STUDY OF GaN LOW DIMENSIONAL STRUCTURES ON SILICON SUBSTRATES GROWN BY THERMAL VAPOR DEPOSITION FOR PHOTODIODE AND SOLAR CELL APPLICATIONS

By

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DEDICATION

To my parents: *Thank you for teaching me to believe in myself while always pushing me to do better. Your advice has helped me to make both the easy and hard decisions and your support has given me the confidence to follow through. I'll need it more than ever in the coming months".*

To my beloved wife and kids: *Who suffered and sacrificed a lot during my absence from Sudan. Thank you for believing in me; for allowing to me further my studies. Please do not ever doubt my dedication and love you.*

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K.M. Saron

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LIST OF SYMBOLS

ε_o	Absolute dielectric constant
T	Absolute temperature
α	Absorption coefficient
N_A	Acceptor concentration
A	Area
D	Average crystal size
k	Boltzmann constant
μ	Carrier mobility
E_C	Conduction band edge
σ	Conductivity
R_c	Contact resistance
β	Contrast ratio of photo and dark current
I	Current
J	Current density
J-V	Current density–voltage
I-V	Current–voltage
W_D	Depletion layer width
V_d	Diffusion voltage
N_D	Donor concentration
N_c	Effective density of states
μ	Effective dipole moment
m^*	Effective mass
ΔV	Electrical polarization
q	Electron charge
m_n	Electron effective mass
m_o	Electron mass
μ_n	Electron mobility
E_F	Fermi level of semiconductor
φ_{BF}	Flat band barrier height
F	Force
n	Free electron concentration
p	Free hole concentration
ν	Frequency
G	Gain
R_H	Hall coefficient
V_H	Hall voltage
m_p	Hole effective mass
μ_p	Hole mobility
θ_i	Hydrogen atoms coverage at the interface
n	Ideality factor
P_{in}	Incident solar power

θ	Incident/Diffraction angle
∞	Infinity
d	Interplanar spacing of the crystal planes
a	Lattice constant along x-axis
c	Lattice constant along z-axis
I_m	Maximum current
J_m	Maximum current density
$\mathrm{P_m}$	Maximum output power
ϕ_m	Metal work function
(hkil)	Miller indices
N_i	Number of sites (dipole moment) per area at the interface
ω	Photon frequency
h	Planck's constant
η	Quantum efficiency
ε_r	Relative dielectric constant
R	Resistance
ρ	Resistivity
S	Responsivity
A^{**}	Richardson's constant
I_o	Saturation current
φ_B	Schottky barrier height
E_g	Semiconductor band gap
χ	Semiconductor electron affinity
ϕ_S	Semiconductor work function
R_s	Series resistance
I_{SC}	Short circuit current
J_{SC}	Short circuit current density
R_{sh}	Shunt resistance
σ_s	Standard deviation
ε_a	Strain along a-axis
ε_c	Strain along c-axis
t	Thickness
τ	Time
L_t	Transfer length
E_v	Valence band edge
V	Voltage
ϑ	Volume
λ	Wavelength
w	Width
W_C	Width of the pad

LIST OF MAJOR ABBREVIATIONS

Al	Aluminum
NH_3	Ammonia solution or gas
NH_4F	Ammonium fluoride
NH_4OH	Ammonium hydroxide
ARC	Anti-reflection coating
a. u.	Arbitrary unit
Ar^+	Argon-ion
BE	Band emission
BH	Barrier height
CVD	Chemical vapor deposition
CB	Conduction band
Cu	Copper
c-Si	Crystalline silicon
DI	Deionized water
DC	Direct current
E_2-H	E_2 (high) phonon mode
EMT	Effective mass theory
e-h	Electron-hole
EDX	Energy dispersive X-ray
Eq	Equation
FF	Fill factor
FWHM	Full width at half maximum
GaN	Gallium nitride
He-Cd	Helium cadmium
HCP	Hexagonal close packed
HMDS	Hexamethyldisilazane
HT	Horizontal tube
HTF	Horizontal tube furnace
HF	Hydrofluoric
InGaN	Indium Gallium nitride
InN	Indium nitride
LPM	Liter per minute

LO	Longitudinal optical
Low D	Low-Dimensional
MIS	Metal insulator semiconductor
MS	Metal semiconductor
MSM	Metal-semiconductor-metal
NBs	Nano belts
NRs	Nano rods
NWs	Nano wires
nm	Nanometer
NBE	Near band edge
Ni	Nickel
PD	Photodiode
PL	Photoluminescence
PV	Photovoltaic
PVD	Physical vapor deposition
KOH	Potassium hydroxide
RCA	Radio Corporation of America
RF	Radio frequency
RT	Room temperature
RMS	Root mean square
rpm	rotation per minute
SEM	Scanning electronic microscopy
SBH	Schottky barrier height
SiO_2	Silicon dioxide
Ag	Silver
AM0	Solar constant
SCLC	Space charge limited current mechanism
Temp	Temperature
T-I-V	Temperature depend on current voltage characteristics
TCVD	Thermal chemical vapor deposition
TE	Thermal evaporation
TVD	Thermal vapor deposition
TE	Thermionic emission

TED	Transmission electron diffraction
TCO	Transparent conductive oxide
UV	Ultraviolet
VB	Valence band
VT	Vapor transport
VLS	Vapor liquid solid
VS	Vapor-solid
WZ	Wurtzite
XRD	X-ray diffraction
Z-B	Zero-bias
ZB	Zinc blende
ZnO	Zinc oxide

KAJIAN STRUKTUR GaN BERDIMENSI RENDAH PADA SUBSTRAT SILIKON YANG DITUMBUHKAN MENGGUNAKAN PEMENDAPAN WAP HABA UNTUK APLIKASI FOTODIOD DAN SEL SURIA

