Summer Internship Report

On

X-Ray and IR Reflectivity of Multilayers

At

Under the guidance of

Dr. BRAJESH SINGH YADAV (SCIENTIST “E” - Characterisation Lab)

SOLID STATE PHYSICS LABORATORY
DEFENCE RESEARCH AND DEVELOPMENT ORGANISATION
Timarpur, Lucknow Road, Delhi-110008

By

MAGESHAN KP (21JE0522)
B.Tech. Engineering Physics

SUBMITTED TO

DEPARTMENT OF PHYSICS
INDIAN INSTITUTE OF TECHNOLOGY DHANBAD
(INDIAN SCHOOL OF MINES)

ORGANISATION PROFILE

Defence Research & Development Organisation (DRDO) works under the Department of Defence Research and Development of the Ministry of Defence. DRDO dedicatedly working towards enhancing self-reliance in Defence Systems and undertakes design & development leading to production of world class weapon systems and equipment in accordance with the expressed needs and the qualitative requirements laid down by the three services.

DRDO is working in various areas of military technology which include aeronautics, armaments, combat vehicles, electronics, instrumentation engineering systems, missiles, materials, naval systems, advanced computing, simulation and life sciences. DRDO while striving to meet the Cutting edge weapons technology requirements provides ample spinoff benefits to the society at large thereby contributing to nation building.

Vision
Make India prosperous by establishing a world-class science and technology base and provide our Defence Services decisive edge by equipping them with internationally competitive systems and solutions.

DRDO has many research and development labs spread across the country. The different R&D labs are meant to work on different projects.one of the labs of DRDO is SSPL (solid state physics laboratory), which is located in Timarpur, Delhi.

Solid State Physics Laboratory (SSPL), one of the establishments under the Defence R&D Organization (DRDO), Ministry of Defence, was established in 1962 with the broad objective of developing an R&D base in the field of Solid State Materials, Devices and Subsystems. The Laboratory has a vision to be the centre of excellence in the development of Solid State Materials, Devices and has a Mission to develop and characterise high purity materials and solid state devices and to enhance infrastructure, technology for meeting the futuristic challenges.

DECLARATION BY THE CANDIDATE

I, **MAGESHAN KP** student of I**NDIAN INSTITUTE OF TECHNOLOGY DHANBAD (INDIAN SCHOOL OF MINES)**, B.Tech in Engineering Physics, declare that the internship on the project titled "Materials Characterization" is my own work conducted under the supervision of **Dr. Brajesh Singh Yadav (Scientist 'E') from SSPL, DRDO, New Delhi.**

I further declare that to the best of my knowledge the project report does not contain any part which has been submitted previously in this organisation or any other university/deemed university without proper citation.

MAGESHAN KP
B .Tech In Engineering Physics
INDIAN INSTITUTE OF TECHNOLOGY DHANBAD
(INDIAN SCHOOL OF MINES)

ACKNOWLEDGEMENT

Firstly, I would like to thank my supervisor **Dr. Brajesh Singh Yadav (Scientist 'E') of Solid-State Physics Laboratory, DRDO** for giving me the chance to take part in the project work which enabled me to accomplish this internship.

I am highly Indebted for the help and support given by **Dr. Anshu Goyal**. I'm grateful for his valuable guidance, timely help and persuasion throughout the program of my study.

I acknowledge **Dr.Thangavel ,Physics Department, Indian Institute of Technology (ISM)** for allowing me to pursue my internship. I express my genuine thanks to everyone for their support and advice to complete my internship in the above said organisation.

I would also like to thank Ms.Bhawana Singh technical staff of SSPL, DRDO, New Delhi for constant help in the characterization process. I'm highly thankful to my team Aaditya Jain and Sanidhya Niranjan for their constant help and endless support in the experimental work.

I am grateful to the whole technical staff at DRDO for their valuable suggestions and guiding me in the project. I would also like to express my gratitude towards my parents for their love and support throughout this session that benefited me in successful completion of this internship.

EXECUTIVE SUMMARY

The internship project at the Solid State Physics Laboratory (SSPL) under DRDO focused on advanced materials characterization methods, particularly using X-Ray Reflectivity (XRR) and Fourier Transform Infrared (FTIR) Spectroscopy. During this period, I gained hands-on experience in thin-film analysis techniques, learning to measure and interpret critical physical properties such as thickness, density, and roughness of thin films and interfaces. The project explored both theoretical and practical aspects of XRR, leveraging the transfer matrix approach and MATLAB-based implementation to calculate reflectivity profiles for multilayered structures. This methodology proved crucial in accurately characterising interfaces in complex material stacks, offering insights into their structural and electronic attributes.

