

CHARACTERIZATION OF EPITAXIAL ALUMINUM NITRIDE THIN FILMS GROWN USING MOCVD METHOD

Submitted in partial fulfillment of the requirements for the award of

Master of Science degree in Physics

By

L. THENMOZHI

(41590024)



DEPARTMENT OF PHYSICS

SCHOOL OF SCIENCE AND HUMANITIES

SATHYABAMA

**INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)**

**Accredited with "A" grade by NAAC | 12B Status by
UGC Approved by AICTE**

JEPPIAAR NAGAR, RAJIV GANDHI SALAI, CHENNAI - 600 119.

May 2023



SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)

Accredited "A" Grade by NAAC | 12B Status by UGC | Approved by AICTE

www.sathyabama.ac.in

DEPARTMENT OF PHYSICS

BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of L. Thenmozhi (41590024) who carried out the project entitled "CHARACTERIZATION OF EPITAXIAL ALUMINUM NITRIDE THIN FILMS GROWN USING MOCVD METHOD" under my supervision from November 2022 to May 2023.

Internal Guide
(Dr. Twisha Sain)

Head of the Department
(Dr. S. Ravichandran)

Submitted for Viva voce Examination held on 9.5.2023 2023

INTERNAL EXAMINER

EXTERNAL EXAMINER

Dr. D. DINESH KUMAR

Associate Professor (Research)

DECLARATION

I L. Thenmozhi hereby declare that the Project Report entitled CHARACTERIZATION OF EPITAXIAL ALUMINUM NITRIDE THINFILMS GROWN USING MOCVD METHOD done by me under the guidance of Dr. Twisha Sain (Internal), Department of Physics, Sathyabama Institute of Science and Technology, Chennai is submitted in partial fulfilment of the requirements for the award of Master of Science Degree in Physics.

DATE: 09-05-2023

PLACE: CHENNAI

A handwritten signature in black ink, appearing to read 'Thenmozhi', is placed within a light gray rectangular box.

SIGNATURE OF THE CANDIDATE

ACKNOWLEDGMENTS

I am pleased to acknowledge my sincere thanks to Board of Management of **SATHYABAMA** for their kind encouragement in doing this project and for completing it successfully. I am grateful to them.

I express my deep sense of gratitude to **Dr. Rekha Chakravathy**, Dean, School of Arts & Science **Dr. S. Ravichandran**, Head of the department, Sathyabama Institute of Science and Technology, Chennai for his expert suggestion and permission to carry out the project work at IGCAR, Kalpakkam.

I express my deep sense of gratitude to my research advisor, **Dr. Twisha Sain**, Assistant Professor, Department of Physics, Sathyabama Institute of Science and Technology, Chennai, for her guidance to complete this work. She never hesitated to help me in during the whole course of project work. She spared her valuable time to make my dissertation a successful one.

I would like to express my heartfelt thanks to my supervisor, **Dr. R. Ramaseshan**, IGCAR for his continuous support and endless guidance.

I also would like to express my gratitude to **Dr. Ch. Kishan Singh** of the same section for his assistance in employing AFM and UV-Vis spectroscopy to perform surface topography and optical analysis. I would also want to convey my gratitude to **Dr. S. Tripura Sundari** and **Mr. K. Venkateswara Reddy** for contact angle measurement. Additionally, I want to convey my gratitude to **Dr. Gomathi Natarajan**, **Mr. Ashok Bhaguna**, **D. T. Sunitha Rajkumari**, and **R. Rajaraman** for their endless guidance and assistance throughout my project work at the IGCAR, Kalpakkam.

I am very grateful to **Dr. B. Venkatraman**, Director of IGCAR, **Dr. R. Divakar**, Director of MSG, IGCAR, and **Dr. Vidya Sundararajan**, Head P & HRMD, SQ & RMG, IGCAR especially for their permission to make use of the laboratory to carry out the project work.

I am very grateful to my parents for their moral support and encouragement throughout my academic career. I would like to express sincere thanks to my friends and all the others who have helped me with my project work

ABSTRACT

AlN epitaxial thin film produced using the MOCVD method with the C-axis orientated. Using HRXRD, the crystal quality has been evaluated and the measured FWHM in the rocking curve (2θ - Ω scan) is 290 arcsec. The UV-Vis NIR spectrum reveals that the transmittance level is very high and the energy band gap is 5.75eV. When this thin film was subjected to nanomechanical characterization, the results showed that the indentation hardness (HIT) was 13.661 ± 0.55 GPa and the indentation modulus (EIT) was 361.59 ± 11.98 GPa at a depth of 30nm from the top surface.

Contents

1	INTRODUCTION	1
1.1	III-V NITRIDE SEMICONDUCTORS	1
1.2	ALUMINUM NITRIDE (AlN)	2
1.2.1	Structure of AlN	3
1.2.2	Phase diagram of AlN	4
1.2.3	Properties of AlN films	4
1.2.4	Application of AlN films	5
1.3	EPITAXIAL FILMS	6
1.4	COMPARISON OF SINGLECRYSTALLINE AND POLY- CRYSTALLINE THIN FILM	8
2	LITERATURE SURVEY	9
2.1	DEPOSITION	9
2.1.1	Epitaxial Growth of Aluminum Nitride on Sap- phire Using Metalorganic Chemical Vapor De- position	9
2.1.2	High quality AlN grown on SiC by metal organic chemical vapor deposition	9
2.1.3	Surface, structural and optical properties of AlN thin films grown on different face sapphire substrates by metalorganic chemical vapor deposition	10

2.2	APPLICATION AND PROPERTIES	10
2.2.1	Stress and piezoelectric properties of aluminum nitride thin films deposited onto metal electrodes by pulsed direct current reactive sputtering . . .	10
2.2.2	The electronic structure of wurtzite and zincblende AlN: an ab initio comparative study	11
3	AIM AND SCOPE OF THE PRESENT INVESTIGATION	12
3.1	AIM	12
3.2	SCOPE	12
4	EXPERIMENTAL AND CHARACTERIZATION TECHNIQUES	13
4.1	PHYSICAL VAPOR DEPOSITION (PVD)	13
4.1.1	Advantage of the PVD	14
4.1.2	Disadvantage of the PVD.....	14
4.2	CHEMICAL VAPOR DEPOSITION (CVD)	15
4.2.1	Advantage of CVD	16
4.2.2	Disadvantage of CVD	16
4.3	COMPARISON OF PVD AND CVD	17
4.4	METAL ORGANIC CHEMICAL VAPOR DEPOSITION (MOCVD)	17
4.5	GROWTH PARAMETER OF AlN.....	19
4.6	CHARACTERIZATION TECHNIQUES	20
4.7	STRUCTURE ANALYSIS	20
4.7.1	X-ray diffraction (XRD).....	20
4.8	SURFACE MORPHOLOGY	23
4.8.1	Atomic force microscopy (AFM)	
4.9	OPTICAL ANALYSIS.....	
4.9.1	Ultraviolet-visible (UV-vis) spectroscopy	25
4.10	MECHANICAL ANALYSIS	27
4.10.1	Nanoindentation.....	27
5	RESULTS AND DISCUSSION	30
5.1	STRUCTURAL ANALYSIS.....	30
5.1.1	X-ray diffraction.....	30
5.1.2	Morphology and surface roughness by AFM.....	31
5.2	OPTICAL ANALYSIS.....	32
5.2.1	UV-Vis-NIR spectrophotometer	32
5.3	MECHANICAL ANALYSIS.....	33

5.3.1	Indentation of hardness and modulus	33
-------	---	----

6	CONCLUSION	36
----------	-------------------	-----------

List of Tables

1.1	Comparison of the physical properties of various nitrides	2
1.2	Comparison of single crystalline and polycrystalline . .	8
4.1	Comparison of PVD & CVD	17

List of Figures

1.1	Periodic Element	1
1.2	a)Crystal structure of AlN; b)Bond configuration of AlN .	3
1.3	Phase diagram of AlN	4
1.4	Epitaxial film growth patterns.....	7
1.5	a)single crystalline.....	8
1.6	b)polycrystalline	8
4.1	PVD Apparatus	14
4.2	Transport and reaction processes in a CVD process	15
4.3	Schematic of metal organic chemical vapor deposition .	19
4.4	Bragg's law of diffraction.....	21
4.5	(a) Schematic of a rocking curve measurement	22
4.6	(b) Example of resultant rocking curves from a film diffraction peak.	23
4.7	Schematic for Atomic Force Microscopy.....	24
4.8	Electromagnetic spetrum.....	25
4.9	Schematic diagram of UV Visible spectroscopy	
4.10	Schematic Diagram of the Berkovich indenter	
4.11	Schematic of a cross section of an indentation with the supposition that piling-up and sinking-in are minimal. Various dimensions that used in the analysis are indicated	
4.12	The load(p) vs displacement(h) curve	29
5.1	HR-XRD pattern for AlN thin film.....	30
5.2	Surface topogrphy of the film by using AFM	31
5.3	Transmittance vs wavelength curve.....	32
5.4	Energy band gap of AlN thin film.....	33
5.5	Load(p) vs depth(h) curve	34
5.6	Hardness value for AlN thin film	35
5.7	Elastic modulus value for AlN thin film.....	35

LIST OF ABBREVIATIONS

WZ	- wurtzite structure
ZB	- Zinc blende
SAWs	- Surface acoustic wave sensors
DMS	- Dilute magnetic semiconductor
PVD	- Physical Vapor Deposition
CVD	- Chemical vapor deposition
MOCVD	- Metal organic chemical vapour deposition
MOVPE	- Metal organic vapor phase epitaxy
XRD	- X-Ray diffraction
UV-	
VIS	- Ultraviolet-visible
NIR	- Near infrared
AFM	- Atomic force microscopy
LED	- Light-emitting diode
FWHM	- Full width at half maximum
MG	- Modulation growth
NL	- Nucleation layer
PALE	- Pulsed atomic layer epitaxy
LVDT	- Linear variable differential transformer

Chapter 1

INTRODUCTION

1.1 III-V NITRIDE SEMICONDUCTORS

Group III nitrides are compounds made of elements from group III and nitrogen from group V of the periodic table.

Periodic Table of the Elements

1 H 1.01																	2 He 4.00	
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18	
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.06	17 Cl 35.45	18 Ar 39.95	
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 51.99	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.38	31 Ga 69.72	32 Ge 72.63	33 As 74.92	34 Se 78.97	35 Br 79.90	36 Kr 83.80	
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.95	43 Tc 98.91	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.6	53 I 126.90	54 Xe 131.29	
55 Cs 132.91	56 Ba 137.33	57-71		72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.20	83 Bi 208.98	84 Po [209.8]	85 At 209.98	86 Rn 222.02
87 Fr 223.02	88 Ra 226.03	89-103		104 Rf [261]	105 Db [262]	106 Sg [266]	107 Bh [264]	108 Hs [269]	109 Mt [278]	110 Ds [281]	111 Rg [280]	112 Cn [285]	113 Nh [286]	114 Fl [289]	115 Mc [289]	116 Lv [293]	117 Ts [294]	118 Og [294]

Figure 1.1: Periodic Element
Image source: Google

The binary nitrides for B, Al, Ga, and In are BN, AlN, GaN, and InN, respectively. These crystals show wurtzite, zinc blende, and rock salt structures. The degree of ionicity determines the crystal structure. High ionicity crystals usually exhibit wurtzite structure. The fourfold coordination of the wurtzite structure in AlN, GaN, and InN is stable at room temperature and pressure, while the fourfold coordination of zinc blende structures is quasistable. Group III elements are represented

by the larger spheres, while group V element atoms are represented by the smaller spheres. The hexagonal crystal of AlN, GaN and InN all have direct transition bandgap structure whereas the cubic structure of AlN and BN exhibit indirect bandgap.

A comparison of properties of various group III nitrides with other common semiconductor have been made in the table given below:

Semi-conductor	Transition type	Band gap(eV)	Thermal conductivity(W/mK)	coefficient of expansion $10^{-6}/^{\circ}\text{C}$
AlN	Direct	6.2	230-320	4.5
GaN	Direct	3.4	130-220	5.6
ZnO	Direct	3.3	43-54	2.9
InP	Direct	1.3	68	4.5
InAs	Direct	0.4	30-50	5.2
GaAs	Direct	1.4	45-54	6.5
Si	Indirect	1.1	140-160	4.1

Table 1.1: Comparison of the physical properties of various nitrides [8, 11, 17, 21]

The difference between AlN, GaN and InN is the existence of d-orbital electrons in the latter two compounds that interact with the N2s electrons. [11]

1.2 ALUMINUM NITRIDE (AlN)

Aluminum nitride (AlN) is a ceramic material having excellent optical and thermal properties. It has a wide bandgap (6.2 eV), high thermal conductivity (320 W/m K), high breakdown voltage, high melting temperature, low coefficient of thermal expansion, UV transparency, high piezoelectric response and excellent dielectric properties [8, 17, 21]. Because of these properties, aluminium nitride is used in several industrial applications, including opto-electronics, electronic substrates, photo-detectors, light-emitting devices, heat sinks and field-effect transistor.

