efficiency of devices and led to red-shifted emission. To demonstrate this, the LEDs on SOI(111) and bulk Si(111) substrates have been driven in the current range of 10 to 100 mA and the micro-EL spectra recorded as shown in Figure 4.5.

Figure 4.5: The micro-EL spectra of LEDs grown on (a) SOI(111) and (b) bulk Si(111) substrates, at different injection currents. Inset: The pictures of (a) green LEDs grown on SOI(111) and (b) blue LEDs grown on bulk Si(111) substrates respectively. The difference in the color emission is due to the In content incorporated in the InGaN/GaN MQWs during growth.

For the case of LEDs grown on bulk Si(111) substrate, the heat generated at the active junctions can be easily dissipated through thermally conductive Si substrate. So at higher driving currents, the blue shift in LEDs on bulk Si(111) substrate may be slightly higher. However, for the case of LEDs on SOI(111) substrate, the heat dissipation through the thin buried oxide layer is inferior and the local heating of the device will try to compensate the blue-shifted EL at higher injection current. A slightly higher junction temperature will show a red-shift of the EL peak and the overall blue-shift at higher driving current could be much lower for LEDs on SOI(111) substrate. From Figure 4.5, the amount of the EL peak shift (energetic position of interference maxima) for LEDs on SOI(111) and bulk Si(111) substrates is in the range of about 2 nm and 4 nm, respectively. Therefore, such SOI substrates would be beneficial for the wavelength stabilization when LEDs are driven at high injection currents.

4.3 *Light extraction studies*

4.3.1 *Incorporation of PhCs*

Cho *et al.* [151] have shown that the extraction efficiency of blue LED on sapphire gradually increases with etch depth until it reaches the MQW active layers. Lee *et al.* [152] have shown that the apex angle of the four facet inverted pyramids at the top surface significantly affect light extraction and efficient out coupling is possible for the case of apex angle between 20° to 70° with a maximum at about 30°. Of course, these enhancement factors are also governed by substrate reflectivity when patterned substrate or reflective substrates are used. A light extraction enhancement of 73% is recently claimed

in the case of unencapsulated thin film LED chips with PhC nanostructures [69]. These reports show the significance of the back side reflector as well as top PhC nanostructures to improve optical power output from LED structures. Thus, in this section, the effects of photonic nano-patterns on light extraction will be discussed. Two different sets of photonic nano-patterns were fabricated on the LED structures grown on SOI(111) substrates. The morphology of the ICP-etched PhCs on the LED surfaces was investigated by performing plane-view and cross-sectional imaging with FESEM as shown in Figure 4.6. For light emission studies, micro-PL measurements were performed.

Figure 4.6: (a) Plane-view and (b) cross-sectional SEM images of rhombic lattice array of nano-holes with 200 nm diameter and 800 nm pitch. (c) and (d) represent plane-view and cross-sectional SEM images of rhombic lattice array of nano-pillars with 200 nm diameter and 400 nm pitch. All the PhC structures are fabricated on LED structures grown on SOI(111) substrate.

The room temperature micro-PL spectra of LED on SOI(111) substrate with and without nano-patterns are shown in Figure 4.7.

Figure 4.7: Micro-PL spectra recorded from LED structures grown on SOI(111) substrate with different shape of nano-patterns: rhombic lattice nano-holes and rhombic lattice nano-pillars.

For the LED surface without nano-patterns, the PL is dominated by multiple reflections at the Fabry-Perot boundaries and well-separated interference peaks with the energetic maxima centered ~ 525 nm. An enhancement in the PL intensity is observed for both LED structures with nano-patterns. With the creation of nano-holes on the LED surface, an increase in the out-coupling of PL emission revealed about four-fold enhancement of the PL intensity. The light extraction effect is more prominent with the creation of nano-pillars on the LED surfaces, revealing almost five-fold enhancement in the PL intensity. The increase is attributed to the increase

in the photons scattering from the sidewalls of the nano-pillars. The creation of nano-pillars leads to an increased in the surface area for photons scattering and thus more pathways for the generated photons to escape.

Other than the enhancement in the PL intensity, a change in the fringe patterns of the PL spectra was also observed. A blue shift in the PL central energetic maxima is observed for both LED structures with nano-patterns, with a larger blue shift observed for the LED structure with nano-pillars. This blue shift in the PL energetic maxima is caused by the band filling effect and the reduction of the piezoelectric field by the strain relaxation of the InGaN/GaN MQWs [153-157]. With nano-patterns on the LED surfaces, the strain in the InGaN/GaN MQWs layers caused by lattice mismatch is released. As a result, the band structure of the InGaN/GaN MQWs become flatter leading to an increase in the overlapping of the wave functions of electrons and holes and hence an enhancement in the radiative recombination.

Another interesting observation is the modulation of the PL spectra at longer wavelengths. For the LED structures with nano-holes, the contribution of the Fabry-Perot fringes to the integrated PL intensity is still prominent. A decrease in the PL spectral modulation at longer wavelength regions was observed for the LED structures with nano-pillars. Due to the presence of GaN pillar/air interfaces at the top surfaces, interference effects from the bottom AlN/Si/SiO₂/Si interfaces are significantly modulated. The pillar-like patterns suppressed the Fabry-Perot cavity effect originating from the AlN/Si/SiO₂/Si interfaces and as a result, led to a decrease in the PL spectral modulation at the higher wavelength regions.

4.3.2 Demonstration of PhC LED on SOI

It is well known that PL is not equivalent to EL. That is, a wafer with high PL efficiency may or may not exhibit high EL efficiency and hence good LEDs. Therefore, in order to demonstrate electrically simulated light emission from PhC-patterned LEDs, full LED device processing has been carried out. The micro-EL spectra recorded from LEDs with and without PhC structures as a function of different injection currents are shown in Figure 4.8. Multiple interference peaks toward the higher wavelength side with the energetic maxima centered ~ 510 nm were observed. The cavity effect due to presence of Fabry-Perot interfaces has led to strong EL intensity modulation as the spectra were obtained from the emission in a small solid angle in microscopic measurements. From the integrated EL spectra, an improvement of about 35-40% in integrated EL intensity is observed in the case of PhC LED when compared to bare LED chip on the same sample without nanopatterns. Although the improvement in the integrated EL intensity is smaller than reported literature [158-161], it is important to note that the improvement of 35-40% in integrated EL intensity is for a LED chip that is already on a reflective substrate (SOI). That is, the improvement in integrated EL intensity by the use of a reflective substrate (SOI) is already embedded in the result. This result shows the use of surface nano-patterning clearly led to an improvement in the light extraction efficiency.

Figure 4.8: Micro-EL spectra of PhC LED on SOI(111) substrate recorded under different injection currents. (a) and (b) represent EL spectra recorded from same LED layers with and without PhCs. (c) The light extraction is shown here with respect to integrated EL spectral intensity of LED chip surface with and without PhCs. Inset: SEM image of the Ni/Au p-contact deposited on top of shallow-etched nano-hole PhC patterned LED surface.

CHAPTER 5

AlGa_xN/GaN-based Heterostructures on SOI Substrate

The experimental results and discussions on the studies performed to show the applicability of the thin AlGa_xN layer grown on GaN template for UV detection are presented in this chapter and are divided into four sections. In the first section, material characterization of the as-grown Al_xGa_{1-x}N/GaN heterostructure on SOI substrate using techniques such as XTEM and HRXRD were discussed. The second section discussed the determination of the dislocation densities using HRXRD and hot H₃PO₄ etching followed by AFM studies. The determination of the Al composition in the thin Al_xGa_{1-x}N layer using a combination of techniques such as HRXRD, TEM and micro-PL was discussed in section three. The results and discussion on the study of the behavior of the optical phonons observed from the 2DEG interface were discussed in section four. UV micro-Raman spectroscopy was used to probe the as-grown layer structure as well as MSM PDs under electrical simulation. In the last section, the electrical properties of the UV PDs were discussed. To demonstrate the applicability of the thin AlGa_xN layer grown on GaN template for UV detection, device processing of the Schottky MSM PDs were carried out. Device characterization was carried out by performing I - V under dark and illumination conditions and spectral response measurements. The I - V characteristics of the devices under illumination are correlated to the responsivity results.