In addition to XRR, I also delved into FTIR spectroscopy, primarily to assess electrical properties and thickness of SiC substrates and epilayers in a nondestructive manner. By analysing IR reflectance spectra, I determined carrier concentrations and mobility in SiC wafers, crucial parameters for power electronics. Using the Modified Dielectric Function (MDF) model, I performed spectral fitting to extract these values with precision, demonstrating the effectiveness of FTIR as a non-contact technique for semiconductors. The project underscored the significance of computational tools in modern material science research, where MATLAB was extensively employed to simulate, fit, and visualize data from both XRR and FTIR experiments.

This internship provided substantial knowledge on thin-film characterization, advanced data analysis techniques, and problem-solving using theoretical models and practical experimentation. Working under the guidance of experienced scientists, I developed proficiency in using XRR and FTIR as robust tools for materials characterization and deepened my understanding of the critical role such techniques play in research and development within the field of solid-state physics.

CERTIFICATE

This is to certify that **Mr Mageshan Kp** is a student of **INDIAN INSTITUTE OF TECHNOLOGY DHANBAD (INDIAN SCHOOL OF MINES)** pursuing **B.Tech In Engineering Physics** has undergone an eight week internship at **Solid State Physics Laboratory (SSPL),DRDO, New Delhi**.

He has successfully completed the project .The project work is original work of the candidate and has not been submitted elsewhere. During the period of training his conduct has been virtuous, exemplary. I wish him success in his approaching career.

Dr. Brajesh Singh Yadav
(Scientist 'E')
Characterization division
SSPL, Delhi

INDEX

CONTENTS

1. CHAPTER 1 : **X-Ray Reflectivity**

1.1. INTRODUCTION.

1.2. X-RAY REFLECTIVITY MEASUREMENT.

1.3. BASICS OF X-RAY CHARACTERISTIC RADIATION.

1.4. GENERATION OF X-RAYS.

1.5. DERIVING ELECTRIC FIELD EQUATIONS FROM MAXWELL'S RELATIONS.

1.6. COMPLEX REFRACTIVE INDEX.

1.7. CONCEPT OF CRITICAL ANGLE.

1.8. FRESNELS REFRACTION COEFFICIENT AND REFLECTIVITY .

1.9. TRANSFER MATRIX APPROACH.

1.10. VERIFICATION OF TRANSFER MATRIX APPROACH.

1.11. COMPUTATIONAL ADVANTAGE OF TRANSFER MATRIX APPROACH AND ITS IMPLEMENTATION.

1.12. MATLAB IMPLEMENTATION FOR A 2-LAYER SYSTEM.

1.13. MATLAB IMPLEMENTATION FOR A 5-LAYER SYSTEM.

1.14. EXPERIMENTAL RESULTS.

1.15. CONCLUSION.

2. CHAPTER 2 : FTIR

2.1 ABSTRACT

2.2 INTRODUCTION

2.3 CHARACTERIZATION METHOD OF THE ELECTRICAL PROPERTIES IN SIC SUBSTRATE USING IR REFLECTANCE SPECTROSCOPY

2.4 MEASUREMENTS OF IR REFLECTANCE SPECTRA OF SIC WAFERS AND ESTIMATION OF ELECTRICAL PROPERTIES

2.5 MATLAB CODE FOR REFLECTANCE SPECTRA OF SUBSTRATE

2.6 CHARACTERIZATION METHOD OF THE ELECTRICAL PROPERTIES AND THICKNESS OF EPILAYERS USING IR REFLECTANCE SPECTROSCOPY.

2.7 METHOD OF OBTAINING THE CARRIER CONCENTRATION, MOBILITY AND THICKNESS OF EPILAYER

2.8 MATLAB CODE FOR REFLECTANCE SPECTRA OF SUBSTRATE AND THE EPILAYER

2.9 CONCLUSION

3. CHAPTER 3 : DETERMINATION OF EIGENSTATE ENERGIES OF A PARTICLE IN A FINITE POTENTIAL WELL

3.1 INTRODUCTION

3.2 OBJECTIVE

3.3 NUMERICAL METHODS FOR SOLVING SCHRÖDINGER EQUATION

3.4 MATLAB IMPLEMENTATION

3.5 RESULT

3.6 VISUALISATION

3.7 CONCLUSION

4. REFERENCES-

- X-ray reflectivity and diffuse scattering
- X-ray Diffraction of Solids and Semiconductors.
- X-ray thin film measurement techniques.
- Nondestructive and Contactless Characterization Method for Spatial Mapping of the Thickness and Electrical Properties in Homo-Epitaxially Grown SiC Epilayers Using Infrared Reflectance Spectroscopy.
- Thickness Determination of Low Doped SiC Epi-Films on Highly Doped SiC Substrates.
- Methods for Thickness Determination of SiC Homoepilayers by Using Infrared Reflectance Spectroscopy.
- Infrared reflectance study of 3C-SiC epilayers grown on silicon substrates.
- Solving Schrödinger Equation for Finite Potential Well Using the Iterative Method.