ABSTRAK

Galium nitrida (GaN) merupakan semikonduktor jurang jalur dengan aplikasi dalam peranti elektronik dan optoelektronik kuasa tinggi. Sel suria heterostruktur yang melibatkan struktur GaN berdimensi rendah (D rendah) pada substrak silikon (Si) berhablur tunggal adalah pilihan yang lebih baik kerana ia mempunyai kecekapan kuantum dalaman yang amat berkesan, voltan litar terbuka yang besar, dan kos pemprosesan yang rendah. Tesis ini mengkaji pertumbuhan struktur GaN berdimensi D rendah pada substrat Si menggunakan teknik pemendapan wap haba (TVD) yang murah untuk sel suria dan peranti fotodiod (PD). Pertumbuhan ini dicapai menggunakan dua kaedah. Kaedah pertama melibatkan pertumbuhan struktur GaN D rendah pada n-Si (111) dalam persekitaran bebas $NH_{3,}$ menggunakan TVD melalui penyejatan haba serbuk GaN di bawah pengaruh gas pembawa, suhu substrat dan masa pemendapan yang berbeza. Keputusan menunjukkan bahawa morfologi dan bentuk struktur GaN D rendah amat bergantung pada setiap parameter. Belauan sinar X dan spektrum Raman daripada struktur GaN D rendah menunjukkan bahawa struktur GaN mempunyai struktur wurtzit heksagon. Persekitaran bebas NH_3 dalam TVD dioptimumkan dengan menggunakan masa pemendapan 1 jam dan suhu pertumbuhan 1000°C untuk memperoleh struktur D rendah yang seragam dengan kualiti hablur yang baik di samping meningkatkan prestasi PD dan peranti sel suria Semasa pendedahan pada cahaya tampak dan UV (365nm) sampel yang dioptimum sebagai PD menunjukkan arus yang tinggi diperoleh pada 522.5 di bawah cahaya tampak dan 11.3 di bawah cahaya UV (ultralembayung). Sebagai sel suria,

kecekapan penukaran adalah setinggi 5.78% di bawah 30 pencahayaan mW/cm^2 Dalam kaedah yang kedua, pertumbuhan saput dan struktur GaN D rendah dalam TVD menggunakan larutan NH_3 dijalankan dengan mengubah kadar aliran gas pembawa N_2 dan satah substrat Si. Sampel yang dioptimumkan (dengan kadar aliran 2 liter/min, (111) satah n-Si) menunjukkan tekanan yang paling rendah dan puncak pemancaran UV tertinggi (363,8 nm) tanpa adanya puncak pemancaran kuning, jika dibandingkan dengan sampel struktur D rendah yang lain. Heterosimpang GaN/n-Si (111) difabrikasikan sebagai PD, yang menunjukkan arus tertinggi 736.8 diperoleh di bawah cahaya tampak dan 5.8 di bawah cahaya UV. Semasa pencahayaan (30 mW/cm^2), sel suria heterosimpang GaN/n-Si (111) menunjukkan kecekapan penukaran yang lebih tinggi iaitu 6.22%, berbanding dengan 3.69% bagi sel suria GaN/n-Si (100). Akhir sekali, konfigurasi logam-semikonduktor-logam (MSM) berasaskan GaN, iaitu saput pada n-Si (111) difabrikasikan untuk pengesanan UV. Semasa pendedahan pada cahaya UV (365 nm) (UV) pada 5 voltan pincang yang dienap selama 45 minit, pengesan MSM UV menunjukkan kebolehresponan yang tinggi 0.29 dan kecekapan penukaran 98.3%. Kajian itu menunjukkan kemungkinan mensintesis struktur GaN D rendah diatas substrat pada kos rendah dengan aplikasi yang berpotensi dalam foto pengesanan detection dan fotovoltan sel suria.

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ABSTRACT

Gallium nitride (GaN) is a greatly promising wide band gap semiconductor with applications in high power electronic and optoelectronic devices. Heterostructure solar cell involving GaN low Dimensional (low D) structures on single crystalline silicon (Si) substrates are the preferable choice as they have excellent internal quantum efficiencies, large open-circuit voltages, and low processing cost. This thesis examines the growth of GaN low D structures on Si substrates using inexpensive thermal vapor deposition (TVD) techniques for solar cell and photodiode (PD) devices. The growth was achieved using two methods. The first method involved the growth of GaN low D structures on n-Si (111) in NH_3-free environments by TVD via thermal evaporation of GaN powder under different carrier gases, substrate temperatures and deposition times. The result showed that the morphology and shape of GaN low D structures are highly dependent on each parameter. The X-ray diffraction and Raman spectra of the low D structures indicated that the GaN structure had a hexagonal wurtzite structure. The TVD is optimized by using 1h deposition time and 1000^{o}C temperature to obtain uniform dense low D structures with good crystalline quality and hence enhanced performance of PD and solar cell devices. Upon exposure to visible and UV (365nm) lights, the optimized sample work as PD showed high current gain of 522.5 under visible light and current gain of 11.3 under UV light. As solar cell, the conversion efficiency is as high as 5.78% under 30 mW/cm^2 illumination. In the second method, the growth of GaN low D structures and films by TVD using NH_3 solution were

carried out by changing the flow rate of N_2 carrier gas and plane of Si substrates. The optimized sample (with flow rate of 2 liter/min, (111) plane of n-Si) shows the lowest stress and highest UV emission at (363.8 nm) peak with almost no yellow emission peak compared to the other low D structures samples. The GaN/n-Si (111) heterojunction was fabricated as PDs, which showed high current gain of 736.8 under visible light and current gain of 5.8 under UV light. Upon illumination (30 mW/cm^2), the GaN/n-Si (111) heterojunction solar cell exhibited higher conversion efficiency of 6.22% compared to 3.69% for GaN/n-Si (100) solar cell. Finally, metal-semiconductor-metal (MSM) configurations based on GaN film on n-Si (111) was fabricated for UV detection. Upon exposure to (365 nm) UV light at a 5 bias voltage for the 45 min deposition time, the MSM UV detector exhibited a high responsivity of 0.29 and a conversion efficiency of 98.3%. The study showed the possibility of fabricating GaN low D structures on Si substrates at low-cost with potential applications in photodetection and photovoltaic solar cell.

CHAPTER 1:

INTRODUCTION

1.1 Introduction

Over the years, intensive researches on semiconductor materials have been conducted to properly investigate their inherent features and applicability. Wide band gap semiconductor material systems (like SiC, ZnO and III-Nitrides related materials) have been developed and regularly applied in electronics, optoelectronics, and numerous other fields [1-3]. Gallium nitride (GaN) has drawn the most attention for future optoelectronic applications due to its unique properties as a semiconductor material [3]. Their distinct features include high electron mobility, high thermal conductivity, large exciton binding energy (~25meV) at room temperature (RT) and wide and direct bandgap (3.4eV). Other distinct features are high breakdown field, due to relatively stable physical properties even under harsh environments, and better chemical stability. These properties make it suitable for several optoelectronic applications such as; field-emission [4], light-emitting diodes [5], short-wavelength optical devices [3, 6], thermoelectrics [5], sensing [7], and energy conversion photovoltaic solar cell [8, 9]. It is also a suitable material for fabricating photodetectors capable of rejecting near infrared and visible regions of the solar spectrum while retaining near unity quantum efficiency in the UV [9]. Moreover, in optoelectronics, GaN is mainly of interest for its potential as a blue and UV light emitter [3].