1.2.1 Structure of AlN

AlN is a member of the III-V semiconductor family due to its unique hexagonal closed-packed wurtzite structure. On the other hand, AlN also exhibits metastable cubic zinc blende (c-AlN) and cubic rock-salt crystal structures, which are stable under specific pressure conditions[11].

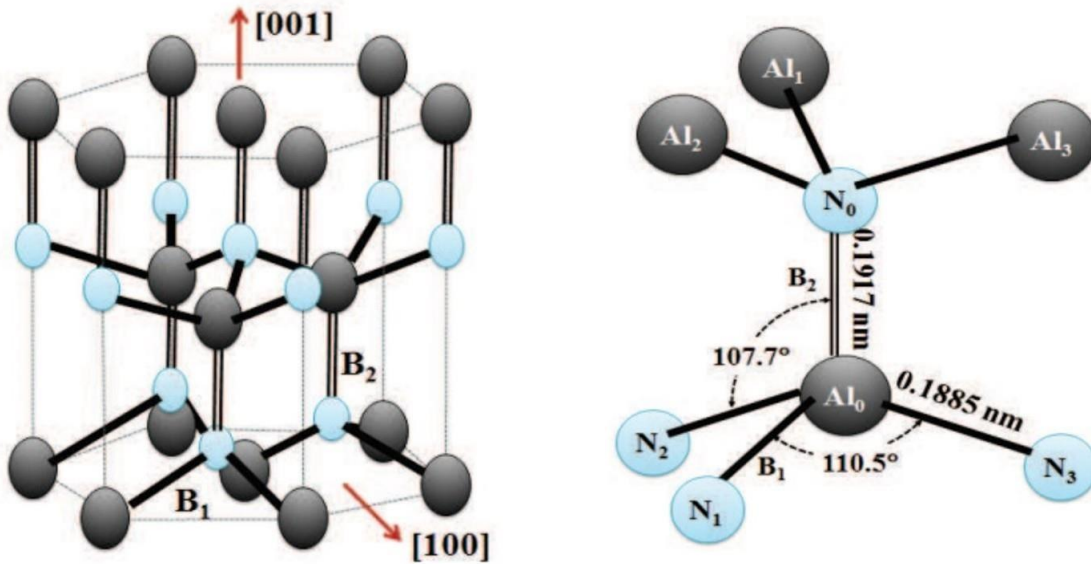


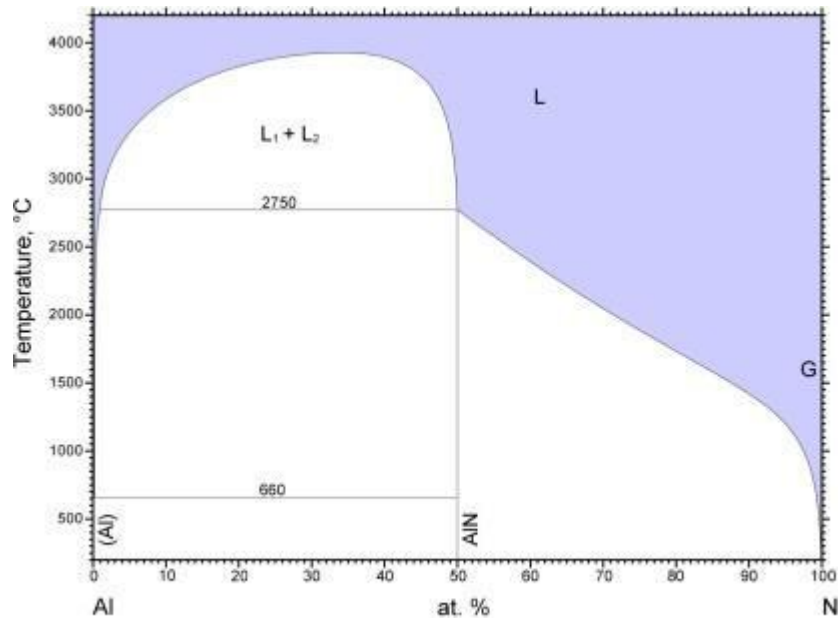
Figure 1.2: a) Crystal structure of AlN; b) Bond configuration of AlN

[19]

The lattice parameters for the a-axis range between 3.110 and 3.113, while for the c-axis, values range between 4.978 and 4.982. The ideal wurtzite structure is deviated from by the c/a ratio, which ranges between 1.600 and 1.602, this deviation is likely caused by lattice instability. In comparison to the other III-V nitride semiconductors, it has greater values for hardness and thermal conductivity.[22]. Four N atoms surround each Al atom, producing a tetrahedron with three B1 bonds between Al-N(i) (i=1,2,3) and one B2 bond between Al-N0 in the c-axis direction. B1 and B2 have respective bond lengths of 0.1885 and 0.1917 nm. The bond angle for N0-Al0-N1 is 107.7° and that for N1-Al0-N2 is 110.5° . The sp^3 hybridization between the semi-full orbits of the Al and N atoms gives rise to the covalent nature of bond B1, meanwhile the coupling of the Al empty orbit and the N full orbit gives rise to the ionic nature of bond B2. The planes along [001], [011], and [111] direction are made up of both B1 and B2 type bonds, as contrast to the planes along [100], [010], and [110] direction, which are composed of B1 type bonds. As a result, compared to the other

directions, the [001] direction has a higher ionic character and a lower bond energy[5, 19].

1.2.2 Phase diagram of AlN



© ASM International 2006 Diagram No. 904240

Figure 1.3: Phase diagram of AlN

AlN is formed with a stoichiometric ratio of 50% Al and N atomic concentration. AlN melts at a temperature of around 2750°C, which is higher than the melting point of pure aluminium (660°C) in an inert atmosphere. The melting temperature linearly reduces as N concentration rises. AlN melts at around 1800°C in a vacuum, while in an atmosphere of air, the surface oxidation happens at temperatures higher than 700°C [19].

1.2.3 Properties of AlN films

The structural, optical, thermal, and piezoelectric properties of AlN.

Structural Properties

Density	3.257
Modulus of Elasticity (GPa)	331
Poisson's Ratio	0.22
Common Crystal Structure	Wurtzite
Lattice constant (Å)	a = 3.112 ; c = 4.982
Hardness (Kg/mm ²)	1100

Optical Properties

Density of states Conduction Band (cm ⁻³)	4.1×10 ¹⁸
Optical phonon energy (meV)	113
Refractive index (vis-ir)	2.15

Thermal Properties

Thermal conductivity (W/mK)	upto 320
Thermal expansion (×10 ⁻⁶ °C)	4.2-5.3
Debye temperature (K)	980
Melting Point (°C)	2200

Electrical Properties

Breakdown field (V/cm)	1.2-1.8×10 ⁶
Mobility electrons holes (cm ² /VS)	135 /14
Dielectric constant (static/high frequency)	8.5-9.14/4.6-4.84
Energy Band Gap (eV)	6.2
Resistivity (Ohm.cm)	10 ¹⁴

1.2.4 Application of AlN films

AlN has high thermal conductivity due to that it is used for electronic packaging and heat sink application. Moreover, AlN has a good chemical stability, high hardness, high electrical resistivity, chemical resistance, thermal shock resistance, low dielectric constant, and thermal expansion coefficient similar to that of silicon crystal, it is frequently used in integrated circuits, automobiles, high-speed rail, IGBT control modules, electrostatic chucks for wafer processing, thermal dissipation, protection against environment and electrical insulation lay-

ers in opto-electronic devices. Aluminum nitride has been utilised in the military for aerospace, defence weaponry, and microwave radar in things like ship navigation systems, missile positioning systems, ground radar systems, and more.

Due to its piezoelectric properties, epitaxially grown crystalline aluminium nitride is also utilized in surface acoustic wave sensors (SAWs) placed on silicon wafers. The electro-mechanical coupling coefficient and acoustic velocity of a-axis oriented AlN are higher than those of c-axis oriented AlN in w-AlN films. A-axis oriented AlN film is therefore expected to perform better for SAW devices.

Magnetic semiconductors are semiconductors that can exhibit ferromagnetism. The transition metal doping in these materials is referred to as dilute magnetic semiconductors (DMS). As a result of the addition of magnetic elements to their lattices, the DMS are semi-magnetic. In general, these materials have spintronic properties, which combine the spin of the electrons with their corresponding electronic charge and magnetic moment.[14]

As from initial discovery of magnetism in Mn-doped GaAs at 100 K. Several III-V based DMSs have been evaluated in that AlN has received the most interest among them as a potential DMS due to its stable mechanical properties, wide band-gap, and high Curie temperature (T_c). Mg, Mn, Co, Cr, Cu, Ni and Fe doped AlN with RT magnetism have been described until now. These transition metals are doped with AlN in order to modify their physical characteristics for use in lasers, deep UV to UV LEDs, sensors, UV polarizers, high-temperature optoelectronic displays, and spin-tunneling apparatus.[26, 27]

1.3 EPITAXIAL FILMS

Regularly oriented growth of one crystalline substance on another is defined as epitaxy. It has two different types of epitaxial growth, homoepitaxy (growth of an epitaxial layer made of the same material as the substrate) and heteroepitaxy (growth of an epitaxial layer made of a material different from the substrate) both of them are used in

semiconductors on Si wafers. Epitaxial films can be formed by using different method, including evaporation, sputtering, molecular beam epitaxy, liquid phase epitaxy, chemical vapor epitaxy, Metal organic chemical vapor deposition.

Epitaxial growth comes in two different forms.

Homoepitaxial layer: The film and the substrate are the same material. Epitaxially grown layer are pure than the substrate and can be doped independently.

Ex: Si on Si

Heteroepitaxy layer: The film and substrate are of different materials.

Ex: Si on sapphire, GaAs on Si

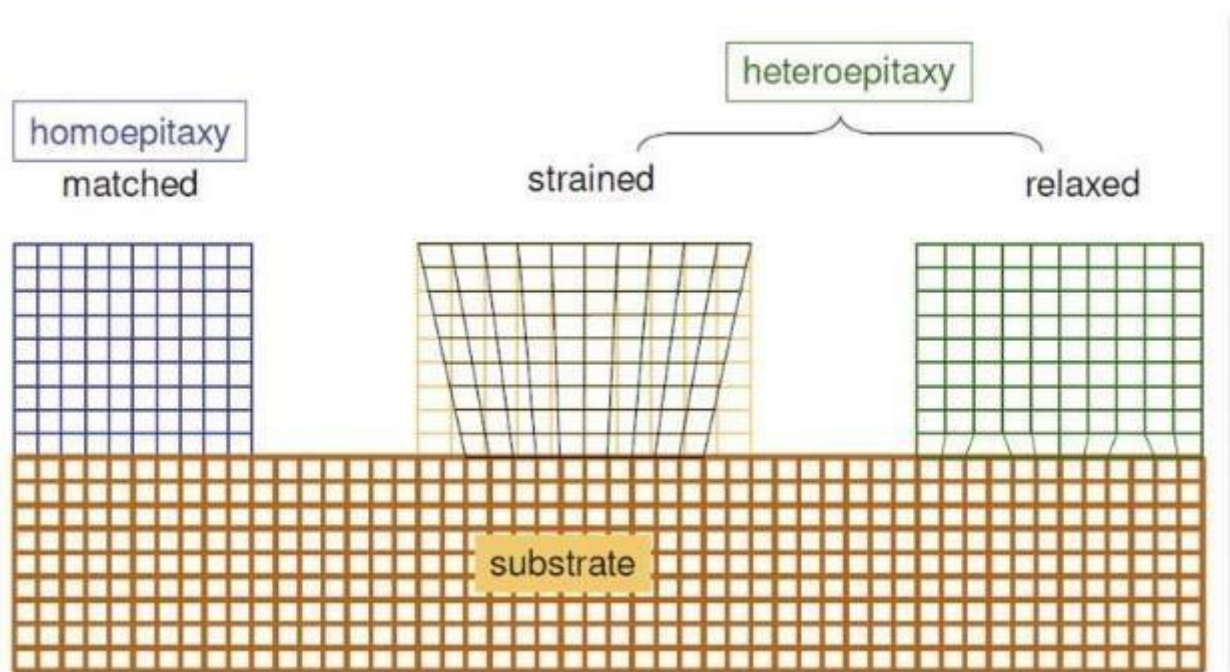


Figure 1.4: Epitaxial film growth patterns
Image source: Google

1.4 COMPARISON OF SINGLECRYSTALLINE AND POLYCRYSTALLINE THIN FILM

PROPERTIES	SINGLECRYSTALLINE	POLYCRYSTALLINE
Definition	In crystalline solids constituent particle(atom,molecule or ions) arrange in a 3 - dimension periodic manner	In polycrystalline solids do not have a consistent arrangement of particle.
Geometry	Have a well defined geometrical form	Does not have well defined geometrical form
Range of order	Have a long range order	long range order has been disrupted
Melting point	Have sharp melting point	Have diffused melting point
Cost	High	low
Boundary	No boundaries	It has boundaries between grains
Crystal growth	Hard	Easy
Example	Diamond, table salt	Metal, ceramics