Chapter 1 - X-RAY reflectivity

1.1 INTRODUCTION

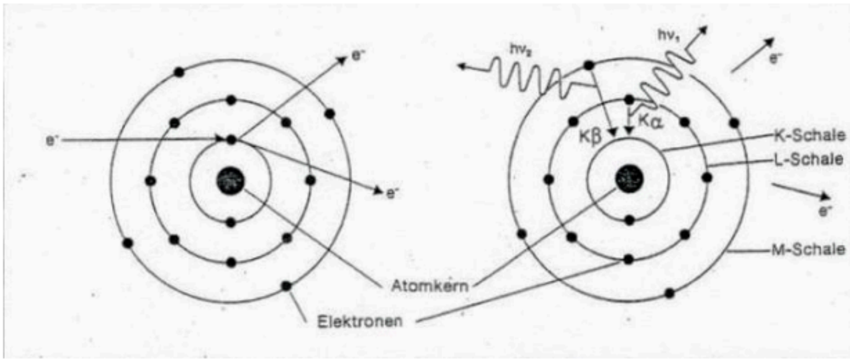
X-ray reflectivity (XRR), also known as X-ray specular reflectivity or X-ray reflectometry, is a common thin film characterization technique. With XRR, it is possible to determine the thickness, density, and roughness of films composed of different materials, such as semiconductive, magnetic, and optical materials.

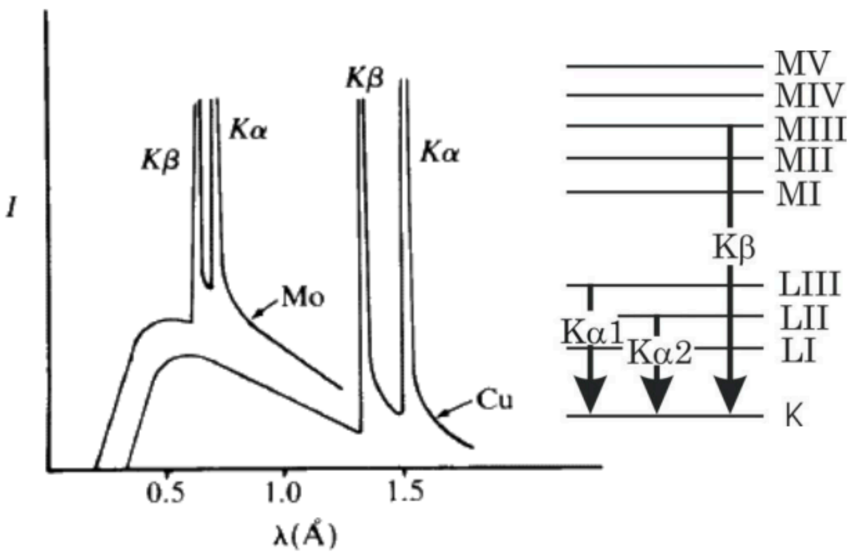
Both crystalline (single crystal or polycrystalline) and amorphous matter in very thin layers can be analyzed, and materials can have single or multiple layers or coatings. The properties of both the surface of the material and the interfaces of the layers can be determined using X-ray reflectivity.

1.2 X-ray reflectivity measurement

1. It can be used to study a single-crystalline, polycrystalline or amorphous material.
2. It can be used to evaluate surface roughness and interface width (arising from roughness and interdiffusion) nondestructively.
3. It can be used to evaluate surface roughness and interface width (arising from roughness and interdiffusion) nondestructively.
4. It can be used to evaluate surface roughness and interface width (arising from roughness and interdiffusion) nondestructively.
5. It can be used to measure film thickness from several to 1000 nm.