Many properties of semiconductor materials are based on their crystalline structure. Two common crystal structures of group III-Nitrides and GaN are the hexagonal close packed (HCP) wurtzite (WZ) and face-centered cubic (FCC) zinc blende (ZB). Wurtzite is the most common crystalline form of GaN due to its

thermodynamic stability in ambient condition, while the ZB is a polymorph derived from WZ at high external pressure. The ZB structure is metastable and may be stabilized by epitaxial growth on Si, GaAs, and SiC under certain growth condition [10, 11]. However, bulk of the research has been centered on the direct-transition bandgap structures of WZ crystal phase, because the growth of the WZ is simpler and less expensive than that of the ZB. In both hexagonal and cubic form, GaN have direct bandgap, indeed, the hexagonal structure is stable and can be grown on various substrates like sapphire, SiC and Si [8]. The most important physical properties of GaN, for both WZ and ZB, significant for electronic devices, are reported and compared with those of Si, AlN and ZnO in the table in Appendix 1 [12, 13].

The past decades has witnessed critical considerations being given to the importance of epitaxial growth in the processing of electronic and optoelectronic devices. Two epitaxial processes are commonly utilized: 1) homo-epitaxy and 2) hetero-epitaxy. Homo-epitaxy involves growth on the substrate of the same material (native substrate) while hetero-epitaxy entails the growth of single crystalline materials on non-native substrates. Hetero-epitaxy is generally used for growing GaN due to lack of homosubstrates. The limitations of GaN-based technology development include; the lack of high quality, large native substrates in large quantities and most of the epitaxial research and device progress depend on heteroepitaxial growth. In the semiconductor technology, most integrated circuits are virtually developed on Si substrates. However, GaN based semiconductor materials have also gained more and more importance in the last two decades. But, Si and conventional III-V materials are not appropriate for fabricating optoelectronic devices in the violet and blue bands of the visible region. Moreover, GaAs based

materials cannot be utilized at soaring temperature. Therefore, GaN is more suited for these areas. GaN based devices are epitaxially grown on Si (111), Al_2O_3 (0001) (sapphire) or SiC (0001) substrates due to the hexagonal surface symmetry and the lack of suitable and cheap homosubstrates [14-16]. However, growth on these substrates is accompanied by a number of deep-level defects, such as dislocations due to disparity in thermal, lattice mismatch and strain (tensile or compressive), which may control the consistency and applicability of GaN-based devices. As far as Al_2O_3 is concerned, the low thermal conductivity makes it less suitable for packaging of high power devices. From the lattice constants and thermal coefficient requirements, SiC is the best option although, it is very expensive. A high-quality 4 inch wafer costs about USD3000, whereas wafers of a larger diameter are currently not available [13]. Silicon (Si) has attracted considerable attention as a substrate material for GaN growth because of its high quality, low cost, wide availability in large diameters, accessibility, promising route for large-scale manufacture, and low-cost mass production [13, 17, 18]. These advantages have made GaN growth on Si highly desirable in the Si-based electronic industry. In addition, the integration of well-established Si electronics with GaN-based photonic devices (optoelectronic integrated circuits (OEICs)) has also proved lucrative in the manufacturing industry.

Recently, low dimensional (low D) semiconductor materials have received great attention due to their unique structure, and superior properties. Low D materials are the class of materials whose structural units are nanoscale low D systems such as quantum dots, rods and wires, quantum fractal networks, nanotubes, etc. Because of the quantum confinement effects, the physical properties of such systems are completely different than those of bulk systems. Such materials are becoming firm ground for the improvement of the rapidly developing area, nanotechnology. Due to

the unusual properties of low D functional materials, their potential to be used in energy- and resource-saving technologies is tremendously high. Among the low D structured materials, GaN nanowires are very interesting with the charge carrier confined in a one-dimension (1D) space owing to their special configuration. GaN nanowires represent unique systems for exploring phenomena at the nanoscale and are expected to play a critical role in future electronic and optoelectronic devices.

Most of the device development depends upon epitaxial growth. The properties of GaN-based optoelectronic (OE) devices are influenced by several variables of the fabrication process of GaN. One of the most significant factors is the growth process of GaN low D structures or films, which controls the structural, optical, and electrical properties of GaN epilayers. However, this growth procedure poses a serious problem as a result of the low decomposition of GaN relative to its high melting temperature, the low solubility of nitrogen in Ga and the high equilibrium vapor pressure of nitrogen on GaN at moderate temperatures. Several studies have made efforts to grow GaN with different morphologies, different optical and electrical properties using various growth techniques. These methods include; metal organic chemical vapor deposition (MOCVD) [19, 20], hydride vapour phase epitaxy (HVPE) [21], molecular beam epitaxy (MBE) [22], physical vapor deposition (PVD) via thermal evaporation techniques [23] and chemical vapor deposition (CVD) [8]. Among the widely studied techniques for GaN nanostructures or film growth, the thermal evaporation technique via vapor phase transport has shown the most potential because of its comparatively uncomplicated experimental procedure, its low melting point, low decomposition or low sublimation point oxides, inexpensive method, and high growth GaN yield [24].

1.2 The Problem Statements

Several essential problems are addressed in this research, and they are summarized as follows: A major issue for the success of GaN based optoelectronics industry is reducing the device cost and simultaneously integrating the GaN based-device with Si electronics on the same chip. GaN based devices are commonly grown by MBE and MOCVD techniques, both requiring expensive equipment and/or reagents. In the particular case of solar cells applications, it would be essential to find inexpensive preparation techniques of GaN semiconductors. Another important issue in growing GaN is that N_2 molecules have a very strong binding energy, and this makes it becomes impossible to decompose N_2 vapor molecules in the growth chamber by thermal means temperatures. But normally, other precursors as NH_3 gas or atomic nitrogen from a radio frequency source are used to grow GaN low D structures or films. Thermal vapor deposition (TVD) is currently employed to deposit GaN by using a direct reaction of Ga with NH_3 gas. In order to promote the formation of GaN, it is necessary to keep the NH_3 gas partial pressure above 1 bar.