Table 1.2: Comparison of single crystalline and polycrystalline

[23]

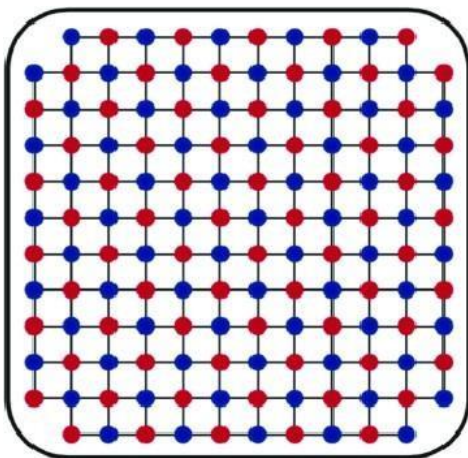


Figure 1.5: a)single crystalline

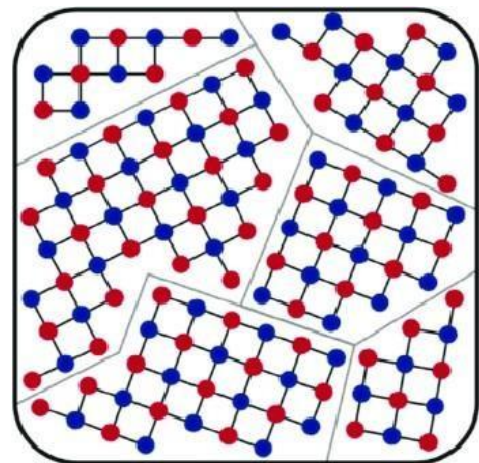


Figure 1.6: b)polycrystalline

Chapter 2

LITERATURE SURVEY

2.1 DEPOSITION

2.1.1 Epitaxial Growth of Aluminum Nitride on Sapphire Using Metalorganic Chemical Vapor Deposition

Epitaxial aluminum nitride (AlN) films were grown on the basal planes of sapphire substrates using metalorganic chemical vapor deposition (MO-CVD), and the following outcomes were obtained. The dependency of the growth rate on the substrate temperature and trimethylaluminum (TMA) content led to the conclusion that mass transport is the growth process limiting factor. Both the substrate temperature and the gas flow pattern have a significant impact on the crystalline perfection of epitaxial layers. Under precisely regulated gas flow patterns, epitaxial growth of single-crystal AlN films at temperatures about 1200 °C is possible. Oriented grains, which correlate to the hillocks seen in the surface morphology, are the primary source of crystalline defect.[16]

2.1.2 High quality AlN grown on SiC by metal organic chemical vapor deposition

Using metal organic chemical vapour deposition, the growth conditions for AlN in two-dimensional (2D) and three-dimensional (3D) growth modes were investigated. Modulation growth (MG), which alternates between 3D and 2D growth modes, was used to produce high-quality AlN layers. AFM images of MG AlN revealed long parallel atomic terraces without step terminations, indicating a decreased dislocation density. Further proof of the low dislocation density in the film was provided by the X-ray diffraction rocking curves, which produced full widths at half maximum (FWHM) of 86 and 363 arcsec.

for the (002) and (102) reflections, respectively. Additionally, 3D-2D MG reduces part of the tensile strain in the AlN film, allowing for the development of thick, crack-free AlN on SiC substrates.[3]

2.1.3 Surface, structural and optical properties of AlN thin films grown on different face sapphire substrates by metalorganic chemical vapor deposition

AlN thin films produced by metalorganic chemical vapour deposition on various face sapphire substrates were thoroughly investigated using a range of methods, such as high resolution X-ray diffraction (HR-XRD), X-ray photoelectron spectroscopy (XPS), Raman scattering (RS), and theoretical calculations. Our findings demonstrated that the early development of AlN is significantly influenced by substrate orientation. The controlling semipolar (101) orientation was visible in the AlN films, although the individual characteristics were a little weaker. AlN films produced simultaneously on several sapphire substrates with varying surface orientations had variable film thicknesses, according to optical reflectance measurements. It was discovered that the dislocation density, crystallite size, and surface oxygen incorporation are all significantly influenced by the surface orientation. Raman line width and XPS results correlated well. The combined analysis helped to clarify the reasons for the varying quality of the AlN films formed on various sapphire faces.[12]

2.2 APPLICATION AND PROPERTIES

2.2.1 Stress and piezoelectric properties of aluminum nitride thin films deposited onto metal electrodes by pulsed direct current reactive sputtering

Platinum, aluminium, and titanium electrodes were coated with polycrystalline aluminium nitride thin films using reactive magnetron sputtering in the pulsed direct current mode. All of the films showed a c-axis texture and a columnar microstructure. These films inherent stress and piezoelectric characteristics were examined in relation to the production environment and the electrode material. Stress levels ranging from intense compression to high tension were recorded, and it was shown that stress was highly dependent on the development

circumstances. It has been demonstrated that the substrate's quality and ionic bombardment affect the piezoelectric $d_{33,f}$ coefficient: The nucleation surface must exhibit hexagonal symmetry, be stable with respect to the nitrogen plasma, and provide adequate energy to the expanding nucleus.[6]

2.2.2 The electronic structure of wurtzite and zincblende AlN: an ab initio comparative study

This research focuses on the electronic characteristics of AlN (wurtzite and zincblende) compounds in various crystal phases, calculated using an all electron ab initio linearized augmented plane wave approach. Band structure, total and partial densities of states, charge density, and the ionicity factor are among the findings. Most of the computed band characteristics for wurtzite-AlN are within 1% of those for c-AlN, including the direct bandgap, total- and upper-valence bandwidths, and antisymmetric gap. Since the characteristics of the charge distributions are comparable, AlN has the same ionicity factor in both configurations.[13]

Chapter 3

AIM AND SCOPE OF THE PRESENT INVESTIGATION

3.1 AIM

- The objective of this project is to create high-quality c-axis-oriented epitaxial grown AlN thin films and evaluate the structural, optical, and mechanical behaviour of these films on appropriate sapphire substrates.

3.2 SCOPE

- Using the MOVPE method, an epitaxial c-axis oriented AlN thin film was synthesised.
- From the rocking curve, the FWHM and crystalline size are calculated.
- Using UV-visible spectroscopy, the transmittance and energy band gap of the AlN film are determined.
- Using nanoindentation technique, the hardness and modulus of the AlN film are determined.
- The developed film directs the usage of AlN in optical devices and also shows that it can be a potential material for mechanical application.

Chapter 4

EXPERIMENTAL AND CHARACTERIZATION TECHNIQUES

4.1 PHYSICAL VAPOR DEPOSITION (PVD)

Physical vapour deposition (PVD), a method for depositing thin films, involves vaporising atoms or molecules of a substance from a solid source in a high vacuum and condensing on a substrate. PVD processes can be used to deposit films of metals, alloys, metal oxides, and some composite materials on a variety of substrates. These procedures are carried out under high vacuum (between 10^{-3} and 10^{-7} mbar) and ultra high vacuum (above 10^{-7} mbar). PVD is used to deposit films ranging from of a few angstroms to thousands of angstroms in thickness.

There are different forms of PVD technique:

- **Thermal evaporation** creates a vapour by heating a substance, which condenses on a substrate to create the coating. There are many ways to heat something up, such as using a hot filament, electrical resistance, an electron or laser beam, or an electric arc.
- **Sputtering** involves the electrical production of a plasma between the coated species and the substrate.
- **Ion plating** is essentially a combination of thermal evaporation and sputtering.[15]

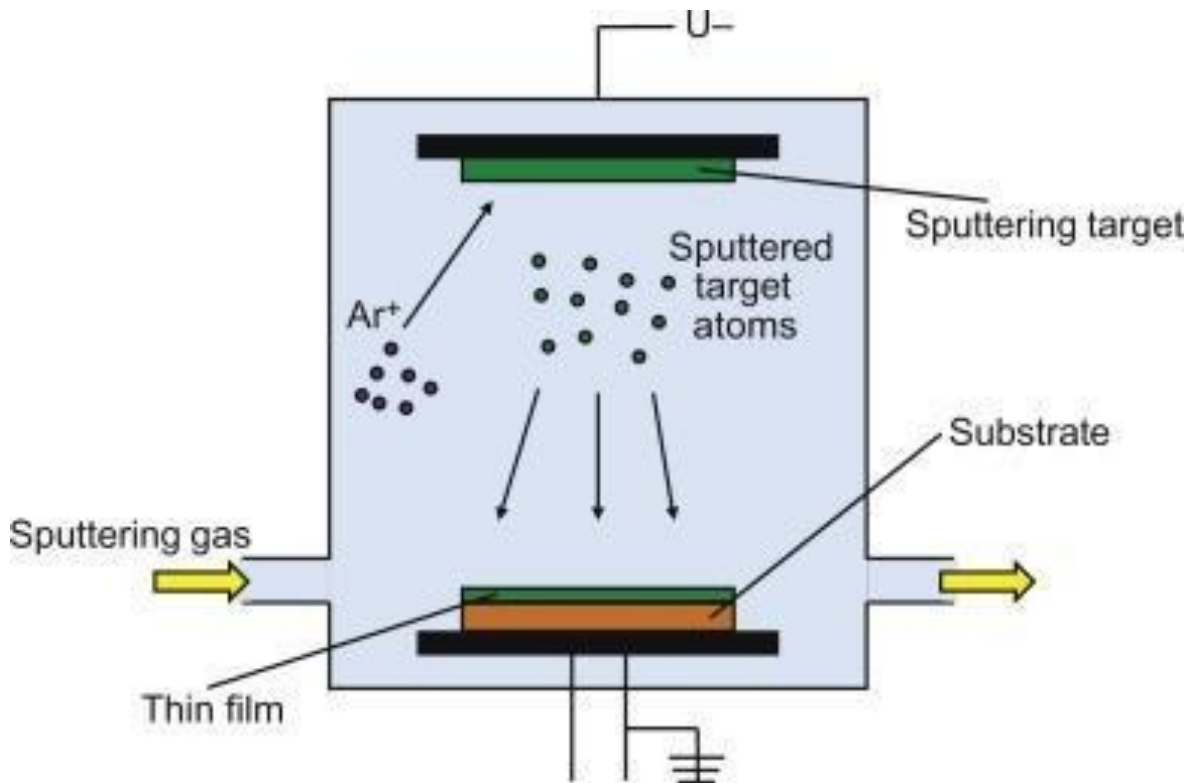


Figure 4.1: PVD Apparatus
Image source: Google

4.1.1 Advantage of the PVD

- PVD is a process that can be used on any inorganic material.
- It has a very low impact on the environment because it doesn't involve the use of chemical reagents or cleaning post-treatments.
- PVD produces coatings with excellent adhesion, resistance, and durability.
- The coating composition and thickness can be greatly controlled using the PVD process.

4.1.2 Disadvantage of the PVD

- The rate of coating deposition is usually quite slow.
- The PVD process requires sophisticated machinery that is expensive.
- Substrates with complicated geometries cannot be processed using the PVD technology.

4.2 CHEMICAL VAPOR DEPOSITION (CVD)

Chemical vapor deposition is a technique for depositing thin films based on chemical reactions involving precursor species of the vapour phase that take place both in the gas phase and on the surface of the substrate. With CVD techniques, it is possible to deposit films with uniform thickness and low porosity not only on flat substrates but also on substrates with intricate shapes. Typically, gas phase and surface reactions are involved in the highly complex CVD processes.[10]

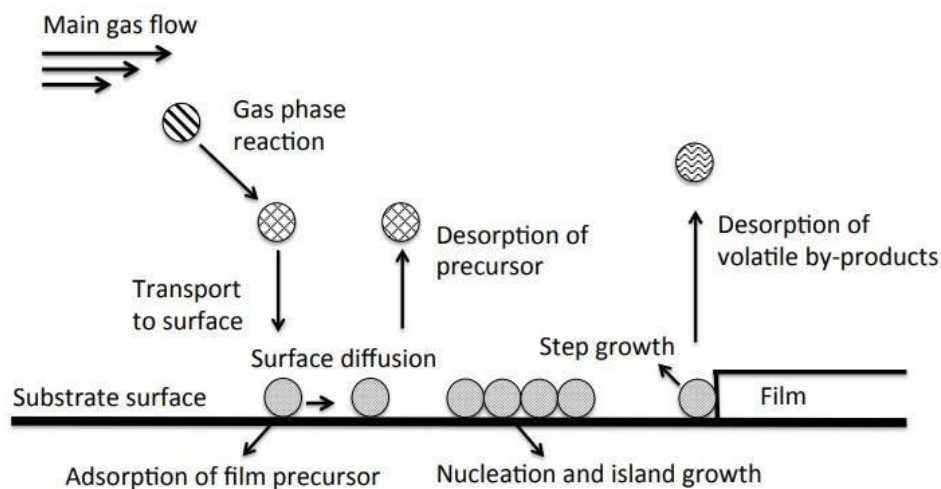


Figure 4.2: Transport and reaction processes in a CVD process
Image source: Google

Steps involved in CVD are shown in the Fig 2.2 and discussed below

1. Evaporation and transport of precursors in the gas flow region into the reactor.
2. Gas phase reactions of precursors in the reaction zone to produce reactive intermediates and gaseous by-products.
3. Mass transport of the reactants to the substrate surface.
4. Adsorption of reactants on the substrate surface.
5. The film formation is caused by surface diffusion to growth sites, nucleation, and surface chemical interactions.
6. Desorption and mass transport of remaining fragments of the decomposition away from the reaction zone.[4]

Precursor molecules are those molecules that contain the elements

required for the thin film to be deposited. In a CVD process, precursors can be inorganic or organic substances, and they can also be in different phases like gas, liquid, or solid. Precursors that are naturally present in a gaseous condition are immediately inserted into the reactor. Examples include NH_3 as a source of nitrogen, O_2 or CO_2 as a source of oxygen. The flow rate is controlled using a mass flow controller (MFC). Organoboron precursors that are volatile in liquid form, such as triethylboron (TEB), triethylgallium (TEGa) and trimethylgallium (TMGa), are stored in specialised containers known as "bubblers," which are often made of stainless steel. The bubbler has one input through which the carrier gas (H_2 , Ar or N_2) enters and transports the precursor vapour through the liquid, and one outlet through which the carrier gas and the precursor vapour are sent to the reactor. The precursor's downstream pressure, which is related to its flow rate, is regulated using an electronic pressure controller (EPC). For CVD precursors, it is often necessary for them to be volatile, thermally stable during transport into the reactor and to have a lower decomposition temperature. In addition to the volatility and stability of the precursor, other significant characteristics include chemical purity, low incorporation or high volatility of byproducts and compatibility with co-precursors[10].