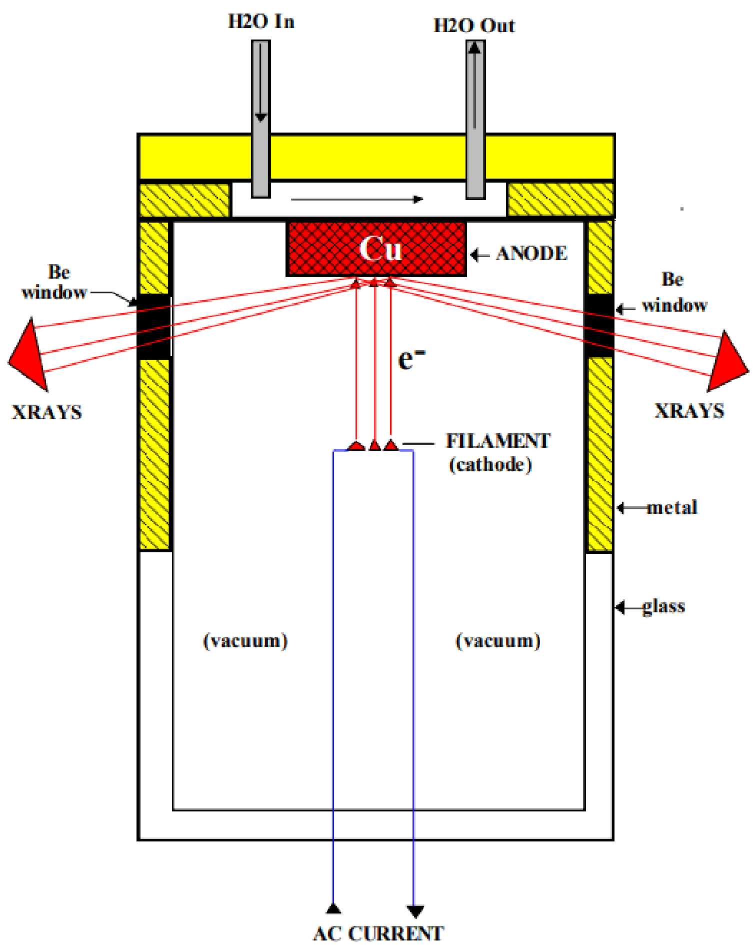
1.3 Basics of Characteristic X-ray radiation





- Electrons from the filament strike the target anode, producing characteristic radiation via the photoelectric effect.
- The electrons knock out electrons of an inner shell (K, L; M etc.), electrons of the outer shells drops down under submission of characteristic X-ray emission.
- Fine structure of the atome shell, orbitals split into sublevels Ka1, Ka2;..
- The anode material (Cu, Mo, Au, …) determines the wavelengths of characteristic radiation.
- While we would prefer a monochromatic source, the X-ray beam actually consists of several characteristic wavelengths of X rays.

1.4 Generation of X-rays-



- Sealed X-ray tubes tend to operate at 1.8 to 3 kW.
- Rotating anode X-ray tubes produce much more flux because they operate at 9 to 18 kW.
  - A rotating anode spins the anode at 6000 rpm, helping to distribute heat over a larger area and therefore allowing the tube to be run at higher power without melting the target.

- Both sources generate X rays by striking the anode target with an electron beam from a tungsten filament.
  - The target must be water cooled.
  - The target and filament must be contained in a vacuum.

1.5 Deriving electric field equation-

The equations governing the electromagnetic phenomena are known as the Maxwell's Equations. They are the divergence & curl relations of the Electric & Magnetic Field.

$$\nabla . E = \rho/\varepsilon_0 \quad - (1) \qquad \nabla \times E = -\partial B/\partial t \quad - (3)$$

$$\nabla . B = 0 \quad - (2) \qquad \nabla \times B = \mu_0 J + \mu_0 \varepsilon_0 \, \partial E/\partial t \quad - (4)$$

Here E & B are Electric & Magnetic Field respectively

ρ is the volume charge density.

J is the displacement current

ε_0 & μ_0 are permittivity & permeability in vacuum.

Since Electric Displacement (D) = $\varepsilon_0 E$

& Magnetic Field Strength (H) = B/μ_0

Therefore, Maxwell's Equation can also be written as →

$$\nabla . D = \rho \quad - (1) \qquad \nabla \times E = -\partial B/\partial t \quad - (3)$$

$$\nabla . B = 0 \quad - (2) \qquad \nabla \times H = J + \frac{\partial D}{\partial t} \quad - (4)$$

→ The first Law of Maxwell is the Gauss Law of Electrostatics.

→ The second Law of Maxwell is the Gauss Law of Magnetostatics.

→ The third Law of Maxwell is the Faraday's Law of Electromagnetic Induction.

→ The fourth Law of Maxwell is the modified form of Ampere's Circuital Law.

Since the Maxwell's Laws of govern the electromagnetic phenomenon, they can be used to define the propogation of Electromagnetic Waves.

Examples of EM waves are visible light, UV rays, X-Rays, Infrared waves etc.