This is even more so that it is practically very difficult to make a fully GaN-based high efficiency solar cell. This is partly related to the relatively inferior quality of GaN crystals grown epitaxially on some heterogeneous substrates, such as SiC and sapphire, as well as to the problems associated with p-type doping in GaN. However, growth of GaN-based device structures on Si is currently achieved by using AlN or Si_3N_4 as buffer layers between the Si and the active layer to reduce defects in the GaN layer. But the insulator properties of Si_3N_4 and AlN have a deleterious effect on transport properties of the junction.

This study, therefore, experimented with a low cost and a conventional TVD method to grow GaN low D structures on Si substrates for photodiodes and solar cells applications. The GaN low D structures were directly grown on Si substrates via the thermal evaporation of two material sources: GaN and Ga in environmental free from NH_3 and by using NH_3 solution. Subsequently, the influence of growth parameters on morphology, structure, optical, electrical properties and as well as the heterojunction devices such as photodiodes, solar cell descriptions were also investigated to understand what the growth of GaN low D structures using TVD will produce. This was to investigate whether it will exhibit a facile and inexpensive method to assemble GaN/Si junctions for developing solar cell application materials.

Since the PVD has serious limitations in achieving conformal coverage on high crystalline and optical quality, TCVD has received recent attention as a deposition method for GaN. Hence, if the growth of GaN is performed in NH_3 solution and the flow rate of N_2 carrier gas, growth temperatures are controlled, the structure and optical properties of the grown GaN should improve. The fixed volatilization of NH_3 from solution is expected to have a beneficial effect in promoting formation of GaN. To circumvent the problems associated with p-type doping in GaN, the researcher grew readily attainable GaN structures on n-type Si substrates, so that p-n junction heterostructures are created for photovoltaic characteristics. High temperature growth of GaN low D structures can therefore, significantly, play a role as auto doping, possibly due to the inter-diffusion of the Ga into the Si substrate to produce heavy p-type doped Si surface. The wide-bandgap window layer embedding GaN low D structures can then be used as a simpler solar cell design strategy.

1.3 Research Objectives

The principal objectives of this project can be summarized in the following points:

1. To determine the optimal growth parameters that influence the structural, optical and electrical properties of GaN low dimensional structures grown on n-Si (111) substrates using physical vapor deposition (PVD) technique.
2. To investigate GaN low dimensional structures and films synthesized on Si substrates using thermal chemical vapor deposition (TCVD) techniques under different conditions.
3. To evaluate the performance of GaN/Si heterostructures fabricated using low cost PVD and TCVD as photodiodes and solar cells.

1.4 Originality of the Research Work

The originality of the study is supported by the following points. First, thermal growth of GaN on Si substrates, in NH_3-free environments is still active area. This technique could provide a new insight into the use of semiconductor materials with wide band gaps in optoelectronic application. This study demonstrates the excellent potential of GaN low D structures on n-Si substrate for use in heterojunction photovoltaic solar cells. Secondly, the investigation the high unintentional doping levels in the Si substrates through the growth of GaN using high growth temperature. Thirdly, the study employs NH_3 solution as the nitrogen source for the synthesis of high-quality GaN low dimensional structures using the thermal evaporation method. A review of contemporary studies has shown that the synthesis of GaN low D structures on catalyst-free Si through the vapor reaction of Ga and NH_3, using NH_3 solution as a gas source has not been conducted. The use of NH_3

solution in thermally grown GaN was found to yield excellent GaN low D structures that exhibit strong photoluminescence properties. Finally, the growth of GaN low D structures using inexpensive method to assemble GaN/Si heterojunction for high performance photodiode that sensing both UV and visible photons was investigated. This achievement, was until now, unreported in current literature.

1.5 Outline of the Thesis

The thesis consists of seven (7) chapters. Chapter 1 provides an overview of the study, from the introduction to originality and objectives of the research. Chapter 2 entails a review of the literature covering growth of GaN and GaN devices, the motivation for the growth of GaN, the principles of thermal evaporation technique and mechanism of GaN growth, the process of growth from the vapor phase, GaN nanostructures formation mechanisms as well as the basic principles of some devices (which have been fabricated in this thesis). Chapter 3 comprehensively describes the methodology and instrumentation used in the study. The results obtained from the research works are analyzed and discussed in Chapters 4, 5 and 6. Chapter 4 elaborates on the properties and applications of the grown GaN low dimensional structures on Si (111) substrate using physical vapor deposition via thermal evaporation of GaN powder under different parameters and conditions. Chapter 5 presents the results of experiments conducted on the thermal vapor deposition of GaN low dimensional structures using NH_3 solution under different parameters Chapter 6 comprises the experimental results of the synthesis of GaN films via thermal evaporation of Ga and GaN powder using NH_3 solution and their application as UV photodetectors. Finally, a summary of this study along with suggestions for future works are presented in Chapter 7.

CHAPTER 2:

LITERATURE REVIEW AND THEORETICAL BACKGROUND

2.1 Introduction

The principles and theories of all subjects involved in this work are presented in this chapter. It begins with a background description and overviews of GaN growth and principles of thermal evaporation method. The review addressed the fundamental principles of thermal evaporation and mechanisms of GaN formation. The fundamental theories of temperature dependence of the current voltage of GaN/Si heterojunction are also addressed. Furthermore, the basic concepts of the devices fabricated in this thesis, which include heterojunction photodiode, solar cell and metal-semiconductor-metal (MSM) photodetector, are briefly described in this chapter.

2.2 Background of GaN Growth

In the early 1930s, GaN was successfully synthesized as a semiconducting material by passing NH_3 gas over hot metallic Ga at high temperatures of 700 to 1000°C (Johnson and Crew, 1932) [25]. In 1971, Pankove *et al.*,[26] reported the first device application of GaN, LED with an insulating-to-n-type structure, but the material was still relatively of low quality and inhibited by large surrounding background electron concentration, resulting from native defects usually considered to be nitrogen vacancies. Those studies encountered significant limitations in obtaining high-quality material. The quality of GaN was significantly enhanced in 1983 with the introduction of an AlN buffer layer that helped to nucleate and produce smooth GaN films [27]. Previous works conducted in the 1983s-1995s mainly focused on the growth of p-type GaN [28-32]. Present studies have improved

the growth of GaN by reducing the room temperature (RT) background electron concentration of GaN films and improved p-type GaN has been reported [29]. The successful p-type doping resulted in a great improvement of device performance [30, 31, 33, 34].