5.1 Material Characterization

5.1.1 Cross-sectional Transmission Electron Microscopy (XTEM)

The imaging of the epitaxial layers of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructure overgrown on a $\text{SOI}(111)$ substrate was carried out using XTEM and the images are shown in Figure 5.1. From the XTEM images, strain compensating low-temperature AlN interlayers within the thick GaN template, the AlGaN/AlN buffer layers as well as the Si overlayers grown on top of the buried oxide layer can be clearly seen. These LT-AlN interlayers are used during the epitaxial growth of GaN layers on SOI substrates to reduce tensile stress and to eliminate cracking of the thick GaN layers [101]. It can be seen from XTEM images that such interlayers are beneficial in reducing the screw dislocation density. From the XTEM images, the thicknesses of the respective layers were also determined.

Figure 5.1: (a) Schematic of the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructure on SOI(111) substrate. (b) The XTEM image of full structure showing thickness of individual epilayers, buffer and AlN/SOI(111) interfaces. (c) High-resolution TEM image of the top active GaN/ $\text{Al}_{0.29}\text{Ga}_{0.71}\text{N}$ /AlN/GaN layers. (d) A high-resolution TEM image of LT-AlN interlayer.

5.1.2 High Resolution X-Ray Diffraction (HRXRD)

The crystalline and structural properties of the LEDs were characterized using HRXRD measurements. The ω -2 θ scan of the (0002) diffraction planes of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ -based heterostructures on SOI(111) substrate is shown in Figure 5.2. The dominant peaks as shown in the HRXRD spectrum were from the thick GaN layers while the peaks at higher Bragg angles were from the AlGaIn buffer and the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer. The experimental Al content in the AlGaIn buffer is ~15% while in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer is ~29%. The FWHM of the (0002) ω scan revealed a value of 633 arcsec for the thick GaN layer and a value of 1024 arcsec for the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer. The observation of satellite diffraction peaks up to the sixth order at low-angles is due to the presence of nitride layers with sharp interfaces. High crystal quality GaN is represented by the nature of these satellites.

Figure 5.2: The HRXRD spectrum of (0002) diffraction planes of Al_xGa_{1-x}N/GaN epitaxial layers on SOI(111) substrate. The spectral features are associated with the high-temperature AlN and AlGaIn buffers, the GaN template and the top Al_xGa_{1-x}N epilayer.

5.2 Determination of dislocation densities

In MOCVD grown GaN epilayers, there are namely three types of TDs which dominated and known as pure-edge TDs, pure-screw TDs or mixed-type TDs. As pure edge TDs do not have a component in the *c*-direction, they are usually emerged into the terraces while step terminations are usually associated with screw/mixed TDs since screw/mixed TDs have a component in the *c*-direction [162]. Figure 5.3 show the $2\ \mu\text{m} \times 2\ \mu\text{m}$ AFM micrographs of the as-grown and etched Al_xGa_{1-x}N/GaN sample. From the AFM images of the as-grown and etched Al_xGa_{1-x}N/GaN sample, the surface and etched pits are mostly found at the step terminations. Hence, the etch pit densities are

attributed to be mostly screw/mixed TDs type and are estimated to be about $1.8 \times 10^9 \text{ cm}^{-2}$.

Figure 5.3: AFM image of the (a) as-grown Al_xGa_{1-x}N/GaN layers on SOI(111) substrate, and (b) same sample surface after etching in H₃PO₄.

HRXRD measurements were performed to obtain the FWHM of x-ray rocking curves of various symmetrical and asymmetrical Bragg reflections and a quantitative evaluation of dislocation densities were calculated using the Ayer's model [163], which is an extension of the Hordon and Averbach model [164]. The model described uses the X-ray linewidth broadening due to TDs with the assumption that the X-ray rocking curves peaks are Gaussian in shape. In other words, the measured rocking curve linewidth (β_m) represents a convolution of the following contributions; the intrinsic rocking curve width of the crystal being examined (β_0), the intrinsic rocking curve width due to the 4-bounce hybrid monochromator (β_d), the rocking curve broadening due to angular rotation at dislocations (β_a), the rocking curve broadening due to strain surrounding the dislocations (β_e), the rocking curve broadening due to crystal size (β_L), and the rocking curve broadening due to curvature of the crystal (β_r).

Therefore, the square of the measured rocking curve linewidth (β_m) is given by:

$$\begin{aligned} \beta_m^2(hkl) = & \beta_0^2(hkl) + \beta_d^2(hkl) + \beta_a^2(hkl) + \beta_e^2(hkl) + \beta_L^2(hkl) \\ & + \beta_r^2(hkl) \end{aligned} \quad (5.1)$$

The intrinsic rocking curve width of the crystal being examined and the intrinsic rocking curve width due to the hybrid monochromator are usually small which is in the range of few arcsec [163]. The rocking curve broadening due to crystal size can be neglected for films thicker than 1.0 μm . The rocking curve broadening due to curvature of the crystal is usually negligible when mismatched heteroepitaxial layers are deposited on substrates which are one hundred times thicker.

Thus, the equation can be further simplified to:

$$\beta_m^2(hkl) - \beta_0^2(hkl) - \beta_d^2(hkl) = \beta_{adj}^2 = \beta_\alpha^2(hkl) + \beta_\varepsilon^2(hkl) \quad (5.2)$$

where β_{adj} is the rocking curve width adjusted to account for the intrinsic rocking curve widths and

$$\beta_\alpha^2 = 2\pi \ln 2 b^2 D = K_\alpha \quad (5.3)$$

$$\beta_\varepsilon^2 = 0.090 b^2 D |\ln(2 \times 10^{-7} \text{ cm} \sqrt{D})| \tan^2 \theta = K_\varepsilon \tan^2 \theta \quad (5.4)$$

where b is the length of the burgers vector ($b_{\text{screw}} = 0.5185 \text{ nm}$, $b_{\text{edge}} = 0.3189 \text{ nm}$) [165] and D is the dislocation density.

Therefore,

$$\beta_{adj}^2 = \beta_\alpha^2(hkl) + \beta_\varepsilon^2(hkl) = K_\alpha + K_\varepsilon \tan^2 \theta \quad (5.5)$$

From the above equation, a linear plot with y-intercept K_α and gradient K_ε is obtained when the square of the FWHM of each rocking curve of reflections is plotted against $\tan^2 \theta$, where θ is the Bragg angle.

The threading dislocation density (D) can then be calculated from the y-intercept of the plot using the relation:

$$D = \text{y-intercept} / 4.36 b^2 \quad (5.6)$$

The screw and edge dislocation densities are then calculated from the plots using the data obtained from symmetrical and asymmetrical reflections, respectively [166-167].

From our HRXRD analysis, the screw and edge dislocation densities are found to be $1.2 \times 10^9 \text{ cm}^{-2}$ and $5.2 \times 10^9 \text{ cm}^{-2}$, respectively. These values closely agree with the etch pit densities and give an estimation of defect density in our GaN/SOI templates with $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /GaN active layers.

Figure 5.4: Plot of the square of the FWHM against $\tan^2 \theta$ for (a) symmetrical reflections and (b) asymmetrical reflections.

5.3 Determination of Al composition

From the literature, it was reported that the lattice constants $c(x)$ and $a(x)$ of the Al_xGa_{1-x}N layer can be determined by performing ω - 2θ scans of symmetric (0004) and asymmetric (10 $\bar{1}2$) reflections, respectively [168]. That is, using Bragg's law:

$$2d_{hkl} \sin \theta = n\lambda \quad (5.7)$$

where d_{hkl} is the lattice plane spacing of the plane (hkl), θ is the Bragg angle, n is the order of diffraction and λ is the Cu K α_1 radiation which is equal to 1.5406 Å; the lattice plane spacing d_{004} can be obtained from the Al_xGa_{1-x}N symmetric (0004) ω - 2θ scan XRD measurement, and hence the lattice parameter $c(x)$ is calculated. Using the same method, the lattice plane spacing d_{102} was determined from the Bragg angle of the (10 $\bar{1}2$) plane. With the calculated lattice parameter $c(x)$ and lattice plane spacing d_{102} , the lattice parameter $a(x)$ can be determined from the d spacing formula for hexagonal crystals:

$$\frac{1}{d_{hkl}^2} = \frac{4}{3} \left(\frac{h^2 + k^2 + hk}{a^2} \right) + \frac{1}{c^2} \quad (5.8)$$

Thus, the lattice constants $c(x)$ and $a(x)$ are 5.120 Å and 3.117 Å, respectively.