If an EM wave is propogating in Free space or vacuum i.e in a region of space where there is no charge or current. The Maxwell's Equations can be written as →

$$\nabla \cdot E = 0 \quad - (1) \qquad \nabla \times E = -\partial B/\partial t \quad - (3)$$

$$\nabla \cdot B = 0 \quad - (2) \qquad \nabla \times B = \mu_0 \varepsilon_0 \frac{\partial E}{\partial t} \quad - (4)$$

Since $\rho = 0 = J$

$\mu = \mu_0$ & $\varepsilon = \varepsilon_0$

Now, taking curl of eqn. (3) →

$$\Rightarrow \vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \vec{\nabla} \times \left(-\frac{\partial B}{\partial t} \right)$$

$$\because \vec{a} \times (\vec{b} \times \vec{c}) = \vec{b}\,(\vec{a}.\vec{c}) - \vec{c}\,(\vec{a}.\vec{b})$$

$$\Rightarrow \vec{\nabla}(\vec{\nabla}.\vec{E}) - \vec{\nabla}^2 \vec{E} = -\frac{\partial}{\partial t}(\vec{\nabla} \times \vec{B})$$

$\because$ $\vec{\nabla}.\vec{E} = 0$ (from eqn (1))

$\vec{\nabla} \times \vec{B} = \mu_0 \varepsilon_0 \dfrac{\partial E}{\partial t}$ (from eqn (4))

$$\Rightarrow 0 - \vec{\nabla}^2.\vec{E} = -\frac{\partial}{\partial t}\left(\mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \right)$$

$$\Rightarrow \vec{\nabla}^2.\vec{E} - \mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} = 0 \quad \text{— (5)}$$

Similiarly, if we take curl of eqn. (4) →

$$\Rightarrow \vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = \vec{\nabla} \times \left(\mu_0 \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \right)$$

we obtain a similiar result →

$$\Rightarrow \vec{\nabla}^2.\vec{B} - \mu_0 \varepsilon_0 \frac{\partial \vec{B}}{\partial t} = 0 \quad \text{— (6)}$$

The equations (5) & (6) are similiar to the wave equation →

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$$

On comparing eqns. (5) & (6) with the wave equation, we get →

$\Rightarrow \quad v^2 = \dfrac{1}{\mu_0 \varepsilon_0} \quad \Rightarrow \quad v = \dfrac{1}{\sqrt{\mu_0 \varepsilon_0}} = 3 \times 10^8$ m/s

Therefore, we can say that the EM waves travel with the speed of light.

Also eqns. (5) & (6) can be written as →

$$\nabla^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad \text{— (5.1)}$$

$$\nabla^2 \vec{B} - \frac{1}{c^2}\frac{\partial^2 \vec{B}}{\partial t^2} = 0 \quad \text{— (6.1)}$$

According to the Fourier Transform, any solution of the wave equation can be expressed as a sum over sinusoidal functions.

Therefore considering sinusoidal functions →

For a wave of single frequency (ω), travelling in the $+j$ direction, independent of x & z dirn., the solutions are →

$$E = E_0 \, e^{i(\omega t - kj)}$$

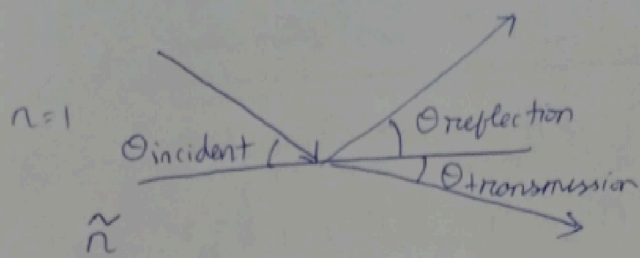
$$B = B_0 \, e^{i(\omega t - kj)}$$

1.6 Refractive Index -

The refractive index for X-rays is less than unity. Mathematically it is given as -

specular reflection

$\theta_{incident} = \theta_{reflection}$



$$\tilde{n} = 1 - \delta - i\beta$$

$$\delta = \frac{\lambda^2}{2\pi} r_e \rho_e \qquad \beta = \frac{\lambda}{4\pi}\mu$$

ρ_e ↓ electron density

$$\rho_e = Z \cdot n = Z \cdot \frac{N_A \rho}{A}$$

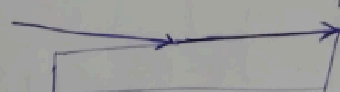
Z = no. of electrons per atom

1.7 Concept of Critical angle-

1. $\cos\theta_{incident} = (1-\delta)\cos\theta_{transmission}$ ★ neglecting absorbtion cofficient