The rapid development in the application of GaN in the past 20 years has been made possible by the constant advances in the fabrication and characterization of increasingly smaller structures. The breakthrough in material processes and phenomena at the nanoscale, in addition to further growth of new theoretical and experimental techniques have provided huge chances for the development of original nanostructured materials. The fabrication of low dimensional structure has indeed provided a number of different physical properties such as electronic structure, morphology, quantum tunneling, surface effect, quantum phase transition, quantum size-effect confinement and nonlinear susceptibility enhancements [35-37]. Moreover, the one dimensional (1D) nanostructures such as nanowires (NWs), nanorods (NRs), nanotubes (NTs) and nanobelts (NBs), in the limit of small diameters can exhibit significantly different optical, electrical and magnetic properties from their bulk three-dimension (3D) crystalline structure [36].

During the last ten years, a good number of research communities have been involved into the epitaxial growth of GaN nanostructures with different shapes using various growth techniques [8, 23, 38-40]. Among various nanostructures, nanowires (NWs) are particularly attractive for future nanotechnology applications in the field of electronic and optoelectronic devices. GaN is of particular interest because it has been shown to yield good quality NWs [41] and can be either grown intrinsically n-type or doped p-type by the incorporation of magnesium during growth [42]. The

semiconducting properties of GaN nanostructures are presently being studied for possible utilization in high-power transistors and low-power lighting. The first successful fabrication of GaN NWs was conducted by Han *et al.,* [43]. Ever since, new applications for GaN NWs have been found in field effect transistors and single nanowire light-emitting diodes. Recently, GaN NWs have been used to fabricate UV photodetector (PD) [38], nanolasers (LDs) [39], nanoscale field effect transistors [44], and light-emitting diodes (LEDs) [40]. Although a majority of GaN NWs usage is still experimental, they have the potential to replace carbon nanotubes in numerous electronic and optoelectronic applications.

2.2.1 Overview of GaN Conventional Growth Techniques

Fabrication of high quality electronics devices like LEDs, LDs, PDs and solar cells requires the growth of high quality GaN doped structures. As a result of the lack of native GaN substrates, GaN based nitride semiconductors have been grown hetero-epitaxially on non-native substrates. However, remarkable progress has been made in the growth of high quality epitaxial GaN nanostructures and films by a variety of methods such as; metal organic chemical vapor deposition (MOCVD) [19, 20], hydride vapour phase epitaxy (HVPE) [21], molecular beam epitaxy (MBE) [22], physical vapor deposition (PVD) [23] and chemical vapor deposition (CVD) [8]. MBE entails the growth of very high quality thin films and nanostructures, however, due to the high cost factor and low growth rate, the method is not commercially feasible. Though MOCVD is a commercially viable method for growth of GaN, the inherent use of hazardous gases and high growth temperatures in the process restricts its application, although it is not a problem for optoelectronic devices. In the case of solar cells applications, it would be vital to use cheap fabrication techniques of III-N semiconductors. Physical vapour deposition (PVD)

via the thermal evaporation of solid materials and thermal CVD using a horizontal tube furnace (HTF) are best suited option because of low-cost and simple experimental procedure [8, 23, 45].

The most desirable technique of growing high purity single crystal group III-nitrides would be those in which these nitrides themselves are used as starting material. This has been an objective of many studies. Slack and McNelly [46] proposed a method where high quality AlN powder from the Al metal can be produced using AlF_3 as an intermediate product. The AlN powder can be transformed to a single crystal by sublimation in a closed tungsten crucible or in an open tube with a gas flow. Over the years, physical vapor transport (PVT) has been intensively explored as the technique for the growth of bulk AlN [47]. However, these techniques have been classified as PVD or thermal CVD, based on vapor-phase approach where elevated temperature is usually required. Each method can then be sub-divided into various respective techniques that will be discussed in the following sections.

2.2.1.1 Growth of GaN Low Dimensional Structures and Films using Physical Vapour Deposition (PVD)

The mechanism of PVD begins when a material is physically released from a source material by heating, and transformed onto a substrate by gas carriers. It explains the solidification of vapour directly onto a surface in a way that no chemical reaction takes place. The most common and important PVD technology for GaN growth is thermal evaporation using a tube furnace. To this point, the best results for the growth of bulk AlN were attained using the PVD method [47]. Several researches have examined the gas composition over heated GaN powder [23, 48-51]. Xiao *et.al.*, [52] studied the thermal stability of GaN by putting GaN powders in

furnace temperatures below 1400°C under a flowing stream of N_2 gas. Stach *et al*., [53] successfully grew GaN NWs on sapphire substrate via a self-catalytic vapor-liquid- solid (VLS) mechanism at high temperature thermal decomposition of GaN.

Furthermore, Lin *et al.,* [54], fabricated vertically aligned GaN NWs array through the thermal evaporation of GaN powder with the support of HCl gas. Tang *et al.,* [23] fabricated high-quality vertically n-GaN (NWs) on p-cuprous oxide (Cu_2O) (111) by thermal evaporation of GaN conventional powders without using any catalyst or template. Rodrıguez *et al.,* [55] synthesized GaN film by close space vapor transport in vacuum using GaN powder as the source material. Recently, Shekari *et al.,* [24, 56] prepared GaN nanostructures from the vapor phase through the thermal evaporation of GaN powder in high temperature furnace on Si and porous Si substrates. They suggested that the growth condition play a vital part in structural morphology and optical characterization of GaN NWs. Herein, we intend to grow GaN low Dimensional structures on the Si substrates without any catalyst and NH_3 gas via the thermal evaporation of GaN powder using a conventional HTF under different conditions.

2.2.1.2 Growth of GaN Low Dimensional Structures and Films by Thermal Chemical Vapour Deposition (TCVD)

Thermal chemical vapor deposition (TCVD) or thermal vapor deposition (TVD) is commonly used to manufacture very pure high-performance solid materials [57]. The process is frequently used in the semiconductor industry to produce thin films. The CVD process involves synthesizing the substrate with one or more volatile precursors, which react and/or decompose on the substrate surface to produce the desired deposit. In the TCVD method, the precursor gas is released on the surface of the substrate, where the reaction occurs under thermal conditions. The TCVD

process requires a pressure level of 10^{-3} Torr. Recently, CVD technology has been discovered as a significant application in the fields of science and engineering. It is effective for the preparation of many advanced products, including bulk materials as well as coatings, films, nanostructures and composites. The TCVD technology can also be used for the manufacture of electronics and optoelectronic materials [57]. However, TCVD GaN materials are generally grown by a vapor phase reaction between GaCl or Ga and NH_3 gas, with N_2 or H_2 utilized as the carrier gas [19, 58, 59]. Chang *et al.,* [60] and Zhou *et al.,* [61] demonstrated an example of thermal CVD process through the Au-catalyzed growth of GaN NWs by evaporating Ga or a Ga_2O_3/Ga mixture under an Ar–NH_3 atmosphere resulting in a morphology of periodic zigzag and diameter-modulated shapes on Si wafers. Recently, studies [8, 62-65] have shown the growth of GaN nanostructures and films by TCVD for electronic application. Nabi *et al.,* [65, 66] synthesized high-quality GaN NWs by pre-treating precursors with aqueous NH_3. They found that aqueous NH_3 effectively enhances the quality GaN NWs.