4.2.1 Advantage of CVD

- Good throwing power and non-line of sight method.
- It has the capacity to manage process parameters to control surface shape and crystal structure.
- A variety of metallic, ceramic, and semiconducting thin films are being deposited by CVD
- Economical to produce since multiple pieces may be coated at once.

4.2.2 Disadvantage of CVD

- Toxic, corrosive, flammable, and explosive precursor gases provide several kinds of chemical and safety risks.
- Due to their high price, size restrictions, and specific use, more advanced reactor and vacuum system designs for CVD variants are

not scalable.

4.3 COMPARISON OF PVD AND CVD

S.No	Description	PVD	CVD
1	Process	Evaporation and collision impact on the solid target	Chemical reaction in gaseous phase impact of fluid dynamics
2	Coating material	Solid	Gas precursor
3	Temperature	Lower(below 450°C)	Higher(600-1100°C)
4	Coating thickness	Thin	Thick and thin
5	State of stress in coating	Compressive	Tensile
6	Wear resistance, toughness	Low,high	High,low
7	Line of sight	Needed	Not needed
8	Cleaning requirement	High	low
9	Cost	More expensive	Less expensive

Table 4.1: Comparison of PVD & CVD

[15, 10]

4.4 METAL ORGANIC CHEMICAL VAPOR DEPOSITION (MOCVD)

A form of chemical vapour deposition technique used to create single or polycrystalline thin films is metalorganic chemical vapour deposition (MOCVD). It is a method for producing complex semiconductor multilayer structures by generating crystalline layers. Metalorganic vapour-phase epitaxy (MOVPE) is another name for metalorganic chemical vapour deposition (MOCVD). In MOCVD, non-reactive carrier gases are often used to inject ultrapure precursor gases into a reactor. For a III-V semiconductor, the group III precursor could be a metalorganic, and the group V precursor could be a hydride. For example, Aluminium nitride can be grown with trimethylaluminium ((CH₃)₃Al) and ammonia(NH₃) precursors.

Precursors undergo pyrolysis when they get close to the semiconductor wafer, and the molecules then absorb onto the surface of the wafer. A new epitaxial layer of the semiconductor crystal lattice is created as a result of the surface reactivity of the precursor material. Growth in the mass-transport-limited growth regime, which is standard for MOCVD reactors, is fueled by chemical species supersaturation in the vapour phase. Films including combinations of group III and group V, group II and group VI, and group IV may be grown using MOCVD. Since it controls the growth rate in the mass-transport-limited regime, the vapour pressure of the group III metal organic source is a significant control parameter for MOCVD growth.

Construction of a typical MOCVD unit is discussed below

A reactor is a chamber constructed from a substance that does not react with the chemicals being implemented. A high temperature must not damage it. A susceptor, a reactor liner, reactor walls, gas injection units, and temperature control units are part of this chamber. Quartz or stainless steel are typically used for the reactor walls. Between the reactor wall and the susceptor, the reactor chamber liner is frequently made of ceramic or specialty glassware, including quartz. Cooling water has to be moving through the channels inside the reactor walls to prevent overheating. A substrate is placed on a susceptor that has a set temperature. The susceptor is constructed from a material that can withstand the temperature and metalorganic compounds utilised; frequently, graphite is used in its fabrication. A specific covering, often made of silicon nitride or tantalum carbide, is required on the graphite susceptor when developing nitrides and related materials to stop ammonia (NH_3) gas deterioration. Bubblers are the apparatuses used to introduce gas. In a bubbler, a carrier gas is bubbled through the metalorganic liquid, which takes up some metalorganic vapour and provides it to the reactor (often hydrogen in arsenide and phosphide development or nitrogen for nitride growth). The quantity of metalorganic vapour carried is influenced by the temperature of the bubbler and the pace at which the carrier gas is pumped through the bubbler. This process is often automated, and the most precise gas control system is one that uses ultrasonic concentration measurement. Toxic waste products need to be transformed into liquid or solid wastes for recycling or disposal (whichever is preferred). Processes should ide-

ally be created to produce as little waste as possible.[24, 2]

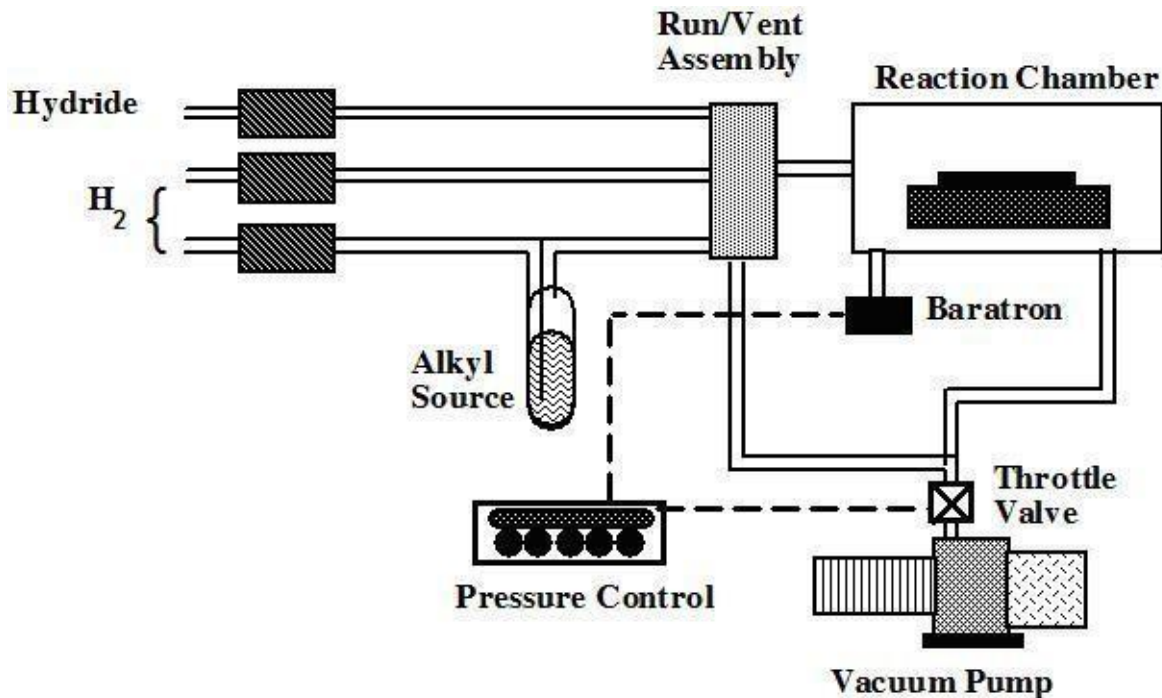


Figure 4.3: Schematic of metal organic chemical vapor deposition

4.5 GROWTH PARAMETER OF AlN

AlN were grown by high temperature MOCVD on 2-inch c-plane substrate in an Aixtron 200/4 RF-S low pressure, horizontal flow MOCVD system with radio frequency (RF) heating to investigate the effect of a TMGa pre-flow. TMAI, TMGa and NH₃ were used as precursors for Al, Ga and N₃ respectively. The mixture of Hydrogen and Nitrogen was used as a carrier gas for the growth and the growth pressure was kept at 50 mbar. Substrates were exposed to in situ Hydrogen atmosphere at 1380°C for 10 min before growth begin. In these studies, an optimized AlN nucleation layer was formed that grows on the substrate at surface temperature of 1080°C and a reactor pressure of 50 mbar. This NL was conventionally grown with simultaneously supplied TMAI (14 sccm) and NH₃ (1200 sccm) and the growth rate was 0.9 nm/s. During the growth the flow rate of TMGa was kept constant at 3.88×10^{-5} mol/min. The appropriate TMGa pre flow time was decided as 2 s with this study. Then AlN layer structure were grown by using the pulsed atomic layer epitaxy (PALE) technique with optimized changing

of TMAI pulses (4-s) and NH₃ pulses (2-s). TMAI and NH₃ flow for this layer were 77 sccm and 900 sccm respectively while the reactor pressure was 50 mbar during the growth. The synthesised thin film has a thickness of 300nm.

4.6 CHARACTERIZATION TECHNIQUES

In this work, a variety of characterisation techniques were employed. Below are a few short summaries of the characterisation techniques.

4.7 STRUCTURE ANALYSIS

4.7.1 X-ray diffraction (XRD)

X-ray diffraction is a powerful characterization technique used in the analysis of crystal structures and inter atomic spacing of material that exhibit long range order. It is a non destructive technique. X-rays are electromagnetic waves of short wavelength ranging from 0.1 to 100Å. X-rays are produced due to sudden deceleration of fast-moving electrons when they collide and interact with the target anode. More than 99 % of the electron energy during this deceleration process is transferred to heat, whereas less than 1% of the energy is transformed into x-rays.

When an incident X ray beam strike the sample, it gets scattered in all the directions. Wave interference is a bedrock for X-ray diffraction techniques. Depending on their phase difference, two light waves of the same wavelength and moving in the same direction can either reinforce or cancel each other. Constructive interference is referred to when the phase difference is $n\lambda$ called in phase in which there will be a peak formation. Destructive interference is referred to when the phase difference is $n\lambda/2$ called out phase in which there will be no peak formation. Bragg's law stated that a crystal may be divided into various sets of parallel planes. Diffraction occurs only when Bragg's law is satisfied.

$$n\lambda = 2d\sin\theta$$

Where,
 n - order of diffraction (integer),
 λ - wavelength of X-ray,
 d - inter planar spacing,
 ϑ - angle of incidence(deg).

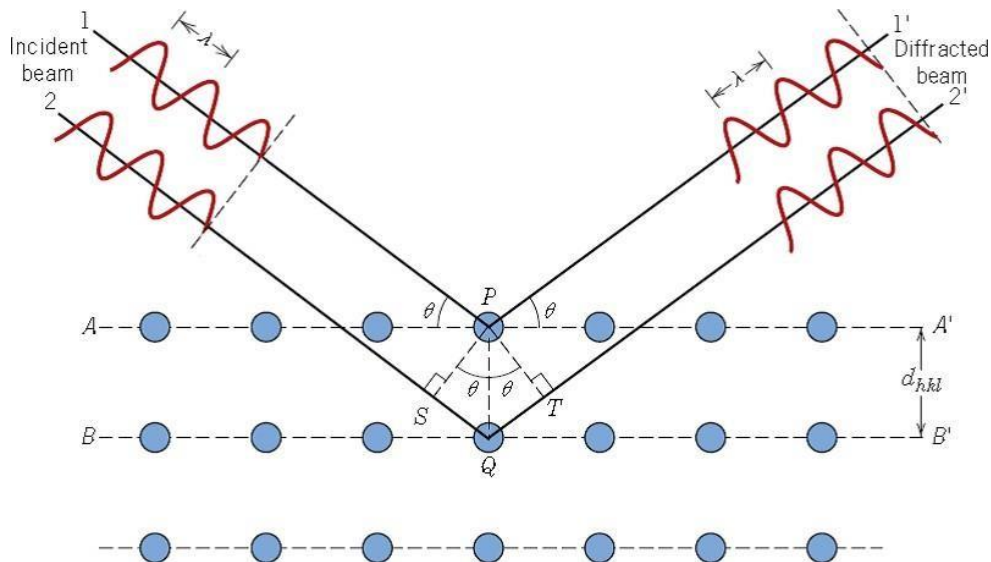


Figure 4.4: Bragg's law of diffraction
Image source: Google

The planar spacing combination, being unique to each material, can be calculated for cubic systems as

$$d = a / (h^2 + k^2 + l^2)^{1/2}$$

where h , k , l are the integers denoting the miller indices which are planes orthogonal to a reciprocal lattice vector. In addition to the other miller indices, hexagonal and rhombohedral systems might contain a redundant fourth index number, usually abbreviated as i .

$$i = -(h + k)$$

Given these well-known variables, constructive interference patterns from x-ray diffraction may be related to certain crystallographic planes.[25]

Rocking Curve (ω scan)

In a rocking curve, the Bragg angle, 2θ is set to the centroid position of a specific reflection in the $2\theta/\omega$ scan and then the sample is tilted (rocked) on the ω axis planes that are no longer parallel with the sample surface are moved onto the Bragg plane. This outcome is a single bell curve, sometimes referred to as a rocking curve, that shows how the distribution of planes changes with tilt. The substrate curvature, dislocation density, and mosaic distribution of the grains, which interfere with the lattice planes' parallel nature, determine the width of the rocking curve. In order to determine the quality of expected epitaxial growth or to identify desired orientation, the full-width half-maximum (FWHM) of the rocking curve is frequently measured. It's important to take care not to confuse the width of the rocking curves with the widths at the $2\theta/\omega$ scan peaks, since they both offer significantly different information.