$\theta_{transmission} = 0$

$\cos(\;''\;) = 1$

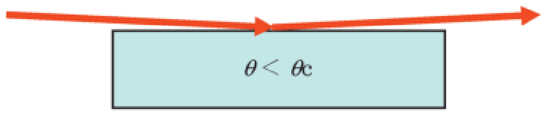


$$\cos\theta_{incident} = 1-\delta$$

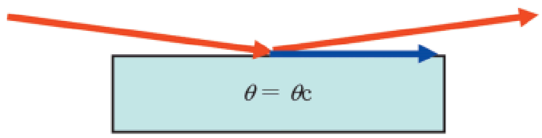
$$\cos(\theta_c) = 1-\delta$$

$$\cancel{1} - \frac{\theta_c^2}{2} = \cancel{1} - \delta$$

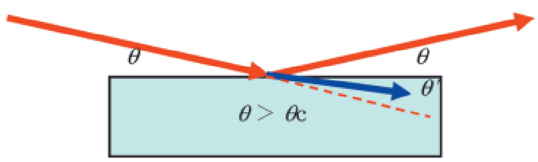
$$\boxed{\theta_c = \sqrt{2\delta}}$$



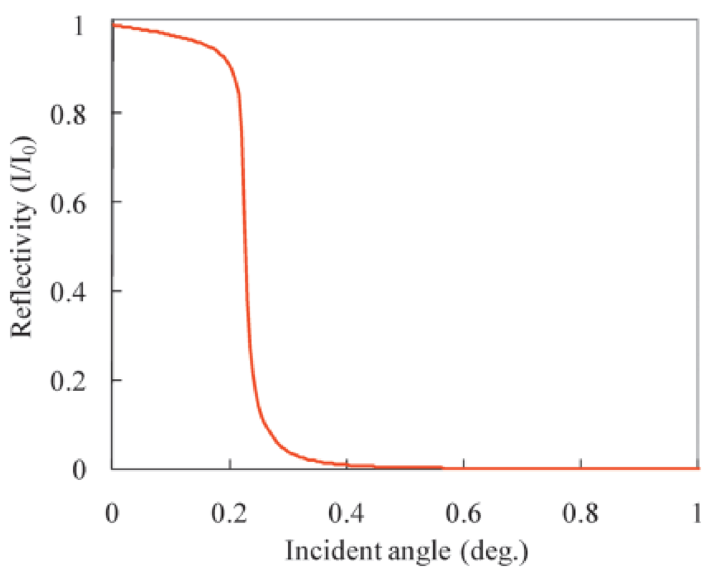
A) Incident angle < Total reflection critical angle
All incident X-rays are reflected.



B) Incident angle = Total reflection critical angle
Incident X-rays propagate along the sample surface.

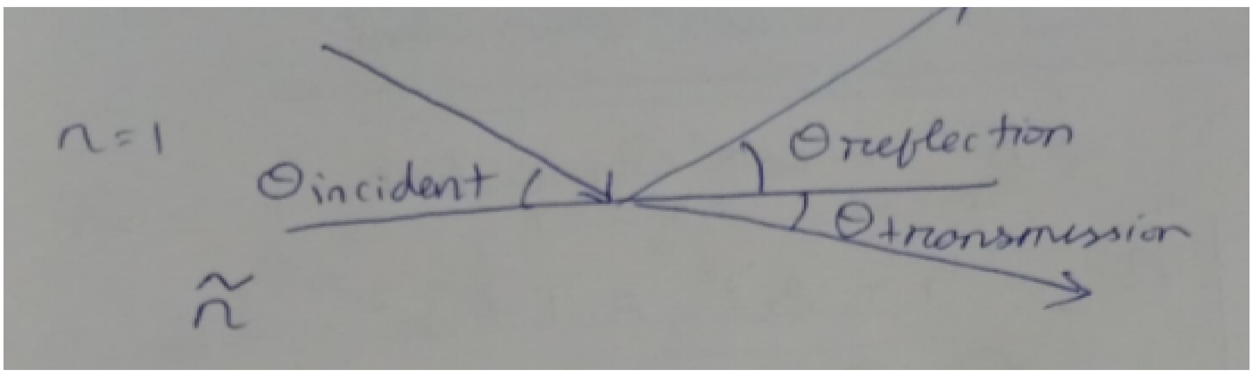


C) Incident angle > Total reflection critical angle
Incident X-rays penetrate into the material by refraction



The above figure shows a calculated X-ray reflectivity curve for bulk Si when an X-ray beam is θimpinged at a grazing angle on to an ideal flat surface of a material, total reflection occurs at below the incident angle θc, and the incident X-rays do not penetrate into the material. X-ray reflectivity decreases rapidly with increasing incident angle, θ above θc. The ratio of specularly reflected X-rays decreases proportionally to θ4.