An evaluation of contemporary studies indicates that the synthesis of GaN nanostructures and films on catalyst-free Si through the vapor reaction of Ga and NH_3, with the use of NH_3 solution as gas source are limited. The use of NH_3 solution is practical because it's cheap, requires no gas controller, as well as its minimal waste production, and rapid, safe reaction with Ga. The NH_3 solution is effective on the structural and optical properties of GaN structures. This study involves the synthesis of GaN low D structures and films using simple and low-cost TCVD method directly on Si substrates through the reaction of metallic Ga and NH_3 solution.

2.2.2 Overview of GaN Applications

Great scientific enthusiasm has been garnered by GaN low dimensional structures because of its possible applications for GaN/Si heterostructures, which could benefit from their distinctive and amenable properties. Some of the various device applications previously reported are discussed in the following.

2.2.2.1 Overview of GaN–Based Heterojunction Photodiode and Solar Cell

In recent times, semiconductor nitrides (III-N) and their ternary alloys have been evaluated as possible options for the fabrication of thin film and tandem solar cells due to their wide range bandgap variation from 0.7 up to 6.2 eV (at 300K), which covers the whole visible range and a large part of the solar spectrum. In addition, they have unique physical, chemical and electric properties and can be obtained as n or p type semiconductors [15, 67]. These features make GaN and related compounds potential materials for the fabrication of p-n junction diode based devices [9, 67, 68]. Nonetheless, advancements in the growth and characteristics of GaN have led to considerable development in device technology. GaN-based photodetectors have been continuously built along with visible-and infrared-range detectors, evolving from Si-based to compound semiconductor based devices such as GaN photodetectors [69]. UV-detecting Schottky diodes using GaN nanostructures were also reported [70]. Photodetectors designed to detect both UV and visible photons are usually based on Si and fabricated using metal Schottky, p-i-n, and p-n structures [69-73]. Therefore, heterojunction diodes involving a wide band gap semiconductor on a single crystalline silicon wafer have a number of prospects such as excellent photoresponse, simple processing steps, and low processing cost compared to that on SiC and Al_2O_3 [74-76]. Consequently, GaN is considered because of its ability to cover visible short-wavelength and UV light as well as its

high heat tolerance. Both undoped and doped GaN films are being used in solar cell devices [8, 68]. However, the growth of GaN on Si substrates has a number of deep-level defects, such as dislocations as a result of lattice mismatch, and strain (tensile or compressive) which may affect the consistency and performance of GaN-based devices. To avoid this problem, a thin crystalline Si_3N_4 or AlN layer was introduced by a nitridation process of the substrate [77-79].

Reichertz *et al.,* [68] reported the growth of p- and n-type GaN dual junction solar cell on a standard n-type Si wafer with a thin AlN buffer layer using MBE. They verified that Al diffusion into the Si substrate during the growth of GaN layers forms a viable silicon solar cell and low series resistance at the GaN/Si heterojunction have been demonstrated [68, 80]. However, the insulating properties of AlN led to a deleterious effect on the transport properties of the junctions. For direct growth of GaN on Si, a thin crystalline Si_3N_4 layer formed by a nitridation process of the substrate has been shown beneficial for subsequent deposition of GaN [78]. Some research groups have employed a metallic surfactant layer and some novel buffer techniques [81]. Although these techniques are said to lead to improved epitaxial films, their superiority in photovoltaic applications remains to be demonstrated. Yamaguchi *et al.,* [82] deposited InN and InGaN on p-type Si (111) by plasma assisted (PA) MBE and observed the rectifying behavior of the junctions, whereas Xu *et al.,* [83] studied n-GaN/p-Si junction but observed no rectifying property, probably due to charge accumulation at the interface layers. Recently, many research groups [8, 83, 84] have grown directly GaN on n-Si substrates and showed rectifying property. However, more results are required to clarify this behaviour and therefore will be demonstrated in this work. Several techniques have been reported for operation of GaN low dimensional structures into well-defined

arrays for integrated devices. Lee *et al*., [85] have fabricated a high-brightness GaN NWs homojunction diode using a dielectrophoresis method. Dislocation free GaN NWs have been grown on Si (111) by MBE and showed the rectifying behavior of the heterostructures [22, 86]. Zhong *et al*., [87] and Tang *et al.,* [88] have synthesized GaN NRs on n-(111) Si based heterojunction diodes solar cell by CVD. The MOCVD method has been used to grow GaN based heterostructures devices [89, 90]. Tang *et al.,* [8] have conducted controlled synthesis of a vertically aligned p-GaN NRs on n-Si substrate based diodes by thermal evaporation technique.

2.2.2.2 Overview of GaN-Based UV-Photodetector Metal-Semiconductor-Metal

The detection of ultraviolet (UV) radiation is significant for several applications such as environmental, space applications, ozone layer monitoring, flame detection, water purification system, and photochemical phenomena detection, and so on. GaN is one of the most suitable materials for the fabrication of high-responsivity and visible-blind UV detectors, because it has a large direct bandgap energy (3.41eV at RT) and a high saturation electron drift velocity of 310 cm/s [91] as well as high temperature resistance and superior radiation hardness in extreme conditions. In recent times, different types of GaN-based photo devices have been suggested, such as blue, near-UV, and violet light-emitting diodes, laser diodes and metal–semiconductor–metal (MSM) photodetectors [92-98]. Among these devices, MSM photodetector have distinctive features, such as a simple structure, easy fabrication, and readily integration [97, 99]. To acquire exceptional UV photodetector devices based on GaN films with large barrier height, a metal with high work function should be chosen such as nickel (Ni). A simple method for the

synthesis of GaN films on n-Si (111) substrate based UV photodetector using NH_3 solution is reported here.