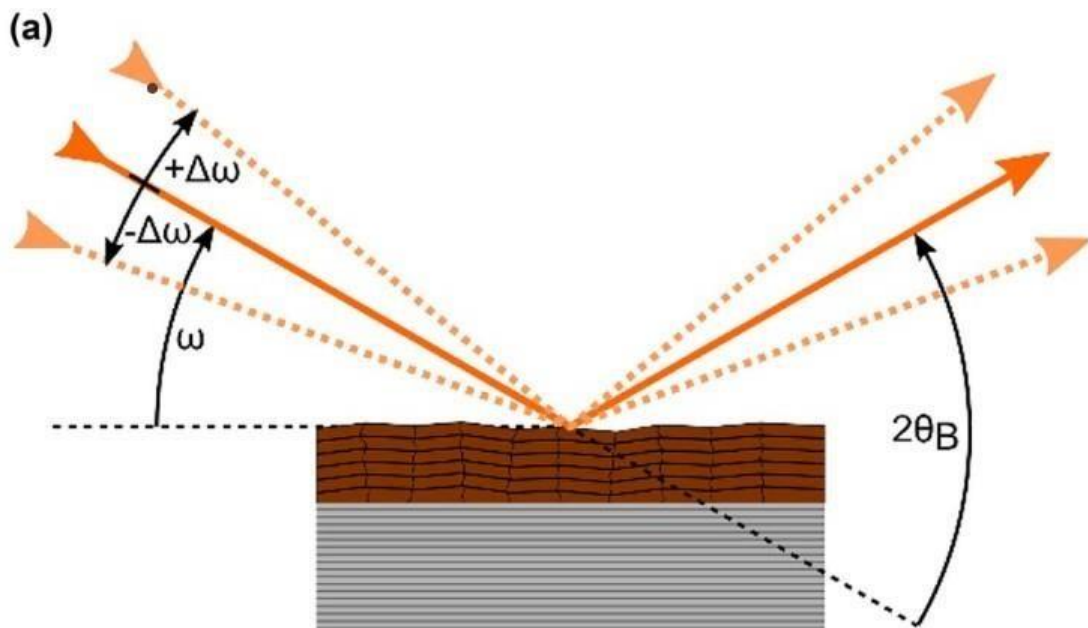


Figure 4.5: (a) Schematic of a rocking curve measurement

Image source: Google

One popular technique is to first run a $2\theta/\omega$ scan, then run rocking curves on each of the detected diffraction peaks. Similar to the $2\theta/\omega$ scan, a diffractometer with a decoupled incidence and detector angle can be used to measure rocking curves instead of an Euler cradle. Due to the beam defocusing that takes place for a divergent beam as

the sample is tilted, parallel beam optics are often required for rocking curves. The primary beam divergence, which is dependent on the optics being utilised, sets a minimum rocking curve width that may be measured. Highly epitaxial films require high resolution optics (primary beam 2- or 4-bounce crystal monochromator).[9]

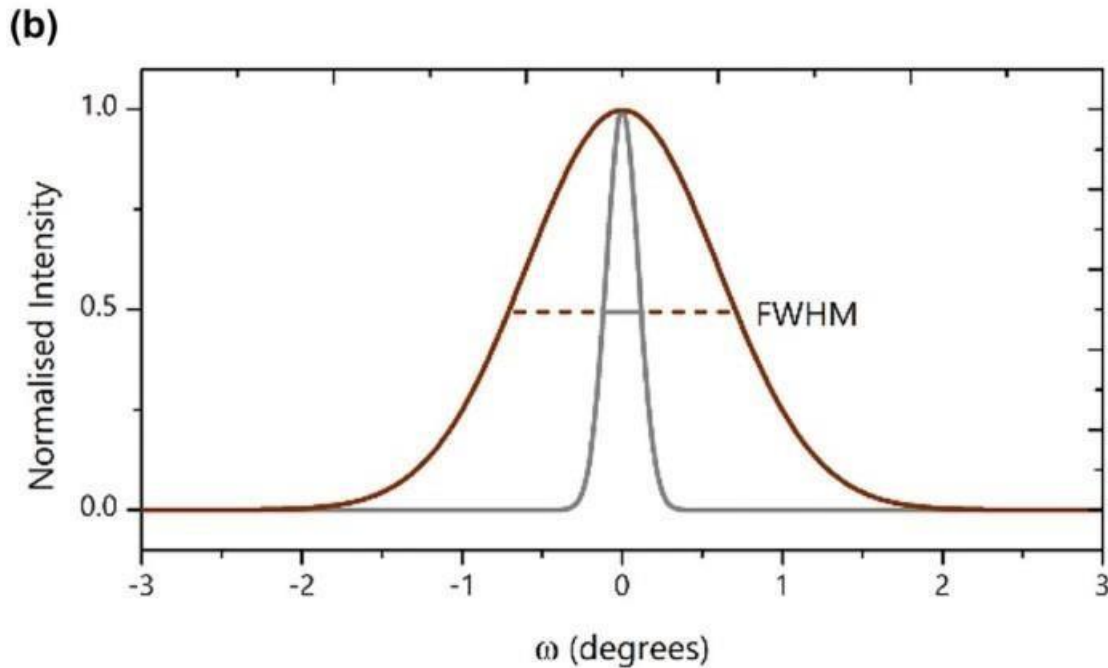


Figure 4.6: (b) Example of resultant rocking curves from a film diffraction peak.
[9]

4.8 SURFACE MORPHOLOGY

4.8.1 Atomic force microscopy (AFM)

AFM is a powerful instrument that provides information on a variety of physical characteristics, such as size, morphology, surface texture, and roughness. High-resolution tip movement and visualisation in 3D images are provided by AFM. Resolution in the vertical direction is constrained by the instrument's vibration environment, whereas resolution in the horizontal direction is constrained by the diameter of the scanning tip. AFM instruments typically have X-Y resolutions of roughly 1 nm and vertical resolutions of less than 0.1 nm.

AFM was created to overcome the fundamental limitation of STM,

which is that it can only capture conducting or semiconducting surfaces. The benefit of the AFM is that it can image practically any surface type, including glass, ceramics, composites, polymers, and biological materials. AFM is made up of a cantilever-mounted sharp tip with a diameter of between 10 and 20 nm. Silicon or silicon nitride is used in the micro-fabrication of AFM tips and cantilevers. The cantilever's dimensions are essential since they determine its stiffness or spring constant. If not adjusted appropriately, this stiffness can lead to poor picture quality as it is crucial to controlling the contact between the AFM cantilever tip and the sample surface. The tip moves in reaction to interactions between the tip and the surface, and the movement is recorded by laser beam focusing on a photodiode.

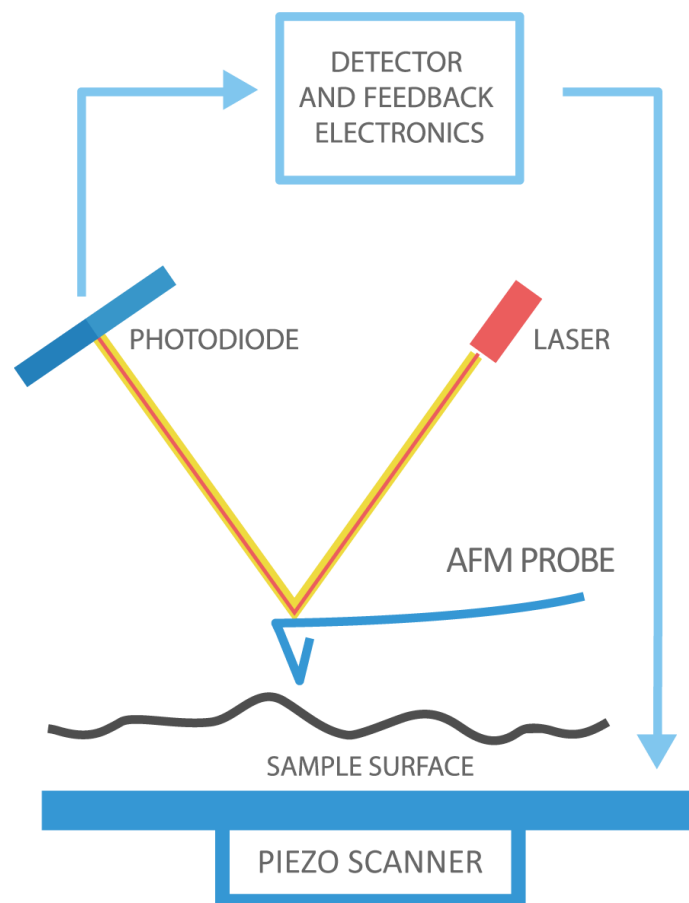


Figure 4.7: Schematic for Atomic Force Microscopy
Image source: Google

4.9 OPTICAL ANALYSIS

4.9.1 Ultraviolet-visible (UV-vis) spectroscopy

Ultraviolet-visible (UV-vis) spectroscopy is used to obtain the absorbance spectra of a compound in solution or as a solid. Only a small portion of the entire electromagnetic spectrum can be detected by the human eye. The visible spectrum, which covers the range of wavelengths from 400 to 800 nm, is the portion of the electromagnetic spectrum that can be seen by human eyes. The UV (ultraviolet) spectrum is the lower wavelength range between 100 and 400 nm. The entire electromagnetic spectrum is shown in figure 4.8.

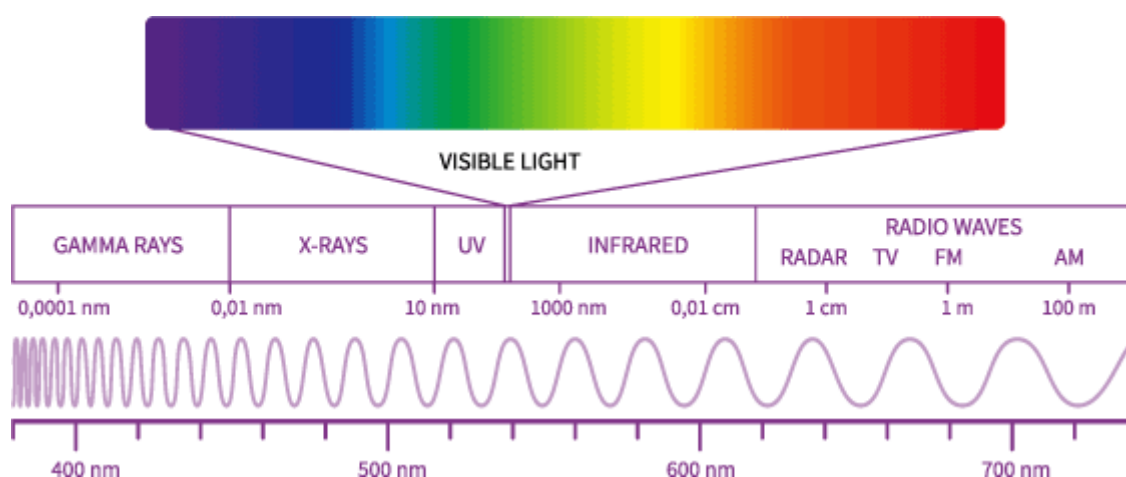


Figure 4.8: Electromagnetic spectrum
Image source: Google

A spectrophotometer is employed to measure the amount of light that a sample absorbs. The instrument operates by passing a beam of light through a sample and measuring the intensity of light reaching a detector. A variety of effects, including absorbance, reflectance, transmittance, and scattering, are produced when electromagnetic radiation interacts with solids and liquids. The compound undergoes an electronic transition as a result of absorbing UV-Visible radiation, in which an electron in the ground state into an energetically excited state. The amount of radiation absorbed is proportional to the energy difference between the ground state and the excited state. When light falls upon a substance it absorbs and reflects a certain amount of radiation. The absorbance (A) is equal to the logarithm of a fraction involving the intensity of light before passing through the

sample (I_0) divided by the intensity of light after passing through the sample (I). The fraction I divided by I_0 is also called transmittance (T), which expresses how much light has passed through a sample. [20, 1]