The Al compositions can be deduced from the following relation [168-169],

$$x = - \frac{a(x)c(x)(1+v) - a(x)c_0^{GaN} - a_0^{GaN}c(x)v}{a(x)c_0^{GaN} - a(x)c_0^{AlN} - a_0^{AlN}c(x)v + a_0^{GaN}c(x)v} \quad (5.9)$$

which takes the tetragonal deformation of the unit cell and strain induced into consideration. We have taken $a_0^{GaN} = 3.189$ Å, $a_0^{AlN} = 3.112$ Å, $c_0^{GaN} = 5.185$ Å, $c_0^{AlN} = 4.982$ Å as the relaxed lattice constants of the binary GaN and AlN.

The Poisson's ratio ν can be determined using the following relation [134,137,170]:

$$\frac{\varepsilon_{zz}}{\varepsilon_{xx}} = \frac{c(x) - c_0}{c_0} \times \frac{a_0}{a(x) - a_0} = -2 \frac{C_{13}}{C_{33}} = \frac{2\nu}{(1 + \nu)} \quad (5.10)$$

which relates the strain components ε_{zz} , ε_{xx} to the elastic constants C_{13} , C_{33} . A variation of elastic constants C_{13} , C_{33} for GaN and AlN were reported in the literature [134,137,170] and a Poisson's ratio of 0.44 used in this study results in the Al composition to be 45% for the Al_xGa_{1-x}N/GaN-based layer structure grown on SOI(111) substrate, which was too high compared to the expected Al composition from growth parameters. The discrepancy in the calculation of the Al composition was attributed to the variation of the Poisson's ratio and that the thin Al_xGa_{1-x}N layers are highly strained. It is important to note that the relations used to calculate the Al composition assumes that the thin Al_xGa_{1-x}N layers are fully strained [171]. To complement the findings, the diffraction patterns from the high resolution TEM images were also used to correlate the lattice constants of the thin Al_xGa_{1-x}N layers as well as from the underlying GaN layers. From TEM, the lattice constants $c(x)$ and $a(x)$ of the underlying GaN layer are 5.056 Å and 3.068 Å, respectively and the lattice constants $c(x)$ and $a(x)$ of the thin Al_xGa_{1-x}N layer are 4.995 Å and 3.090 Å, respectively. As expected, strain is presented in the layers as evidenced from the lattice constants. In addition, the in-plane lattice constants of the thin Al_xGa_{1-x}N layers and GaN obtained from the TEM analysis were not the same, supporting that the thin Al_xGa_{1-x}N layers were not fully strained. This observation supports the discrepancy in calculation of the Al content using the equations used in XRD analysis since the thin Al_xGa_{1-x}N layers are not fully

strained. The degree of relaxation in the thin Al_xGa_{1-x}N layer can be calculated using the following relation [172]:

$$R = \frac{a_s - a}{a_s - a_0} \quad (5.11)$$

where a refers to the measured lattice constant of the Al_xGa_{1-x}N layer by TEM, a_s refer to the in-plane lattice constant of the underlying GaN layer measured by TEM and a_0 refers to the in-plane lattice constant of the fully relaxed Al_xGa_{1-x}N layer, respectively. The lattice constants of the fully relaxed Al_xGa_{1-x}N layer can be determined from the following relations by assuming Vegard's law, which states that the lattice constants of an alloy will vary linearly between end members [134,168,171].

$$c_0^{AlGaN}(x) = c_0^{GaN}(1 - x) - c_0^{AlN}(x) \quad (5.12)$$

$$a_0^{AlGaN}(x) = a_0^{GaN}(1 - x) - a_0^{AlN}(x) \quad (5.13)$$

Therefore, using the relaxed lattice constants of the binary GaN and AlN, $a_0^{GaN} = 3.189 \text{ \AA}$, $a_0^{AlN} = 3.112 \text{ \AA}$, $c_0^{GaN} = 5.185 \text{ \AA}$, $c_0^{AlN} = 4.982 \text{ \AA}$ and 29% for the expected Al composition from the growth parameters, the lattice constants of the fully relaxed Al_xGa_{1-x}N layer are calculated to be $a_0^{AlGaN}(x) = 3.167 \text{ \AA}$, $c_0^{AlGaN}(x) = 5.126 \text{ \AA}$. Therefore, with the lattice constants of the Al_xGa_{1-x}N layer ($a = 3.090 \text{ \AA}$) measured by TEM, the in-plane lattice constant of the underlying GaN layer ($a_s = 3.068 \text{ \AA}$) measured by TEM, and the in-plane lattice constant of the fully relaxed Al_xGa_{1-x}N layer ($a_0 = 3.167 \text{ \AA}$) calculated by assuming Vegard's law, the degree of relaxation in the thin Al_xGa_{1-x}N layer is calculated to be ~22%.

With the lattice constants and thickness of the layers obtained from TEM, the Al composition was obtained by performing the simulation and fitting of the

(002) diffraction pattern as shown in Figure 5.5. With an Al composition of 29% and relaxation of 22% for the thin Al_xGa_{1-x}N layer respectively, the simulated and fitted peaks matched. Hence, an Al composition of 29% was thus obtained for the thin Al_xGa_{1-x}N layer for the Al_xGa_{1-x}N/GaN-based structure grown on SOI(111) substrate. The Al composition profile was also determined from the PL data. In the PL spectrum shown in Figure 5.6, the peak position at 3.42 eV corresponds to a near-band-edge transition from GaN while the peak located at 4.00 eV corresponds to the Al_xGa_{1-x}N layer with an Al composition of 29% as estimated from the following relation [173]:

$$E_g(x) = (1-x) E_g(\text{GaN}) + xE_g(\text{AlN}) - bx(1-x) \quad (5.14)$$

where $E_g(x)$ is the bandgap of Al_xGa_{1-x}N, x is the Al fraction, $E_g(\text{GaN})$ is the bandgap of GaN = 3.42 eV, $E_g(\text{AlN})$ is the bandgap of AlN = 6.20 eV, and b is the bowing parameter = 1.0 eV.

Figure 5.5: Simulated and fitted peaks of the (0002) diffraction planes.

Figure 5.6: The PL spectrum of this $\text{Al}_{0.29}\text{Ga}_{0.71}\text{N}/\text{GaN}$ epitaxial layer on SOI(111) substrate taken at room temperature.

5.4 2DEG interface vibrational properties by UV Micro-Raman Spectroscopy

In Raman experiments, the use of different laser excitation wavelengths allows the selective probing of phonon and material properties. For example, in GaN (bandgap of 3.4 eV), material properties can be probed under visible excitation wavelengths (514 nm), whereas surface properties can be studied using UV excitation (325 nm). With 325 nm excitation, the optical penetration depth is less than 40 nm in GaN [147-148]. Therefore, UV micro-Raman is used to probe the as-grown top layer structure as well as MSM PDs under electrical simulation to address the 2DEG interface vibrational properties.

Figure 5.7: (a) The UV micro-Raman spectrum recorded with a 325 nm resonant excitation from a He-Cd laser at 0 V bias. DARS: disorder-activated **Raman** scattering. (b) The behaviors of the intensities of interface phonon modes at 608 cm^{-1} and 720 cm^{-1} in UV Raman spectra with different applied bias voltages.