2.3 Thermal Evaporation Process Principles of GaN

The thermal evaporation method is based on the vapour-solid (V-S) mechanism. Evaporation is a thermal separation process used for concentrating solid into liquid form or (solutions, suspensions, and emulsions). Thermal evaporation technique has been extensively used for growing semiconductor materials in vacuum chamber or in furnace tube. A number of very remarkable nanostructures have been obtained via this method [24, 45, 53, 100]. The conventional TVD growth mechanism remains suitable to account for the growth phenomena of GaN. The growth mechanism can be explained as follows: GaN powder can be thermally evaporated at high temperatures of 1150ºC. The decomposition of the GaN nanoparticles generates N atoms and isolated nanoscale Ga droplet. Lvov [48] suggested that GaN decomposes at temperatures above 850ºC in high vacuum via the following possible reactions:

$$\mathrm{GaN(s)} \xrightarrow{850°\mathrm{C}} \mathrm{Ga}(l) + 0.5\,\mathrm{N}(g) + 0.25\,\mathrm{N_2}(g) \qquad (2.1)$$

It has also been suggested and experimentally shown that congruent sublimation of GaN is likely, which yields diatomic or polymeric vapor species [48, 101].

$$\mathrm{GaN(s)} \xrightarrow{850°\mathrm{C}} \mathrm{GaN}(g)\ \mathrm{or}\ [\mathrm{GaN}]_x(g) \qquad (2.2)$$

Initially, decomposition of the GaN powder leads to the formation of isolated liquid Ga nanoparticles. The resultant vapor species is composed of the atomic nitrogen and diatomic or polymeric GaN. The occurrence of this decomposition in the course of

the thermal evaporation of GaN powder in a furnace tube at 1150ºC can be observed to result in low D structures growth in real time and at high spatial resolution [45].Therefore, it can be deduced that Ga droplets become self-catalytic growth elements of GaN via V-S growth mechanism. Many factors can influence the decomposition and growth of GaN via thermal evaporation of GaN powder such as gas flow rate, type of carrier gas, growth temperatures and growth time.

The second method involves the growth of GaN low D structures and films via the thermal evaporation of Ga under NH_3 gas flow. The growth of GaN in a HTF through the reaction of metallic Ga and NH_3 solution as source materials and N_2 as carrier gas is clarified by the following process: N_2 gas carries volatile NH_3 from the solution into the HTF, then as the temperature of the furnace reached growth temperature (T>950ºC), Ga vapor subsequently reacts with gaseous NH_3 to form the nucleus of the GaN. GaN low D structures prepared by a direct reaction of Ga and NH_3 gas in the furnace tube at temperature above 950ºC can be expressed by [102];

$$2Ga(s) + 2NH_3(g) \xrightarrow{\Delta} 2GaN(s) + 3H_2(g) \qquad (2.3)$$

The gaseous NH_3 flow can be managed by fluctuating the rate by which (N_2 or Ar) gas carries volatile NH_3 from the NH_3 solution into the HTF. In thermal CVD processes, the surface reaction rate on the substrate increases with temperature. Therefore, shape, morphology, and density of nanostructures can be controlled by varying the growth condition such as gas flow rate, growth duration *etc*. [45].

2.3.1 Synthesis of GaN Low Dimensional Structures

Several synthetic methods have been developed to successfully fabricate high crystalline quality low D structures for a number of diverse materials ranging from

metals and semiconductors to oxides. For the PVD process, only the vapor-solid growth mechanisms can occur while both vapour-liquid-solid (V-L-S) and V-S growth mechanisms can occur in CVD process. For V-L-S method, catalyst seeds are needed. During the reaction, the catalyst seeds are in liquid form, and the droplets provide preferential sites for absorption of the gas phase reactant. Factors such as deposition time, temperature and carrier gas flow are vital for the growth mechanism that controls the final structural features of GaN nanostructures. GaN nanostructures fabricated explicitly for applications in electronic and optoelectronic nanodevices are typically synthesized using thermal evaporation, a form of self-growth mode control [23]. For nanomaterial fabrication using CVD, reactants are transported from a liquid or gas source to the substrate surface, which absorbs the reactants. The self-induced approach is a valuable growth mode to form GaN nanowires on a wide number of substrates for optoelectronic devices. However, their nucleation and growth processes should be distinguished from the usual growth modes in chemical and physical vapor deposition.

The self-induced growth of GaN in low D structures is more promising than common catalyst-induced growth, since such an approach has the significant advantage to limit the potential nanostructures contamination. Thus, there are increasing efforts to grow low dimensional structures by catalyst-free methods, but in this case a model forecasting the low dimensional structures (NW, NR, etc.) properties is lacking. We synthesized GaN low dimensional structures in the catalyst-free approach on Si substrates via V-S mechanism. Various hierarchical semiconductor nanostructures through the V-S growth mode have also been reported [23, 42, 54]. It must be mentioned here that nanostructures size can be varied by changing the evaporation conditions but no precise control of spatial arrangement

can be achieved. The thermal evaporation basically follows the V-S mechanism. Usually GaN powders are placed inside a HTF, and then GaN powder will be heated up by a heating source to its vapour point once the appropriate pressure within the furnace tube is reached. The vaporized GaN will condense along the surfaces of substrates through the vapour-solid mechanism. The kinetics of this growth process has been reported [103, 104]. As apparent from Figure 2.1, the self-catalytic growth involves two different steps, mainly nucleation and growth. For low pressure, GaN nucleation is free from catalysts and the growth is expected to be via the V-S route.

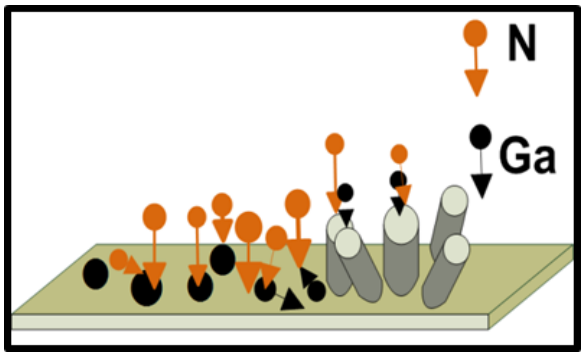

Figure 2.1. Quasi-aligned vertical standing GaN NWs under reduced pressure which follows V-S transformation [104].