1.8 Fresnel refraction coefficient and reflectivity-



Fresnal Refraction coefficient (γ)

$$\gamma = \frac{n_{air} \sin\theta\ incident - \tilde{n} \sin\theta_{transmission}}{n_{air} \sin\theta\ incident + \tilde{n} \sin\theta_{transmission}} \quad -(1)$$

$$\sin\theta_{transmission} = \sqrt{1-\cos^2\theta_{transmission}} \quad -(2)$$

$$\Rightarrow n_{air} \sin(90-\theta_{incident}) = \tilde{n} \sin(90-\theta_{transmission})$$

$\hookrightarrow$ From Snell's Law

$$\Rightarrow n_{air} \cos\theta_{incident} = \tilde{n} \cos\theta_{transmission} \quad -(3)$$

Substituting eqn (2) & (3) in eqn (1) $\rightarrow$

$$\Rightarrow \gamma(\theta) = \frac{\sin\theta_{incident} - \sqrt{\tilde{n}^2 - \cos^2\theta_{incident}}}{\sin\theta_{incident} + \sqrt{\tilde{n}^2 - \cos^2\theta_{incident}}}$$

$$\because \tilde{n}^2 = (1-\delta)^2 = 1 + \delta^2 - 2\delta$$

$$= 1 - 2\delta$$

$$= 1 - \theta_c^2$$

$$\because \cos^2\theta_{incident} = \left(1 - \frac{\theta^2_{incident}}{2}\right)^2 = 1 + \cancel{\frac{\theta_{incident}}{4}}^{\,0} - \theta^2_{incident}$$

$$\Rightarrow \gamma(\theta) = \frac{\theta_{incident} - \sqrt{1-\theta_c^2 - 1 + \theta^2_{incident}}}{\theta_{incident} + \sqrt{1-\theta_c^2 - 1 + \theta^2_{incident}}}$$

$$\Rightarrow \gamma(\theta) = \frac{\theta_{inc} - \sqrt{\theta^2_{inc} - \theta_c^2}}{\theta_{inc} + \sqrt{\theta^2_{inc} - \theta_c^2}}$$

$$\because R = \gamma\gamma^* = \left| \frac{\theta - \sqrt{\theta^2 - \theta_c^2}}{\theta + \sqrt{\theta^2 - \theta_c^2}} \right|^2$$

$$\therefore \text{Reflection intensity } (R) = \left| \frac{\theta - \sqrt{\theta^2 - \theta_c^2 - 2i\beta}}{\theta + \sqrt{\theta^2 - \theta_c^2 - 2i\beta}} \right|^2$$

The above relation is obtained when we consider the absorption.

$$\because q = \frac{4\pi}{\lambda} \sin\theta = \frac{4\pi}{\lambda} \theta$$

$$R = \left| \frac{q - \sqrt{q^2 - q_c^2 - \frac{32 i \pi^2 \beta}{\lambda^2}}}{q + \sqrt{q^2 - q_c^2 - \frac{32 i \pi^2 \beta}{\lambda^2}}} \right|^2$$

For $[\theta_{incident} > \theta_{critical}]$ X-Rays can penetrate the material.

$$d \approx \frac{\lambda}{2\Delta\theta} \qquad [\because \lambda = 2d\theta]$$

$$d = \frac{\lambda}{2(\theta_{m+1} - \theta_m)}$$

[θ_{m+1} & θ_m are the angles at which the adjacent maximum or minimum interferences are located]