UV Raman resonantly excites the top Al_xGa_{1-x}N/AlN/GaN interfaces and the top-most region of the GaN 2DEG channel. The Raman experiments were performed with a micro-Raman setup in a backscattering geometry $z(x, -)z$, along the (0001) axis of the MSM PDs surface. From the Raman spectrum in Figure 5.7a, instead of just the typical E_2 -high and A_1 (LO) modes permitted in this backscattering geometry [146-147], three peaks at 608, 702 and 720 cm^{-1} are detected along with GaN E_2 -high mode. The position of the E_2 -high phonon of underlying GaN layer is observed at 568 cm^{-1} . Since unstrained GaN is characterized by an E_2 frequency of 567 cm^{-1} [146-147], the mode at 568 cm^{-1} indicates that the stress in the underlying GaN template is low. Compared with GaN and AlN, Al_xGa_{1-x}N alloys exhibit a lower structural quality (FWHM in HRXRD) and therefore, a disorder-activated phonon density of states (DOS) can manifest itself in the first-order spectra. Moreover, the disruption of the ordering at the Al_xGa_{1-x}N/AlN/GaN leads to the breakdown of the Raman selection rules and hence, the appearance of forbidden optical phonon peaks. It has been reported in literature that the phonon DOS of Al_xGa_{1-x}N alloys must have a corresponding singularity within the range 695–725 cm^{-1} [174], corresponding to the disorder-activated Raman scattering (DARS) phonon mode observed around 702 cm^{-1} in Figure 5.7a.

The other two modes observed at 608 cm^{-1} and 720 cm^{-1} seems to appear from the 2DEG interface and are thought to be interface modes. This was confirmed by measuring other Al_xGa_{1-x}N/GaN HFETs structures with high Al content in the Al_xGa_{1-x}N layer and similar optical vibration peaks were found in an molecular beam epitaxy (MBE)-grown Al_{0.39}Ga_{0.61}N/GaN

structure [175]. In HFETs structures with Al content $< 25\%$ which are transparent to the 325nm excitation wavelength, the $A_1(\text{LO})$ modes were clearly observed. In addition, there might be a query if the peak observed at 608 cm^{-1} belongs to the $A_1(\text{TO})$ of the thin AlN buffer layer used in the layer structure. However, this is impossible as the $A_1(\text{TO})$ is forbidden in the $z(x, -)z$ configuration used and the Raman excitation source probes maximum depth $< 40 \text{ nm}$.

Within the macroscopic dielectric continuum model (DCM) modified for uniaxial crystals, the frequencies for interface and confined modes can be deduced theoretically [176-178]. However, these theoretical analyses have been confined to highly symmetric and/or simple structures such as single or double quantum wells composed of binary semiconductors. When the structure is asymmetric or has multiple heterointerfaces, application of the DCM model becomes highly complicated due to the coupling between adjacent interfaces. A general method was developed by Lü et al. [179] to solve the equations for wurtzite multi-interface heterostructures by using the transfer matrix method [179-184] which reduces the complex derivation of the potential to a simple matrix multiplication. Following their method and applying it to air/GaN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /AlN/GaN system, there exist three interface modes as shown in Figure 5.8. Under the quasi-backscattering conditions in the Raman measurements with 325 nm excitation, the maximum wavevector $q_{\parallel}/d$ is around 0.3 (d is the thickness of GaN/ $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /AlN). From Figure 5.8, with $q_{\parallel}/d \approx 0.3$, three interface modes around 610 cm^{-1} (IF1), 715 cm^{-1} (IF2) and 790 cm^{-1} (IF3) at low in-plane wavevectors were found which matches

well with the experimental observations. Thus, the modes around 608 and 720 cm^{-1} are attributed to be interface modes.

Figure 5.8: Dispersion relations for the optical phonon interface (IF) modes in a GaN/Al_xGa_{1-x}N/AlN/GaN system. The Al content in the Al_xGa_{1-x}N layer is taken to be 29%.

In order to have a better understanding of the electrical properties of the MSM PDs, UV micro-Raman was performed to check on the behavior of the interface phonon modes by simultaneously probing the MSM PDs electrically. It has been suggested that interface phonon scattering plays an important role in the mobility of electrons in semiconductor heterostructures especially in the Al_xGa_{1-x}N/GaN heterostructures [185-189] since carriers transport in such heterostructures are mostly localized in the 2DEG close to the Al_xGa_{1-x}N/GaN interface. Indeed, changes in the UV-Raman intensity of the interface peaks as a function of an applied bias voltage were observed in

Figure 5.7(b). Differences in the frequency position of the peaks lie within the spectrometer resolution. By plotting the peak intensity as a function of the applied voltage, the quenching of the intensity of the phonon mode at 608 cm⁻¹ with increasing voltage was observed. The peak intensities have been normalized to the non-polar E_{2h} mode of the underlying GaN layer and to their own intensity at 0 V. Both peaks showed an anti-correlated trend in intensity with applied voltage. While the peak at 720 cm⁻¹ slightly increases with voltage, the one at 608 cm⁻¹ is strongly quenched. The quenching of the intensity of the phonon mode at 608 cm⁻¹ with increasing voltage is a clear indication of its strong electrostatic character. Such mode is supposed to lead the interaction with electrons and contribute most part of the scattering rates [188]. It was shown through theoretical calculations that an increase in the confinement degree of the electron states will lead to an increase in the electron-optical-phonon scattering rates in wurtzite semiconductor structures [188]. This would explain the voltage-dependent Raman results. The application of an external voltage in the Al_xGa_{1-x}N/GaN heterostructures modified the electronics bands such that the 2DEG is further confined to the interface. In a case where the Al_xGa_{1-x}N/GaN heterostructures is without the thin AlN spacer layer, the stronger confinement will lead to a penetration of the electron wave function into the Al_xGa_{1-x}N barrier layer which results in substantial alloy scattering rates. That is, with increasing bias, the electron-optical-phonon scattering rates increases. However, in our GaN/Al_xGa_{1-x}N/AlN/GaN structures where a thin AlN spacer layer is inserted, the penetration of the electron wave function from the GaN layer into the Al_xGa_{1-x}N barrier layer is prevented due to an increase in the conduction-band

discontinuity between the Al_xGa_{1-x}N barrier layer and the thick GaN layer, suppressing alloy scattering [187,189]. The electron-optical-phonon scattering rates is reduced which explains the quenching of the intensity of the phonon mode at 608 cm⁻¹. The different behavior observed for the mode at 720 cm⁻¹ suggests that it could not be an interface mode but instead, the mode could be the A₁(LO) phonon mode which arises from the GaN underneath and shifted from its typical value due to the screening effects of the 2DEG gas at the interface.

5.5 Device characterization

5.5.1 *I-V* and Responsivity measurements

In order to test out the applicability of such a thin Al_xGa_{1-x}N layer on a GaN/SOI template for UV detection, device processing of Schottky MSM UV PDs has been carried out. The *I-V* characteristics of the fabricated MSM PDs taken under the dark as well as illuminated conditions are shown in Figure 5.9(a). The photocurrent-to-dark current contrast ratio at 5 V applied bias is about 3 at 325 nm illumination. The dark current remains the same while the photocurrent increases with respect to applied voltage. The photo-to-dark current contrast ratio presented here is at a fixed intensity of 16 mW/cm². Although the photoexcitation from the 325 nm laser shows a low photo-to-dark current contrast ratio, the absolute value of the observed photocurrent below 320 nm excitation wavelengths could be very high considering our MSM design. This is because the Al content in the top Al_xGa_{1-x}N layer is >25% and we have used a 325 nm laser illumination which is lower than the bandgap of Al_xGa_{1-x}N layer. A higher dark current observed in this case is due to the

relatively high sheet carrier density of the 2DEG with the insertion of the thin AlN spacer (sheet carrier density $> 10^{13} \text{ cm}^{-2}$) along with an internal polarization field in this layer configuration on SOI [187,189]. However, this charge confinement at the 2DEG interfaces also leads to strong detector responsivity at shorter wavelength excitation $< 320 \text{ nm}$ as shown in Figure 5.9(b).

From the I - V plot in Figure 5.9(a), it was clear that photocurrent and dark current start to saturate at a bias voltage of 4 V. This saturation is caused by the complete depletion of the 2DEG channel below the cathode contact at the pinch-off voltage (V_p) when the flat-band conditions are reached and the electric field at the anode becomes zero [90,190-191]. At low bias voltages $< V_p$, the 2DEG with its high sheet carrier density acts as an equipotential plane. That is, the electric field and depletion region is confined within the AlGaIn layer, between the 2DEG and the Schottky contact. In this case, the capacitance of the device is mainly due to the carriers in the 2DEG channel. As bias voltage increases $> V_p$, the depletion region penetrates into the GaN layer underneath the channel. In this case, the capacitance of the device is dominated by the depletion region at the cathode side which is due primarily to the background donors in the GaN channel layer since the 2DEG channel is depleted at this side. The depletion of the 2DEG below the cathode contact leads to an increase in the channel resistance and absorbs any further increase in the applied bias. As a consequence, the photocurrent saturates and becomes less dependent on the bias voltage. The saturation is also observed in the responsivity measurements in Figure 5.9(b).