Low D structures can be grown without extra metal catalysts by thermally evaporating a suitable source material near its melting point and then depositing at cooler temperatures [105]. The growth of GaN low D structures on a Si substrate by the supply of sufficient metal Ga under atmospheric pressure in TVD system can be explained in the following way. Initially, the Ga vapor can be transported to the substrate at high temperatures which forms liquid droplets with a small size. The supply of NH_3 and carrier gas contributes to the Ga rich GaN nucleation. The adatoms diffusion of nitrogen radicals in the Ga liquid droplet is expected to be high under atmospheric pressure, favoring crystallization at the substrate–liquid interface

and then growth proceeds by a continuous supply of Ga and NH_3 that keeps the liquid droplets alive on the tip of the structures. In the case of self-catalytic GaN low D wires, the Ga metal droplet is normally not observed on the apex as the growth proceeds at a higher temperature and results in consumption or desorption of Ga [103]. When NH_3 is added to the reaction tube furnace, the liquid droplets solidify quickly by nitrogen and the formation of GaN low D wires can eventually be observed [105].

The substrate plane and crystalline structure also affect the growth process. Since Si has a diamond structure, there are two commonly used faces of Si substrates with directions of (111) and (100). Several groups have reported high quality GaN epitaxy directly on Si (111) and Si (100) substrates [63, 106]. GaN grown on Si (100) usually has mixed phases due to the large lattice mismatch and the formation of an amorphous Si_xN_y layer at the interface of GaN/Si, which degrades the crystal quality [107]. However, growth of GaN on Si (100) is very challenging due to the different crystallographic surface symmetries: GaN has six-fold symmetry, while Si (100) has four-fold symmetry [106]. The Si (111) substrate is usually preferred for GaN epitaxy due to the six-fold surface symmetry, which already gives a good rotational matching for GaN [106]. Therefore, good crystalline quality GaN structures have been obtained on Si (111) substrate [88, 108].

2.4 Strain and Stress of the Single Crystalline GaN

It is acknowledged that epitaxial GaN films or nanostructures with high crystalline quality are required in many optoelectronic applications [8, 9, 88]. However, the epitaxial GaN films have been fabricated on Si (111), Al_2O_3 (0001) (sapphire) or SiC (0001) substrates due to the hexagonal surface symmetry [109,

110]. These substrates exhibit different thermal and lattice mismatch compared to GaN, which result in tensile or compressive strain subsequently resulting in the formation of defects such as misfit dislocations. Drawbacks of Si substrates include large mismatches in lattice constants (17%) and thermal expansion coefficients (33%), which lead to strain in the grown layer thereby resulting in the formation of cracks [13, 18, 99, 109, 111]. The thermal expansion coefficient for the silicon substrate is $\alpha_{Si} = 2.6\times10^{-6}\ K^{-1}$, which is smaller than that ($\alpha_{GaN} = 2.6\times10^{-6}\ K^{-1}$) of GaN. The huge mismatch in thermal expansion coefficients can cause thermal tensile stress and result in severe cracking of the GaN layer during the post-growth cooling process [112]. This problem can be prevented by alternating layers in order to withstand the strain and produce high-quality crystal [110, 111]. In GaN epilayer on Si, stress develops largely from lattice and thermal mismatch between the film and the substrate and growth process [110]. The calculated stresses and the interfacial energy corresponded to the case where the misfit between the GaN layer and the substrate lattice constants is fully relaxed or partially by an array of evenly-spaced edge dislocations. Such a situation is shown schematically in Figure 2. 2 (a). For a partially relaxed layer two cases are possible:

(1) $a_{epi} < a_s$ the layer is under tensile stress

(2) $a_{epi} > a_s$ the layer is under compressive stress

where a_{epi} is the lattice constant of epitaxial layer and a_s lattice constant of substrate. For GaN/Si the lattice constant (a_{epi}=3.189 Å) of GaN layer is smaller than c–Si (a_{Si} = 5.4309 Å), which indicate that the GaN layer under tensile strain (Figure 2. 2 (b)) [113, 114]. The growth on such a substrate allows us to investigate the impact of strain on the optical properties within a single substrate. The stress in GaN can be

estimated from the X-ray diffraction peak positions of GaN planes, and from the Raman scattering peak.

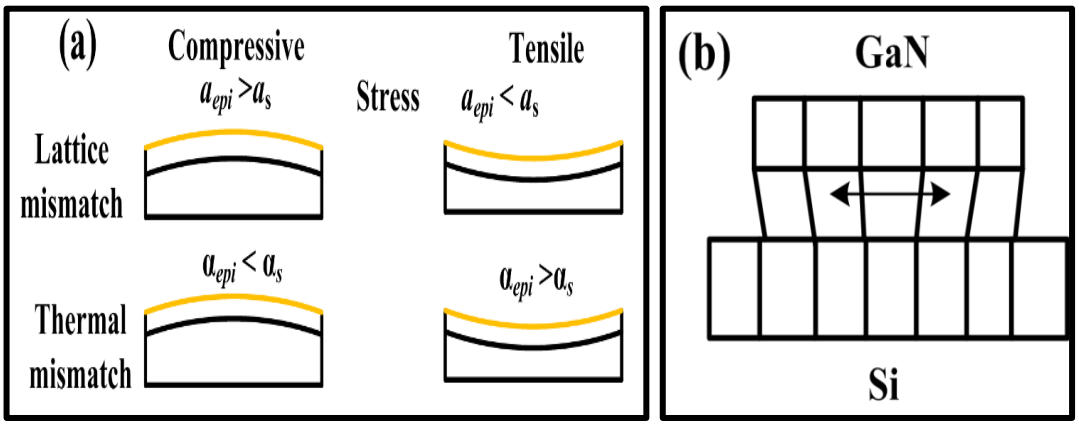

Figure 2.2. Schematic for the biaxial stress/strain resulting from the lattice and thermal mismatches between layer and substrates: (a) stress between layer and two different substrates and (b) stress/strain between GaN and Si substrate [114].

2.4.1 Stress Calculation from XRD Data

Stress and lattice constants are important aspects considered in evaluating the deformation state of crystalline materials. Therefore, the lattice constants, *c* and *a*, obtained from the XRD measurements can be derived from the peak positions of (100) and (002) planes [115, 116]. The ratio of elastic stiffness constants for epilayer can be inferred from experimental XRD data of GaN epitaxial layer, lattice constants c_{epi} and a_{epi}. These are compared with the lattice constants a_0 and c_0 of bulk GaN at 3.189 and 5.185 Å, respectively. Using these values, the in-plane, (ε_a), and out-of-plane, (ε_c), strain components of the GaN layer can be calculated based on the following expressions [110, 117];

$$\varepsilon_a = \frac{(a_{epi} - a_0)}{a_0} \tag{2.4}$$