Transmittance, $T = I / I_0$

Absorbance, $A = \log_{10}(I_0 / I) = \log_{10}(1/T) = -\log_{10}(T)$

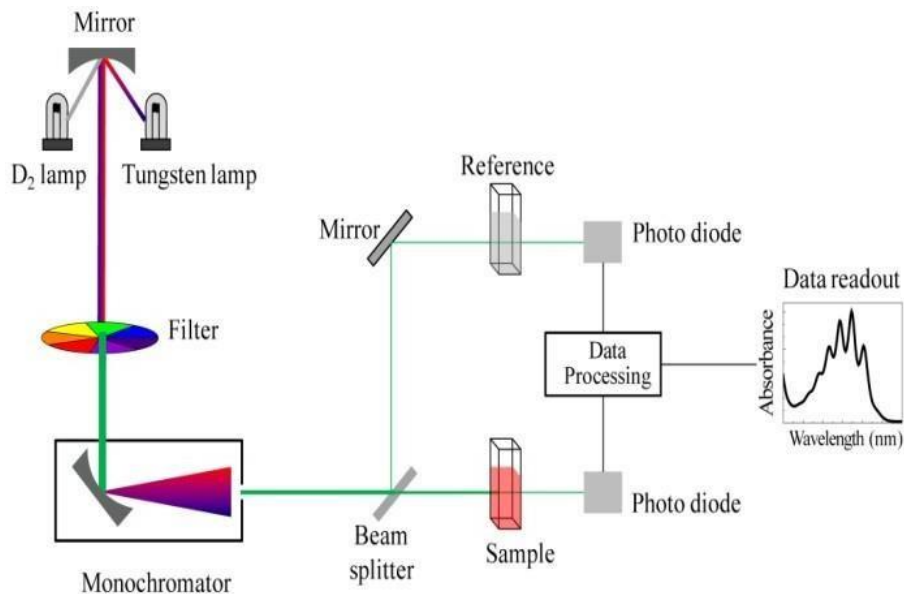


Figure 4.9: Schematic diagram of UV Visible spectroscopy
Image source: Google

All of these devices have a light source (typically a tungsten or deuterium lamp), a sample holder, and a detector, though some also have a filter for selecting out one wavelength at a time. A prism or diffraction grating separates a beam of light from a visible or UV light source into its individual wavelengths. A half-mirrored device divides each monochromatic beam into two beams of equal intensity. One of the beams passes through the target sample, while the other beam passes to the reference sample. The final result is determined from the sample beam and reference beam. In this work an UV Vis NIR spectrophotometer (Hitachi made) has been used to find the film transmittance.

4.10 MECHANICAL ANALYSIS

4.10.1 Nanoindentation

Nanoindentation is a powerful technique for analysing the mechanical characteristics of a material, such as its hardness, elasticity, and plasticity which determines its capacity to withstand persistent deformation when under stress. The measurement of forces in the mN range with high accuracy and precision and the depth of penetration to nm resolution are its primary concerns. The applied load divided by the area of the projected contact surface in the material gives the hardness. When a load is applied, the bonds between the atoms stretch and cause elastic deformation. When the load is removed, the object returns to its original shape. When a force is placed past the elastic limit, plastic deformation occurs, and permanent distortion results. Tensile testing is often utilised for bulk samples, however nanoindentation may also evaluate soft tissues, polymeric materials, thin film coatings, and other materials. Indenters with various shapes, including Berkovich for E and H, spherical for stress-strain, flat punch for complex modulus, cube corner for fracture toughness, spherical cone for scratch measurements and wedge for three-point bending, can be used to test the desired characteristics.

This method is frequently employed to figure out the mechanical characteristics of thin films, coatings, particles, fibres, embedded phases, and patterned structures. The loads are applied in nanoindentation equipment electro-magnetically, electrostatically, or by spring deflection. To measure the displacement, a capacitance gauge or a linear variable differential transformer (LVDT) are utilised. The Berkovich indenter is the indenter that is most often used in nanoindentation. It is a three-sided pyramid with the benefit that, as compared to a Vickers indenter, the three planes may be more easily machined to come together at a single point, enabling a more exact indentation operation. The sample's surface is indented using a diamond probe with a tip as small as 30 nm. These have equilateral triangle shapes that have curved sides. From load displacement curves, hardness and elastic modulus are calculated.

During the loading and unloading cycles, the load and indenta-

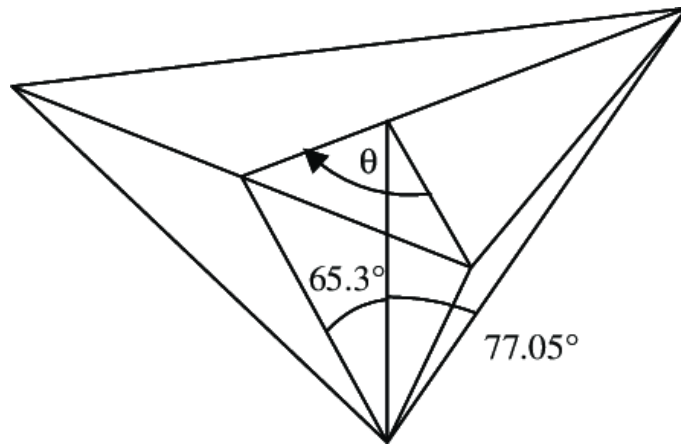


Figure 4.10: Schematic Diagram of the Berkovich indenter
Image source: Google

tion displacements are measured. The unloading area of the load-displacement curve is typically thought to be entirely elastic. The load displacement curves (P-h curves) may be used to measure three essential factors. The elastic limit, maximum displacement, and maximum load Determined is the modulus or stiffness $S = dP/dh$, which is equal to the slope of the top part of the unloading curve. Thin film measurement on a substrate is difficult because the information volume has to be free of substrate effects. This is accomplished by restricting the indentation depth at 10% of the film thickness.

$$\text{Hardness} = F_{max}/A_p(h_c) \text{ in pascal}$$

where,

F_{max} =Load applied (mN/min),

A_p =projected area,

h_c =contact depth.

$$1/E_r = (1-(r_i)^2)/E_i + (1-(r_s)^2)/E_s$$

where,

E_r =Reduced modulus,

E_i =Indenter modulus,

E_s =Specimen modulus,

r_i =poisons ratio of indenter,

r_s =poisons ratio of specimen.[7, 18]

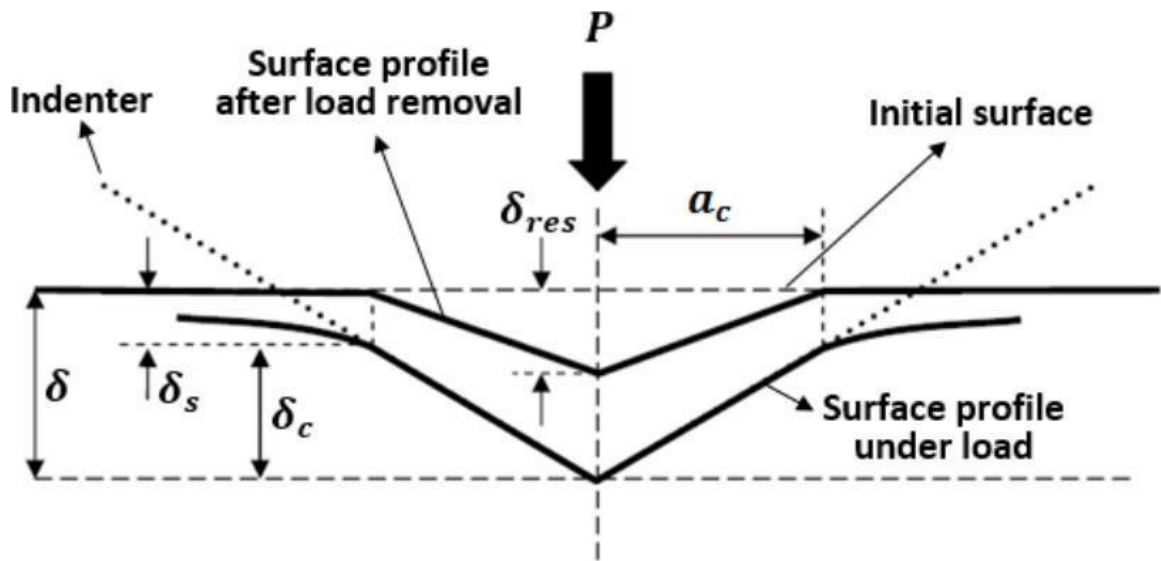


Figure 4.11: Schematic of a cross section of an indentation with the supposition that piling-up and sinking-in are minimal. Various dimensions that used in the analysis are indicated