Figure 5.9: (a) I - V curves of $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ MSM PD on SOI(111) substrate measured under dark and illuminated conditions in reverse bias conditions. The inset shows the MSM configuration of the PDs. (b) The spectral responsivity plots of such PDs at different bias voltages.

The spectral responsivity curves versus wavelength plots at different applied bias are shown in Figure 5.9(b). It was observed that the measured responsivities at a wavelength of 250 nm varied from 1500 A/W at -3 V bias to 7800 A/W at -5 V bias. A saturation in the spectral response of such PDs was observed when spectral response tests were conducted with increased applied bias, which agreed with the saturation photocurrent observed in the I - V plot. The slight cut-off observed at a wavelength below 310 nm corresponds to the absorption band-edge of the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer with Al composition of 29% while the sharp cut-off around the 362 nm is due to the absorption band of GaN. Even for the low voltage bias of -3 V, the 2DEG interface acts as a barrier for the depletion layer where the upper $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer contributes to the photocurrent in the UV spectral regions resulting in a sharp increase in responsivity. The evidence of detectable photocurrent even at very low excitation intensity of 0.1 mW/cm^2 at 325 nm and the high spectral response in the UV spectral range signifies the high sensitivity of these MSM PDs fabricated on a composite SOI substrate.

CHAPTER 6

Conclusions

This thesis presents world's first demonstration of InGaN/GaN-based LEDs and AlGaIn/GaN-based detectors on large compliant 6-inch (111) SOI substrates. The improvements in device performance brought about by the utilization of such compliant substrate were studied in relation to the structural, optical and electrical properties. Since two different GaN-based devices are studied in this thesis, the conclusions and original contributions generated from this thesis are summarized with respect to the devices and are as follows:

InGaN/GaN-based LEDs

1. A look at the FWHM of the (0002) ω scan rocking curve reveals similar crystalline quality when the same InGaIn/GaN MQW LED structures grown on SOI(111) and bulk Si(111) substrates. From micro-Raman measurements, stress-free LED epilayers grown on SOI(111) and bulk Si(111) substrates were achieved. As evidenced from TEM, Crack-free thick GaN layers can be grown such highly refractive nanoscale SIMOX SOI substrates. Thus, the SOI(111) substrate serve as a potential alternative to replace bulk Si(111) substrate as the low cost approach to grow high crystalline quality and crack-free GaN epilayers for nitride-based LED devices.
2. LEDs were fabricated on both SOI(111) and bulk Si(111) substrates and an enhancement in the EL integrated intensity was observed for the LED

structures grown on SOI(111) substrate. The enhancement in the EL integrated intensity for the LEDs on SOI(111) substrate was due to

- a. A lesser visible light absorption by the SOI(111) substrate as compared to bulk Si(111) substrate,
- b. Fabry-Perot interference effects due to cavity form as a result of the high refractive index contrast at the AlN/SOI/SiO₂/Si interfaces.

Therefore, with the use of SOI(111) substrates for LEDs, an increased in the out-coupling of visible light can be achieved.

3. Despite similar layer structures and growth conditions, a difference in the emission wavelength from the LED structures was due to a difference in the In incorporation in the MQWs giving a green emission ~525 nm and a blue emission ~485 nm from the LED structures grown on SOI(111) and bulk Si(111) substrate, respectively. As a consequence of a lower surface temperature of the SOI wafer during MQW growth, a higher In content was incorporated in the MQWs. With this higher In-incorporation, LEDs emitting in the spectral region known as the green-gap were produced. It is a known fact that to produce LEDs with high quantum efficiencies in the green-gap spectral range (530 nm to 580 nm) is very challenging and usually in this spectral range which requires high In-incorporation, a decreasing internal quantum efficiency is expected. Instead, a higher EL integrated intensity was observed for such LEDs on SOI(111) substrate as compared to the LEDs grown on bulk Si(111) substrate. That is, with the use of SOI(111) substrates for LEDs, devices emitting efficiently in the green-gap spectral range can be produced. The realization of such devices

is highly desirable as they can improve the production of color displays based on red, green and blue LEDs.

4. A check on the amount of EL peak shift at high drive currents for the LEDs on SOI(111) and bulk Si(111) substrates shows a smaller EL peak shift for the LEDs on SOI(111) substrate. At high drive currents, a blue-shift in the EL emission peak occurs due to the band filling effect and the reduction of the piezoelectric field by the strain relaxation of the InGaN/GaN MQWs. On the other hand, the high drive currents lead to a red-shift in the EL emission peak due to local heating effects and temperature rise in the LED devices. For LEDs on SOI(111) substrate, the heat generated at the active junctions is less easily dissipated through the thin buried oxide layer as compared to the thermally conductive Si substrate. That is, the local heating of the device will lead to a larger red-shift in the EL peak which will compensate the blue-shifted EL at higher injection current. Therefore, the use of SOI substrates for LEDs is beneficial for wavelength stabilization to maintain color chromaticity when LEDs are driven at high injection currents.
5. From the light extraction studies, it was shown that with the creation of nano-patterns on the LED surfaces, an enhancement in the PL intensity can be achieved. However, this enhancement is dependent on factors such as etch depth, shape and periodicity of the nano-patterns as observed from the experimental results. Generally, the enhancement is due to an increased in surface area for photons scattering which generate more pathways for photons to escape and hence a higher PL. However, since a high PL measured from MQWs from unprocessed samples does not necessary

meant high EL from finished LEDs, full LED device processing was carried out completed with PhCs and light emission from the finished devices were recorded by performing micro-EL measurements. An improvement of about 35-40% in integrated EL intensity was observed in the case of PhC LED when compared to bare LED chip on the same sample without nanopatterns. Since the PhCs are used on LEDs grown on a SOI(111) substrate, the improvement of the integrated EL intensity from the use of the reflective substrate (SOI) is already embedded in the result. This study demonstrated that with the incorporation of photonic structures, light extraction efficiency of GaN LEDs on SOI substrates can be improved.

Al_xGa_{1-x}N/GaN-based PDs

1. The FWHM of the (0002) ω scan of the thick GaN layer which reveals a value of 633 arcsec shows that the crystalline quality of the Al_xGa_{1-x}N/GaN heterostructure grown on the SOI(111) substrate is comparable to an Al_xGa_{1-x}N/GaN heterostructure grown on a 6-inch silicon (111) substrate [192]. From micro-Raman measurements, stress-free Al_xGa_{1-x}N/GaN epilayers grown on SOI(111) substrate were achieved. Thus, the SOI(111) substrate can be considered as an alternative to bulk Si(111) substrate as a low cost approach to grow high quality and crack-free GaN epilayers for nitride-based PD devices.
2. A study on the dislocation densities values for the Al_xGa_{1-x}N/GaN heterostructure grown on 6-inch SOI(111) substrates was performed and was found to be in the range of $1.2 \times 10^9 \text{ cm}^{-2}$ to $5.2 \times 10^9 \text{ cm}^{-2}$. The

typical value of dislocation densities in GaN epilayers grown on sapphire has been reported to be in the range of 10^8 to 10^{10} cm^{-2} [134,193]. 4H-SiC substrate has been reported to give a better material quality of GaN epilayers and hence a lower defect density value when compared to GaN epilayers grown on sapphire substrates [194]. When silicon substrates are used for GaN growth, the typical value of dislocation densities in GaN epilayers were reported to be in the range of 10^9 to 10^{10} cm^{-2} [195-196]. Till date, there is no reference available in the literature to compare the defect density level in GaN epilayers on 6-inch SOI(111) substrate. Thus, the dislocation densities analysis performed gave an estimation of defect density for GaN/SOI templates with $\text{Al}_x\text{Ga}_{1-x}\text{N}$ /GaN active layers for field-effect transistor or 2DEG PD applications.