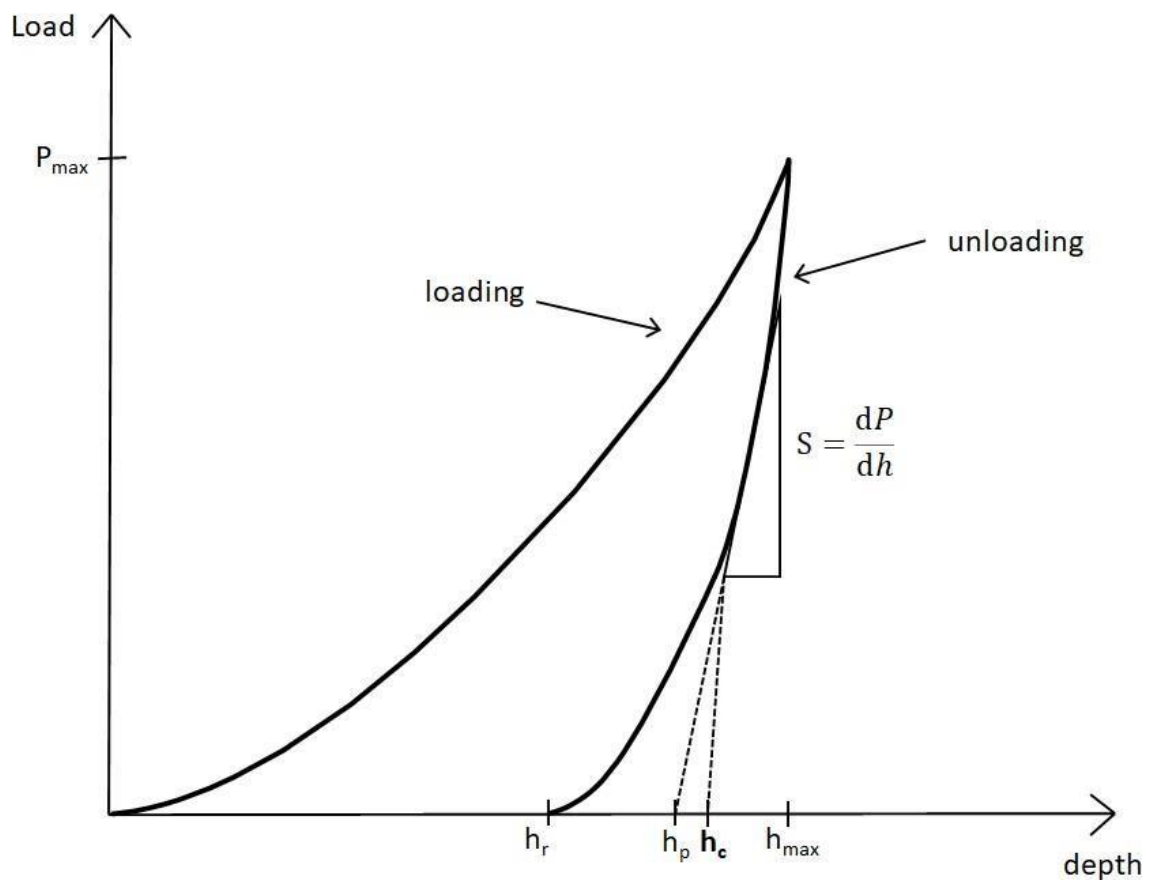


Figure 4.12: The load(p) vs displacement(h) curve

Chapter 5

RESULTS AND DISCUSSION

5.1 STRUCTURAL ANALYSIS

5.1.1 X-ray diffraction

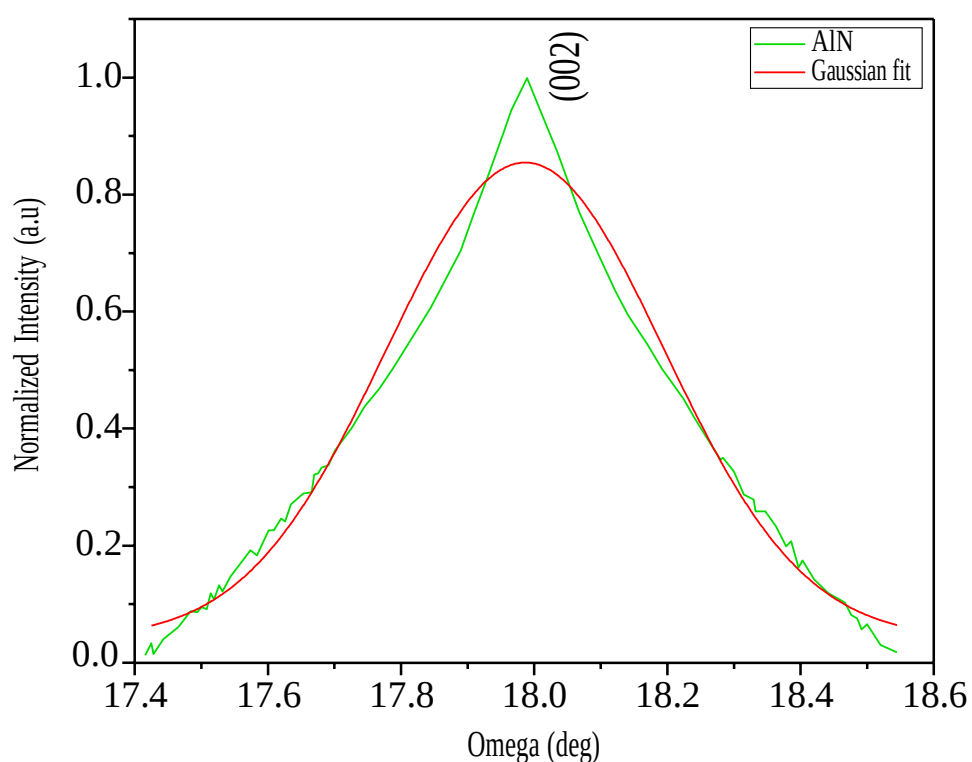


Figure 5.1: HR-XRD pattern for AlN thin film

High resolution XRD rocking curve measurements were made to understand the structural properties of the MOCVD grown thin film. Peak position and the broadening observed in the 2θ - Ω scans mea-

sured with HR-XRD may show the relaxation and crystalline quality of the sample. The sharp gaussian peak close proximity to the sample peak shows that the sample is highly epitaxial and of exceptionally high quality. The peak, which appears at a 36 deg angle, is part of the 002 plane in the $2\theta/\theta$ a powder pattern. However the angle at 18 deg shown in the Fig. 5.1. The FWHM of this peak found as 290 arcsec, which signifies to be a epitaxial film.

5.1.2 Morphology and surface roughness by AFM

The 2D surface topography of the film is explored using afm over an area $1 \times 1 \text{ } \mu\text{m}^2$. The presence of microscopic features can be attributed to the growth process and defects present. The rms roughness of the film is 1.13 nm as shown in the Fig. 5.2

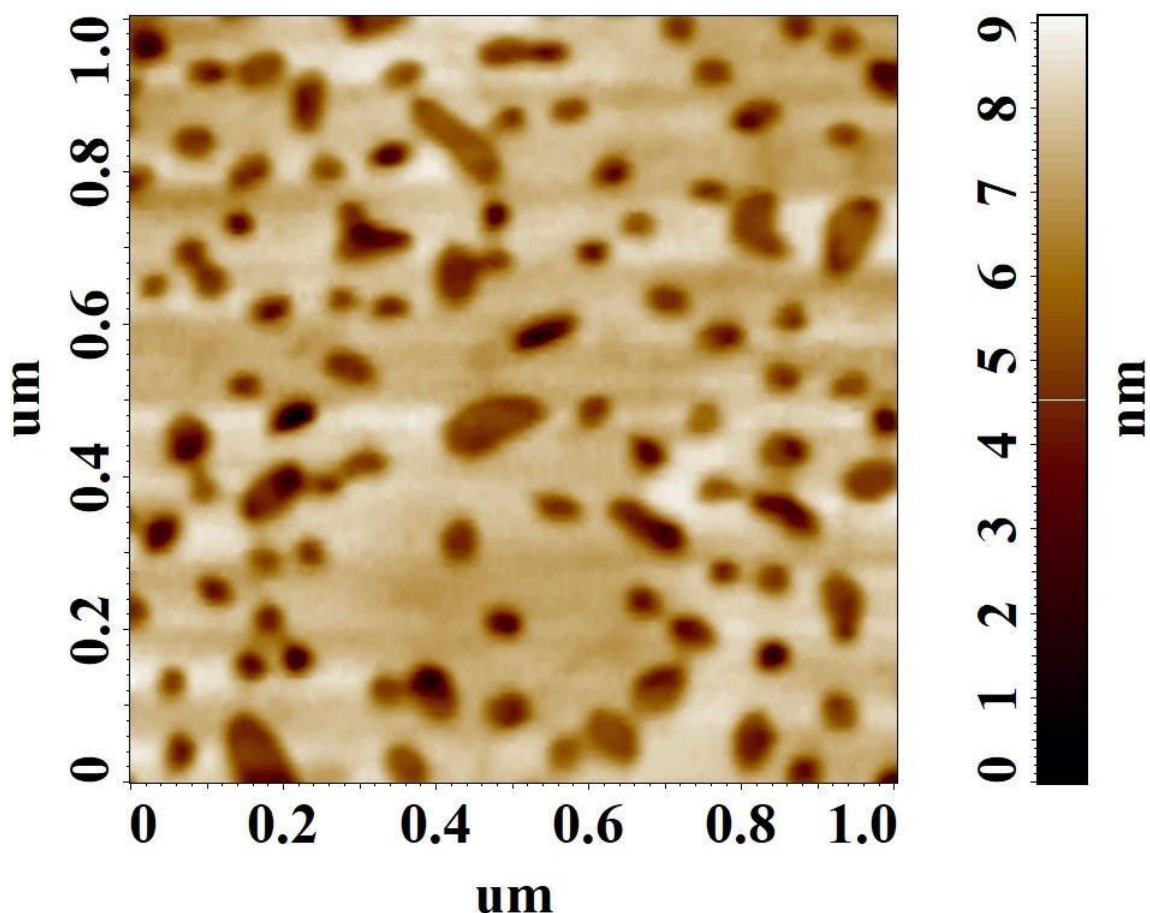


Figure 5.2: Surface topography of the film by using AFM

5.2 OPTICAL ANALYSIS

5.2.1 UV-Vis-NIR spectrophotometer

A UV-Vis-NIR spectrophotometer has been used to examine the AlN sample optical characteristics. Presence of defects strongly impact the optical properties of AlN based optoelectronic device. The spectra reveal a crisp interface between AlN thin film and substrate, as seen by well defined interference pattern. Moreover, there are many studies in the literature show that the transmittance level decrease when surface roughness of the thin film increase. The present thin film exhibits interference pattern in the wavelength range from 240 to 1000nm. This is probably because the very thin film interferes with the substrate, and it may also be because there are defects in the films, as shown in the Fig. 5.3. The band gap of the grown aln film is 5.75 ev. Thus, it is a wide bandgap system as shown in Fig. 5.4.

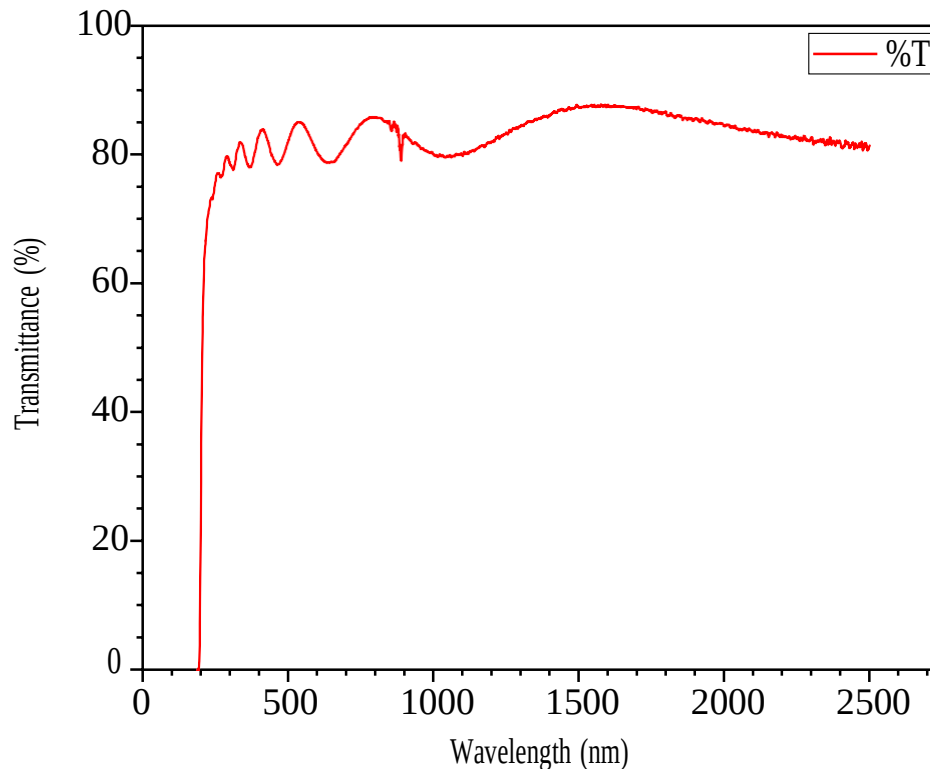


Figure 5.3: Transmittance vs wavelength curve

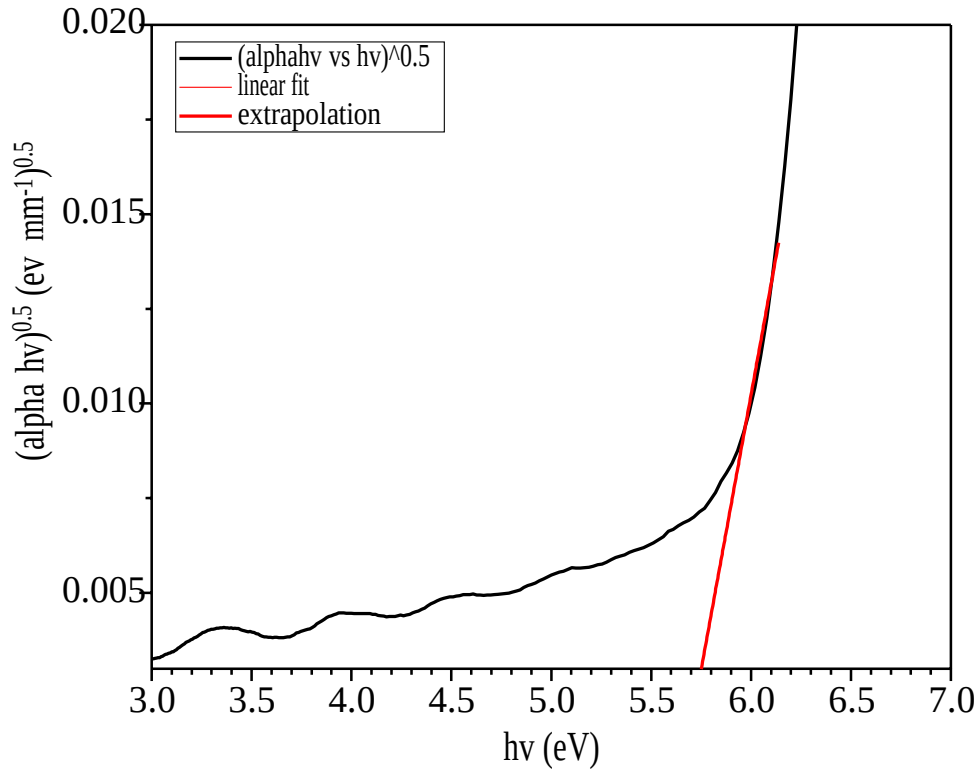


Figure 5.4: Energy band gap of AlN thin film

5.3 MECHANICAL ANALYSIS

In this work, Indentation hardness and modulus studies were performed using a Nanoindentation (M/s. Anton Paar, switzerland) at a max depth of 130 nm, loading rate 10 mN/min and unloading rate 10 mN/min for this thin film using continuous stiffness measurement technique.

5.3.1 Indentation of hardness and modulus

Mechanical property measurements based on depth sensing techniques where the load and displacement data are collected throughout the indentation process have been commonly used to determine hardness and Modulus of elasticity. Indentation mean hardness measurement on the surface of AlN thin film at depth of 30nm is 13.661 ± 0.55 GPa respectively. Fig. 5.6 shows the indentation mean hardness profile for AlN thin film. Hardness describe the ability to resist plastic deformation.