3. An over-estimation of the Al composition in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer occurs when only HRXRD was used. This was due to the wide range of values for Poisson's ratio available in the literature and the assumption used in the HRXRD relation for the calculation of the Al content; that the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer is fully strained. A check on the in-plane lattice constants of the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers and GaN obtained from the TEM analysis shows that the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer was not fully strained and explained the discrepancy in the calculation of the Al content using the HRXRD relations. Therefore, complementary techniques such as TEM and micro-PL should be used along with HRXRD for accurate Al content determination in thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers.
4. UV-micro Raman experiments with 325nm excitation and performed in a backscattering geometry $z(x, -)z$, along the (0001) axis of the MSM PDs

surface shows the appearance of forbidden optical phonon modes at 608, 702 and 720 cm^{-1} . While the mode at 702 cm^{-1} was attributed to be a disordered activated phonon mode, the modes at 608 and 720 cm^{-1} were thought to be interface modes. To confirm this, theoretical calculations incorporating the transfer matrix method was performed and 3 interface modes at 610, 715, and 790 cm^{-1} were found from the dispersion plot. From literature, it has been shown that interface phonon scattering plays an important role in the mobility of electrons in semiconductor heterostructures especially in the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures since carriers transport in such heterostructures are mostly localized in the 2DEG close to the interface [185-189]. Thus, in order to confirm if the modes observed at 608 and 720 cm^{-1} were interface modes, UV Raman spectroscopy is used to probe the MSM PDs under electrical simulation. With increased bias, changes in the UV Raman intensities of these two modes were observed with an anti-correlation trend. With increased bias, the intensities of the peak at 720 cm^{-1} was observed to increase slightly while the one at 608 cm^{-1} was strongly quenched. The quenching of the intensity of the phonon mode at 608 cm^{-1} with increasing voltage is a clear indication of its strong electrostatic character as such mode is supposed to lead the interaction with electrons and contribute to most part of the scattering rates. This confirms the phonon mode at 608 cm^{-1} to be an interface mode. Due to a different behavior observed for the mode at 720 cm^{-1} , this mode was attributed to be the $A_1(\text{LO})$ phonon mode which arises from the GaN underneath and shifted from its typical value due to the screening effects of the 2DEG gas at the interface.

5. The intensity of the interface modes was shown to be strongly dependent on the bias voltage applied to the MSM PD simultaneously probed electrically, and thus, to the photoresponse characteristics influenced by the electron-phonon interaction. The application of an external voltage in the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterostructures modified the electronics bands such that the 2DEG is further confined to the interface. In our structures where a thin AlN spacer is inserted between the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier layer and the thick GaN layer, electron penetration from the GaN channel into the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ barrier layer is suppressed which led to a reduction in the alloy disordering scattering. As a result, quenching of the intensity of the phonon mode at 608 cm^{-1} was observed in the voltage-dependent Raman measurements due to a reduction in the electron-optical-phonon scattering rates. However, the increased confinement of the 2DEG to the interface with a reduction in the electron-optical-phonon scattering rates also led to a strong detector responsivity at shorter wavelength excitation $< 320\text{ nm}$.
6. The I - V characteristics of the fabricated MSM PDs taken under the dark and illuminated conditions showed a low photocurrent-to-dark current contrast ratio of 3 at 5 V applied bias with 325 nm illumination with a fixed intensity of 16 mW/cm^2 . The low photocurrent-to-dark current contrast ratio was due to the high dark current. The high dark current is a consequence of the relatively high sheet carrier density of the 2DEG due to the insertion of the thin AlN spacer (sheet carrier density $> 10^{13}\text{ cm}^{-2}$) along with an internal polarization field. The observation of high dark current seems to suggest deleterious effects with the insertion of the thin AlN spacer at the $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ heterointerface. However, from the

spectral response curves, strong detector responsivity at shorter wavelength excitation < 320 nm was observed as a result of the charge confinement at the 2DEG interfaces.

7. Saturation of both the photocurrent and dark current was observed in the I - V as well as in the spectral response plots. The saturation is caused by the complete depletion of the 2DEG channel below the cathode contact at the pinch-off voltage (V_p) when flat-band conditions are reached and the electric field at the anode becomes zero. The completion depletion of the 2DEG below the cathode contact led to an increase in the channel resistance and absorbed any further increase in the applied bias. As a consequence, the photocurrent become less dependent on the bias voltage and led to saturation.
8. H. Jiang et al reported a peak responsivity of 114 mA/W at 350 nm with an applied bias of 15 V for a visible-blind Schottky MSM PDs fabricated on an undoped AlGaIn/GaN HEMT structure [90]. Another group reported a resultant responsivity at 360 nm varied from 0.11 to 0.12 A/W when the device was biased from 2 to 5 V for an UV MSM PDs based on the AlGaIn/GaN HEMT structure with the LT-AlGaIn intermediate layer [191]. The measured spectral responsivity of the fabricated device in this study varied from 1500 A/W at -3 V bias to 7800 A/W at 250 nm with an applied bias of -5 V which is much higher than these reported literature. An extremely high PD responsiveness at an incident light wavelength of 240 nm of 5.2×10^9 A/W was reported for an UV MSM PDs based on a 2DEG AlGaIn/GaN heterostructure on sapphire [88]. Since this is the first time data from a 6 inch Si-based substrate technology is being reported,

the results obtained in this thesis are quite comparable to data from such nitride layers on sapphire substrates.

9. The cut-offs observed at a wavelength below 310 nm and around 362 nm corresponds to the absorption band-edge of the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer with Al composition of 29% and the absorption band of GaN, respectively. The evidence of detectable photocurrent even at very low excitation intensity of 0.1 mW/cm^2 at 325 nm and the high spectral response in the UV spectral range indicates that by correctly tuning the the cutoff wavelength with Al content in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer to the desired UV wavelengths, highly sensitivity photo sensors can be designed.

In summary, bright electroluminescent InGaN/GaN-based LEDs and high sensitivity 2DEG AlGaIn/GaN-based MSM PDs on SOI platform were demonstrated. In an attempt to enhance light extraction, the fabrication of PhCs to create nano-patterned LED surfaces on SOI platform was also demonstrated. The results shown that with the benefits offered by the SOI substrate together with combination of PhCs, high brightness LEDs can be realized. An important study was made by performing UV Raman studies which shows the influence of the interface modes in the AlGaIn/GaN-based 2DEG structures and their scattering behaviors on the electrical properties of UV PDs. From the results, it was shown that by tuning the cutoff wavelength with Al content in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer to the desired UV wavelengths, such MSM PDs could be useful for highly sensitivity photo sensors.

CHAPTER 7

Recommendations for Future Work

In this thesis, nitride-based devices on a SOI platform were demonstrated for the first time. Therefore, there is still a lot of room for improvement with regards to the device performance on such a compliant substrate. Hence, we would like to make some recommendations for future work based on the current experimental results:

1. The growth of InGaN/GaN-based LED structures on the SOI platform shows comparable material quality to the Si platform. In addition, an improvement in the output of light was observed from the benefits offered by the SOI platform as well as with the incorporation of PhCs. However, the current LEDs demonstrated could only be useful for low power LEDs due to the poor heat dissipation of the SOI substrate. At high injection currents, excessive heating occurs which will lead to a degradation in the device performance. To target high power and high brightness LEDs, the fabrication of vertical LEDs sandwiched by two electrodes is highly desirable. That is, the growth of InGaN/GaN-based LED structures can be performed on a SOI platform to take advantage of the compliant principle to reduce the dislocation densities and achieve a better material quality. Upon which, transfer the as-grown LED structures to a substrate with high electrical and thermal conductivity such as copper for better heat

dissipation allowing higher injection currents to be applied so as to achieve high power and high brightness LEDs.

2. The growth of AlGaIn/GaN-based heterostructures on the SOI platform as UV PDs shows comparable material quality to reported work on a Si platform. Highly sensitive UV photosensors were also demonstrated when combined with a 2DEG with a substantial improvement in the responsivities compared to reported literature. The dislocation densities reported for such AlGaIn/GaN-based heterostructures on the SOI platform was comparable to similar such AlGaIn/GaN-based heterostructures on a Si platform used for HEMTs applications. Work for such AlGaIn/GaN-based heterostructures on the SOI platform can be explored for HEMTs applications.