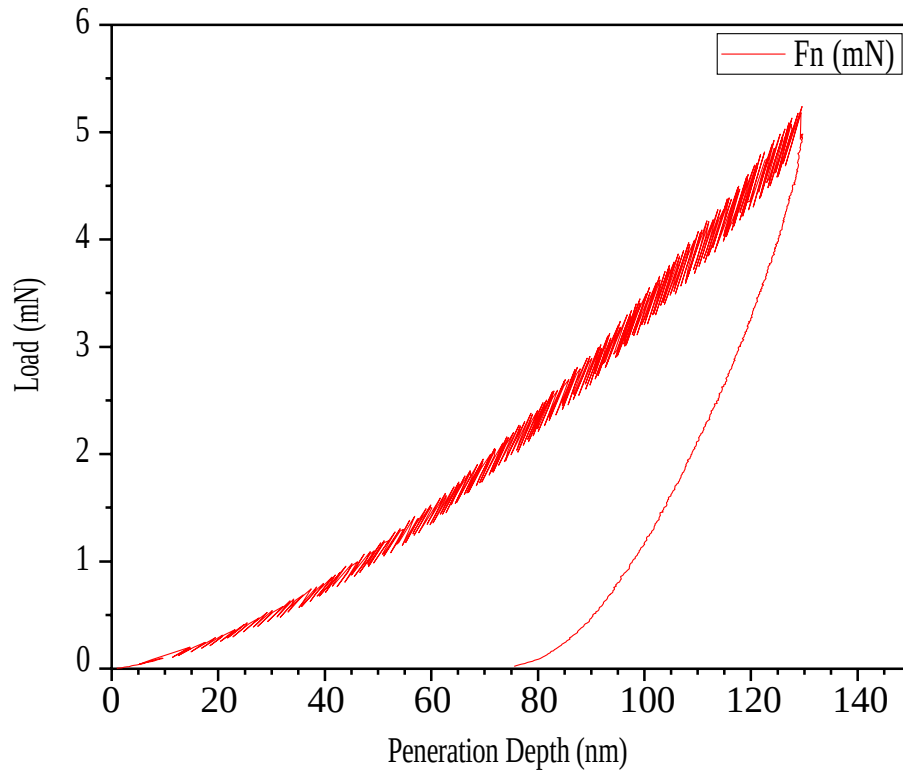


Figure 5.5: Load(p) vs depth(h) curve

Nanoindentation experiments also yielded the elastic modulus. The stiffness of the material (resistance to elastic strain) is represented by the material's modulus of elasticity. Fig. 5.7 shows the indentation mean modulus profile for AlN thin film. Due to a tip artifact (tip rounding off), the initial indentation mean modulus of AlN thin film falls. AlN thin film have a 361.59 ± 11.98 GPa mean modulus.

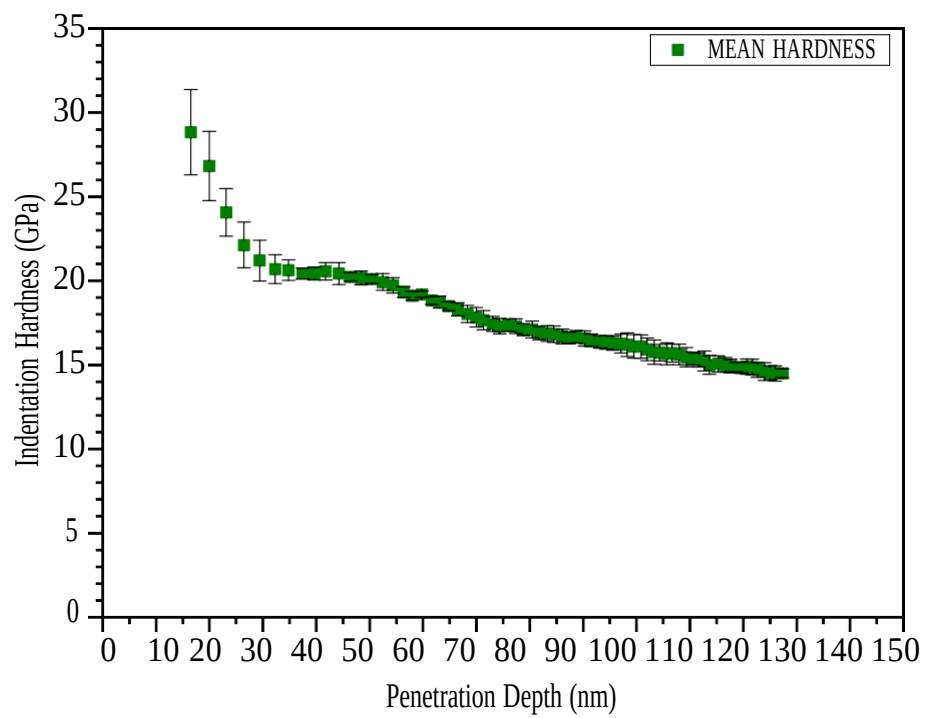


Figure 5.6: Hardness value for AlN thin film

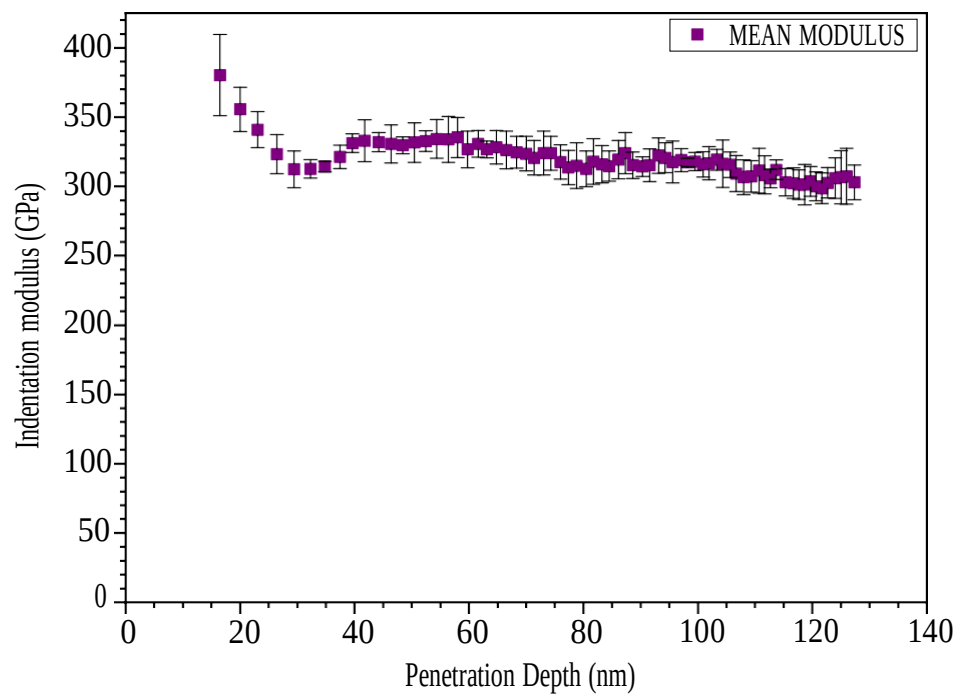


Figure 5.7: Elastic modulus value for AlN thin film

Chapter 6

CONCLUSION

An epitaxial c-axis oriented AlN thin film was synthesized using MOCVD technique. These thin films were characterized using high resolution XRD, AFM, UV-Vis-NIR spectroscopy and nanomechanical techniques. High resolution XRD was used to identify the (002) orientation quality by (2θ - Ω scan) from that the FWHM observed was 290 arcsec. Small value confirms that the epitaxial thin film is highly oriented single crystal. The transmittance study by UV-VIS spectroscopy confirms the high transparency of the thin film and the energy band gap of the film is 5.57eV. Also, the substrate roughness is very less led to high transparency and the rms roughness of the film is 1.13 nm. The nanomechanical characterization using nanoindentation system using Continuous Stiffness Measurement technique exhibited an indentation hardness (HIT) of 13.661 ± 0.55 GPa and indentation modulus (EIT) of 361.59 ± 1.98 GPa at a depth of 30nm from the top surface.

Bibliography

- [1] CE Adeeyinwo, NN Okorie, and GO Idowu. Basic calibration of uv/visible spectrophotometer. *International Journal of Science and Technology*, 2(3):247–251, 2013.
- [2] Yiren Chen, Hang Song, Dabing Li, Xiaojuan Sun, Hong Jiang, Zhiming Li, Guoqing Miao, Zhiwei Zhang, and Yue Zhou. Influence of the growth temperature of aln nucleation layer on aln template grown by high-temperature mocvd. *Materials Letters*, 114:26–28, 2014.
- [3] Z Chen, S Newman, D Brown, R Chung, S Keller, UK Mishra, SP Denbaars, and S Nakamura. High quality aln grown on sic by metal organic chemical vapor deposition. *Applied Physics Letters*, 93(19):191906, 2008.
- [4] KL Choy. Chemical vapour deposition of coatings. *Progress in materials science*, 48(2):57–170, 2003.
- [5] V Cimalla, Joerg Pezoldt, and Oliver Ambacher. Group iii nitride and sic based mems and nems: materials properties, technology and applications. *Journal of Physics D: Applied Physics*, 40(20):S19, 2007.
- [6] Marc-Alexandre Dubois and Paul Muralt. Stress and piezoelectric properties of aluminum nitride thin films deposited onto metal electrodes by pulsed direct current reactive sputtering. *Journal of Applied Physics*, 89(11):6389–6395, 2001.
- [7] Anthony C Fischer-Cripps. Critical review of analysis and interpretation of nanoindentation test data. *Surface and coatings technology*, 200(14-15):4153–4165, 2006.
- [8] T Hanada. Basic properties of zno, gan, and related materials. *Oxide and nitride semiconductors: processing, properties, and applications*, pages 1–19, 2009.

- [9] George F Harrington and José Santiso. Back-to-basics tutorial: X-ray diffraction of thin films. *Journal of Electroceramics*, 47(4):141–163, 2021.
- [10] Anthony C Jones and Michael L Hitchman. *Chemical vapour deposition: precursors, processes and applications*. Royal society of chemistry, 2009.
- [11] Adarsh Sandhu Kiyoshi Takahashi, Akihiko Yoshikawa. Wide bandgap semiconductors. (*fundamental properties and modern photonic and electronic devices*), pages 36–38, 1983.
- [12] Yao Li, Chi Zhang, Xuguang Luo, Yuanlan Liang, Dong-Sing Wu, Chin-Che Tin, Xiang Lu, Kaiyan He, Lingyu Wan, and Zhe Chuan Feng. Surface, structural and optical properties of aln thin films grown on different face sapphire substrates by metalorganic chemical vapor deposition. *Applied Surface Science*, 458:972–977, 2018.
- [13] F Litimein, B Bouhafs, Z Dridi, and P Ruterana. The electronic structure of wurtzite and zincblende aln: an ab initio comparative study. *New Journal of Physics*, 4(1):64, 2002.
- [14] VI Litvinov and VK Dugaev. Ferromagnetism in magnetically doped iii-v semiconductors. *Physical review letters*, 86(24):5593, 2001.
- [15] Donald M Mattox. *Handbook of physical vapor deposition (PVD) processing*. William Andrew, 2010.
- [16] Mizuho Morita, Norihiko Uesugi, Seiji Isogai, Kazuo Tsubouchi, and Nobuo Mikoshiba. Epitaxial growth of aluminum nitride on sapphire using metalorganic chemical vapor deposition. *Japanese Journal of Applied Physics*, 20(1):17, 1981.
- [17] Hadis Morkoç. *Handbook of Nitride Semiconductors and Devices, GaN-Based Optical and Electronic Devices, Volume*, volume 53. Wiley Online Library, 2008.
- [18] Warren C Oliver and Georges M Pharr. Measurement of hardness and elastic modulus by instrumented indentation: Advances in understanding and refinements to methodology. *Journal of materials research*, 19(1):3–20, 2004.

- [19] Padmalochan Panda. *Synthesis and Characterization of Pristine and Doped (Ti and Cr) AlN Thin Films*. PhD thesis, HOMI BHABHA NATIONAL INSTITUTE, 2019.
- [20] Heinz-Helmut Perkampus. *UV-VIS Spectroscopy and its Applications*. Springer Science & Business Media, 2013.
- [21] YU Peter and Manuel Cardona. *Fundamentals of semiconductors: physics and materials properties*. Springer Science & Business Media, 2010.
- [22] Eliseo Ruiz, Santiago Alvarez, and Pere Alemany. Electronic structure and properties of aln. *Physical Review B*, 49:7115, 1994.
- [23] Raymond E Smallman and AHW Ngan. *Physical metallurgy and advanced materials*. Elsevier, 2011.
- [24] Gerald B Stringfellow. *Organometallic vapor-phase epitaxy: theory and practice*. Elsevier, 1999.
- [25] Challapalli Suryanarayana, M Grant Norton, C Suryanarayana, and M Grant Norton. *X-rays and Diffraction*. Springer, 1998.
- [26] Kenji Ueda, Hitoshi Tabata, and Tomoji Kawai. Magnetic and electric properties of transition-metal-doped zno films. *Applied Physics Letters*, 79(7):988–990, 2001.
- [27] SG Yang, AB Pakhomov, ST Hung, and CY Wong. Room-temperature magnetism in cr-doped aln semiconductor films. *Applied physics letters*, 81(13):2418–2420, 2002.