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APPENDIX A- LIST OF ABBREVIATION

$a_0^{\text{GaN}}, c_0^{\text{GaN}}$	Relaxed lattice constants of the binary GaN
h_f	Thickness of the epilayer
h_s	Thickness of the substrate
E_F	Fermi level
E_c	Critical energy
$\{G\}$	Reciprocal lattice vectors
P_{pe}	Piezoelectric polarization
P_{sp}	Spontaneous polarization
V_f	Forward voltage
a_0	In-plane lattice constant of the fully relaxed $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer
$a_0^{\text{AlGa}}(x), c_0^{\text{AlGa}}(x)$	Lattice constants of the fully relaxed $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer
$a_0^{\text{AlN}}, c_0^{\text{AlN}}$	Relaxed lattice constants of the binary AlN
a_f	In-plane lattice constant of the epilayer
a_s	In-plane lattice constant of the substrate
a_s	In-plane lattice constant of the underlying GaN layer measured by TEM
d_{hkl}	Lattice plane spacing of the plane (hkl)
$k_{ m}$	In-plane wavevector of guided mode
k_0	Original in-plane wavevector
n_{GaN}	Refractive index of GaN
n_{air}	Refractive index of air
n_s	Refractive index of the active layer
n_{sc}	Sheet carrier concentration
t_{eff}	Effective critical thickness
K_α	y-intercept of the plot of the square of the FWHM of each rocking curve of reflections against $\tan^2\theta$
K_ε	gradient of the plot of the square of the FWHM of

	each rocking curve of reflections against $\tan^2\theta$
β_{adj}	Rocking curve width adjusted to account for the intrinsic rocking curve widths
η_{ext}	External quantum efficiency
η_{extr}	Light extraction efficiency
η_i	Internal quantum efficiency
θ_c	Critical angle
θ_i	Incident angle
θ_m	Angle of propagation within the active layer
σ_f	Biaxial stress in the film
σ_s	Biaxial stress in the substrate
σ_{xx}	Biaxial stress in the LED structures
ϵ_0	Total strain of the system due to the lattice mismatch
ϵ_f	Biaxial strain in the film
ϵ_s	Biaxial strain in the substrate
$\Delta\omega$	Raman shift
2D	2-dimensional
2DEG	Two dimensional electron gas
3D	Three-dimensional
a	Measured lattice constant of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer by TEM
AFM	Atomic-force microscopy
AlAs	Aluminum arsenide
AlGaN	Aluminum gallium nitride
AlN	Aluminum nitride
Ar	Argon gas
Au	Gold
b	Bowing parameter
$b, b_{\text{screw}}, b_{\text{edge}}$	Length of the burgers vector
BCl_3	Boron trichloride gas
BOX	Buried oxide

BSE	Backscattered electron imaging
$c(x)$, $a(x)$	Lattice constants or lattice parameters
C_{13} , C_{33}	Elastic constants
Cl_2	Chlorine gas
CMOS	Complementary metal-oxide-semiconductor
CHF_3	Trifluoromethane gas
D	Dislocation density
DARS	Disorder-activated Raman scattering
DCM	Dielectric continuum model
DI	Deionized
DOS	Density of states
EBL	Electron beam lithography
E_g	Bandgap of semiconductor
$E_g(\text{AlN})$	Bandgap of GaN
$E_g(\text{GaN})$	Bandgap of GaN
$E_g(x)$	Bandgap of $\text{Al}_x\text{Ga}_{1-x}\text{N}$
EL	Electroluminescence
Fe	Iron
FESEM	Field emission secondary electron microscope
FIB	Focused Ion Beam
FWHM	Full-width-at-half-maximum
GaAs	Gallium arsenide
GaN	Gallium nitride
GaP	Gallium phosphide
H_3PO_4	Phosphoric acid
HCl	Hydrochloric acid
He-Cd	Helium-Cadmium
HEMTs	High electron mobility transistors
HFETs	Heterostructure field effect transistors
HRXRD	High resolution X-ray diffraction
HT	High-temperature
$h\nu$	Energy of light
ICP	Inductively coupled plasma

InGaN	Indium gallium nitride
InN	Indium nitride
InP	Indium phosphide
I - V	Current-voltage
K	Elastic constant of the system
L	Thickness of the active (GaN) layer
LEDs	Light emitting diodes
LT	Low-temperature
m	Mode number
MBE	Molecular beam epitaxy
MOCVD	Metal-organic chemical vapor deposition
MOEMs	Micro-opto-electromechanical systems
MQWs	Multi-quantum wells
MSM	Metal-semiconductor-metal
n	Order of diffraction
N_2	Nitrogen gas
Ni	Nickel
OEICs	Optoelectronic-integrated-circuits
PDs	Photodetectors
PECVD	Plasma enhanced chemical vapor deposition
PhC	Photonic crystal
PL	Photoluminescence
Pt	Platinum
QCSE	Quantum confined Stark effect
RF	Radio frequency
RIE	Reactive-ion-etching
S.I.	Semi-insulating
SEI	Secondary electrons imaging
Si	Silicon
SiC	Silicon carbide
SIMOX	Separation by implantation of oxygen
SiN	Silicon nitride
SiO ₂	Silicon dioxide

SOI	Silicon-on-insulator
TDs	Threading dislocations
Ti	Titanium
TIR	Total internal refraction
UID	Unintentionally doped
UV	Ultraviolet
ν	Poisson's ratio
V_p	Pinch-off voltage
XTEM	Cross-sectional transmission electron microscopy
β_0	Intrinsic rocking curve width of the crystal being examined
β_d	Intrinsic rocking curve width due to the 4-bounce hybrid monochromator
β_L	Rocking curve broadening due to crystal size
β_m	Measured rocking curve linewidth
β_m	Measured rocking curve linewidth
β_r	Rocking curve broadening due to curvature of the crystal
β_α	Rocking curve broadening due to angular rotation at dislocations
β_ε	Rocking curve broadening due to strain surrounding the dislocations
$\varepsilon_{zz}, \varepsilon_{xx}$	Strain components
θ	Bragg angle
λ	Wavelength of light or radiation source
ω	Omega
$\omega-2\theta$	Omega-2theta
R	Degree of relaxation in the thin $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layer
n	Refractive index
x	Al composition
σ	Polarization induced sheet charge density

By applying the general method developed by Lü et al [179] to solve the equations for wurtzite multi-interface heterostructures using the transfer matrix method [180-184], the complex derivation of the potential is reduced to a simple matrix multiplication. Following the equation (12) in reference [179], we solve $M_{22} = 0$ to get the dispersion relation for the air/GaN/Al_xGa_{1-x}N/AlN/GaN system. The thickness of the air/GaN/Al_xGa_{1-x}N/AlN/GaN system is $\infty/2\text{nm}/17\text{nm}/1\text{nm}/2650\text{nm}$. After performing the calculations, it was found that the thin GaN capping layer ($\sim 2\text{nm}$) and the AlN spacer layer ($\sim 1\text{nm}$) did not affect the results. Thus, a simpler system air/Al_xGa_{1-x}N/GaN system with thickness $\infty/17\text{nm}/2650\text{nm}$ respectively will be derived here.

The equation in reference [179] states the following:

$$\begin{aligned}
 M_{22} = & (1 - \alpha_{45})(1 + \alpha_{34})(1 + \alpha_{23})(1 - \alpha_{12})e^{j(k_2d_2+k_3d_3+k_4d_4)} \\
 & + (1 - \alpha_{45})(1 + \alpha_{34})(1 - \alpha_{23})(1 + \alpha_{12})e^{j(-k_2d_2+k_3d_3+k_4d_4)} \\
 & + (1 + \alpha_{45})(1 - \alpha_{34})(1 + \alpha_{23})(1 - \alpha_{12})e^{j(k_2d_2+k_3d_3-k_4d_4)} \\
 & + (1 + \alpha_{45})(1 - \alpha_{34})(1 - \alpha_{23})(1 + \alpha_{12})e^{j(-k_2d_2+k_3d_3-k_4d_4)} \\
 & + (1 - \alpha_{45})(1 - \alpha_{34})(1 - \alpha_{23})(1 - \alpha_{12})e^{j(k_2d_2-k_3d_3+k_4d_4)} \\
 & + (1 - \alpha_{45})(1 - \alpha_{34})(1 + \alpha_{23})(1 + \alpha_{12})e^{j(-k_2d_2-k_3d_3+k_4d_4)} \\
 & + (1 + \alpha_{45})(1 + \alpha_{34})(1 - \alpha_{23})(1 - \alpha_{12})e^{j(k_2d_2-k_3d_3-k_4d_4)} \\
 & + (1 + \alpha_{45})(1 + \alpha_{34})(1 + \alpha_{23})(1 + \alpha_{12})e^{j(-k_2d_2-k_3d_3-k_4d_4)} = 0
 \end{aligned} \tag{B.1}$$

where

$$\alpha_{i,i+1} = \frac{k_i \varepsilon_{i,z}}{k_{i+1} \varepsilon_{i+1,z}}, \tag{B.2}$$

$$k_i = \sqrt{-(\varepsilon_p/\varepsilon_z)q}, \tag{B.3}$$

ε_p and ε_z are the dielectric constants of the respective materials in the direction parallel and perpendicular to the heterointerface respectively, d_i is the thickness of each layer and i is the order of the material in the whole system.

For the air/Al_xGa_{1-x}N/GaN system which consists of 3 layers where,

$$d_3 = d_4 = d_5 = d_{\text{GaN}}, \quad (\text{B.4})$$

$$\varepsilon_3 = \varepsilon_4 = \varepsilon_5 = \varepsilon_{\text{GaN}}, \quad (\text{B.5})$$

$$k_3 = k_4 = k_5 = \sqrt{-(\varepsilon_{(\text{GaN})p}/\varepsilon_{(\text{GaN})z})}q = i\sqrt{(\varepsilon_{(\text{GaN})p}/\varepsilon_{(\text{GaN})z})}q \quad (\text{B.6})$$

$$\alpha_{34} = \frac{k_i \varepsilon_{i,z}}{k_{i+1} \varepsilon_{i+1,z}} = \frac{k_3 \varepsilon_{3z}}{k_4 \varepsilon_{4z}} = 1 \quad (\text{B.7})$$

$$\alpha_{45} = \frac{k_i \varepsilon_{i,z}}{k_{i+1} \varepsilon_{i+1,z}} = \frac{k_4 \varepsilon_{4z}}{k_5 \varepsilon_{5z}} = 1 \quad (\text{B.8})$$

Substituting the above (B.4) to (B.8) into equation (B.1),

$$\begin{aligned} M_{22} &= 4(1 - \alpha_{23})(1 - \alpha_{12})e^{j(k_2 d_2 - k_3 d_3 - k_4 d_4)} \\ &+ 4(1 + \alpha_{23})(1 + \alpha_{12})e^{j(-k_2 d_2 - k_3 d_3 - k_4 d_4)} = 0 \end{aligned} \quad (\text{B.9})$$

Rearranging the above,

$$\begin{aligned} &4e^{-j(k_3 d_3 + k_4 d_4)}[(1 - \alpha_{23})(1 - \alpha_{12})e^{j(k_2 d_2)} \\ &+ (1 + \alpha_{23})(1 + \alpha_{12})e^{-j(k_2 d_2)}] = 0 \end{aligned} \quad (\text{B.10})$$

Rearranging and expanding,

$$\begin{aligned} &1[e^{j(k_2 d_2)} + e^{-j(k_2 d_2)}] - \alpha_{12}[e^{j(k_2 d_2)} - e^{-j(k_2 d_2)}] \\ &- \alpha_{23}[e^{j(k_2 d_2)} - e^{-j(k_2 d_2)}] + \alpha_{12}\alpha_{23}[e^{j(k_2 d_2)} + e^{-j(k_2 d_2)}] = 0 \end{aligned} \quad (\text{B.11})$$

Introducing hyperbolic functions where

$$\sinh x = [(e^x - e^{-x})]/2, \quad (\text{B.12})$$

$$\cosh x = [(e^x + e^{-x})]/2 \quad (\text{B.13})$$

And noticing the exponential functions carry an imaginary number, we let

$$k' = jk \quad (\text{B.14})$$

The equation (B.11) becomes

$$2\cosh k'_2 d_2 - 2(\alpha_{12} + \alpha_{23}) \sinh k'_2 d_2 + 2\alpha_{12}\alpha_{23} \cosh k'_2 d_2 = 0 \quad (\text{B.15})$$

Simplifying,

$$1 - (\alpha_{12} + \alpha_{23}) \tanh k'_2 d_2 + \alpha_{12}\alpha_{23} = 0 \quad (\text{B.16})$$

For the air/AlGa_N/GaN system,

$$k_1 = \sqrt{-(\varepsilon_{1p}/\varepsilon_{1z})}q = \sqrt{-(\varepsilon_{(air)p}/\varepsilon_{(air)z})}q = iq \quad (\text{B.17})$$

$$\begin{aligned} k_2 &= \sqrt{-(\varepsilon_{2p}/\varepsilon_{2z})}q = \sqrt{-(\varepsilon_{(AlGaN)p}/\varepsilon_{(AlGaN)z})}q \\ &= i\sqrt{(\varepsilon_{(AlGaN)p}/\varepsilon_{(AlGaN)z})}q \end{aligned} \quad (\text{B.18})$$

$$\begin{aligned} k_3 &= \sqrt{-(\varepsilon_{3p}/\varepsilon_{3z})}q = \sqrt{-(\varepsilon_{(GaN)p}/\varepsilon_{(GaN)z})}q \\ &= i\sqrt{(\varepsilon_{(GaN)p}/\varepsilon_{(GaN)z})}q \end{aligned} \quad (\text{B.19})$$

$$\alpha_{12} = \frac{k_1 \varepsilon_{1z}}{k_2 \varepsilon_{2z}} = \frac{1}{\sqrt{\varepsilon_{2p}\varepsilon_{2z}}} \quad (\text{B.20})$$

$$\alpha_{23} = \frac{k_2 \varepsilon_{2z}}{k_3 \varepsilon_{3z}} = \sqrt{\frac{\varepsilon_{2p}\varepsilon_{2z}}{\varepsilon_{3p}\varepsilon_{3z}}} \quad (\text{B.21})$$

Substituting the above (B.17) to (B.21) into equation (B.16) and simplifying,

$$\sqrt{\varepsilon_{2p}\varepsilon_{2z}}(\sqrt{\varepsilon_{3p}\varepsilon_{3z}} + 1) - (\sqrt{\varepsilon_{3p}\varepsilon_{3z}} + \varepsilon_{2p}\varepsilon_{2z}) \tanh(k'_2 d_2) = 0 \quad (\text{B.22})$$

Substituting in (B.14) and (B.18) :

$$\sqrt{\varepsilon_{2p}\varepsilon_{2z}}(\sqrt{\varepsilon_{3p}\varepsilon_{3z}} + 1) + (\sqrt{\varepsilon_{3p}\varepsilon_{3z}} - \varepsilon_{2p}\varepsilon_{2z}) \tanh\left(qd_2 \sqrt{\frac{\varepsilon_{2p}}{\varepsilon_{2z}}}\right) = 0 \quad (\text{B.23})$$

The dispersion relation for the optical phonon interface modes in the air/GaN/Al_xGa_{1-x}N/AlN/GaN system [Figure 5.8] can then be obtained by solving equation (B.23) where

$$\varepsilon_{i,p}(\omega) = \varepsilon_{i,p}^{\infty} \frac{\omega^2 - \omega_{i,p,L}^2}{\omega^2 - \omega_{i,p,T}^2} \quad (\text{B.24})$$

for E_1 phonons and

$$\varepsilon_{i,z}(\omega) = \varepsilon_{i,z}^{\infty} \frac{\omega^2 - \omega_{i,z,L}^2}{\omega^2 - \omega_{i,z,T}^2} \quad (\text{B.25})$$

for A_1 phonons.

ε_p^{∞} and ε_z^{∞} are the optical dielectric constants of the materials, i is the order of the materials in the system, $\omega_{p,L}$ and $\omega_{z,L}$ are the zone center longitudinal $E_1(\text{LO})$ and $A_1(\text{LO})$ phonon frequencies, and $\omega_{p,T}$ and $\omega_{z,T}$ are the zone center transverse $E_1(\text{TO})$ and $A_1(\text{TO})$ phonon frequencies of the bulk materials.