$$\gamma_{rough} = \gamma_{flat} \cdot e^{-q^2\sigma^2/2}$$

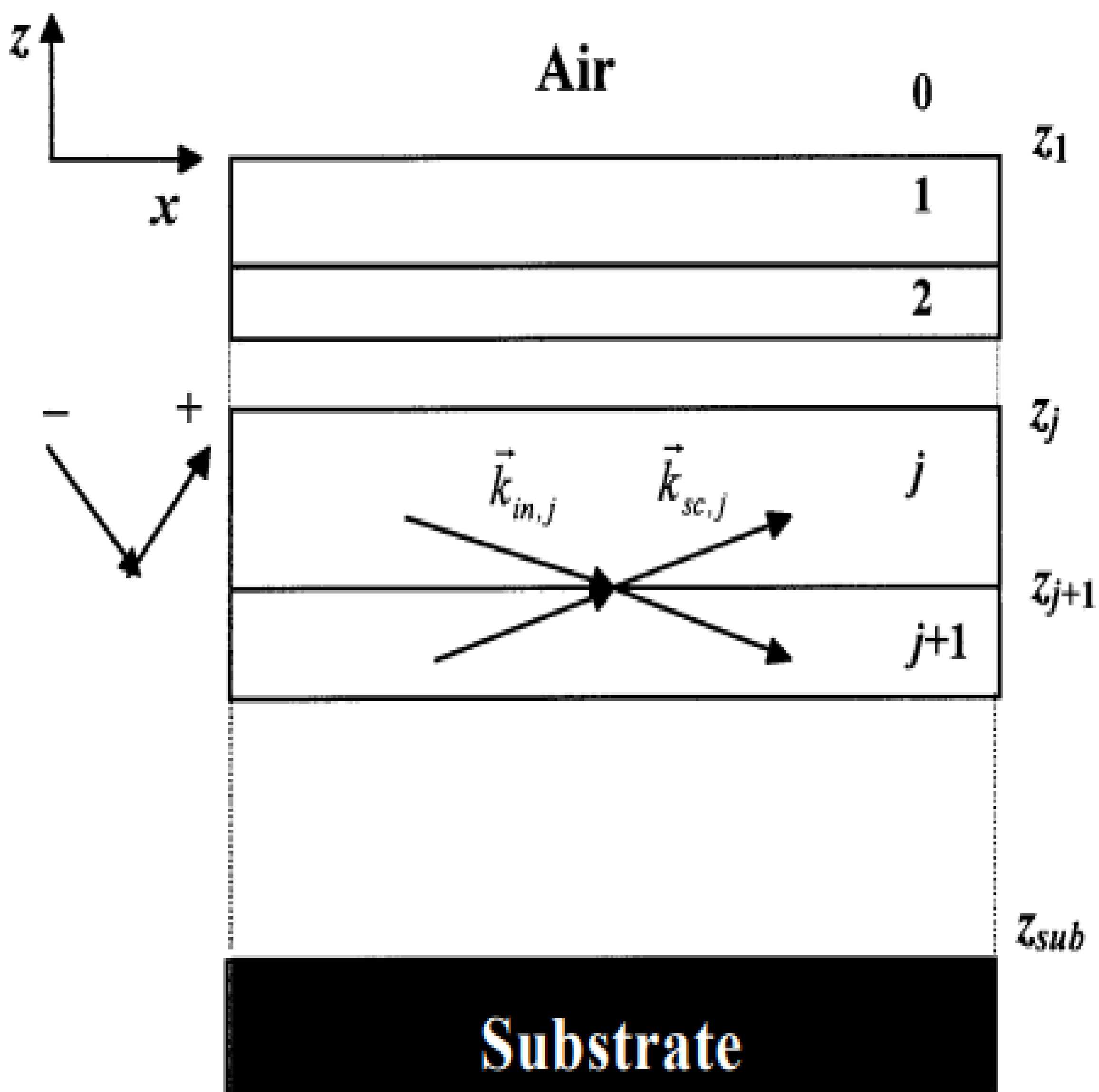
$$\left[\begin{array}{l} \sigma = \text{roughness} \\ q = \frac{4\pi}{\lambda} \sin\theta \end{array} \right]$$

The above reflectivity formula works fine for a particular layer and one may have to apply the same formulation again and again to solve a given system of layers on a substrate. This gives rise to an essential need of having a better approach to solve such problems.

An interesting solution to this is , by using matrix approach or transfer matrix method. The method is common to many optics problem and provides computational easiness and feasibility over traditional approaches.

Upnext is, utilisation of transfer matrix method.

1.9 The Transfer Matrix approach-



For a plane wave polarized in the direction perpendicular to the plane of incidence (s) and propogating in the medium (m), the solution of Helmholtz equation for the electric field is →

$$E^{+} = A^{+} e^{i(\omega t - K_x x + K_z z)} \quad \text{(wave travelling +z dirn)}$$

$$E^{-} = A^{-} e^{i(\omega t - K_x x - K_z z)} \quad \text{(wave travelling -z dirn.)}$$

where $K_x = K \cos\Theta$ (x component of wave vector)

$K_z = \pm K \sin\Theta = \pm\sqrt{K^2 - K_x^2}$ (z component of wave vector)

The superposition of E^{+} & E^{-} at the interface of the medium at depth z gives the electric field

$$E(x,z) = E^{+} + E^{-}$$

$$E(x,z) = A^{+} e^{i(\omega t - K_x x + K_z z)} + A^{-} e^{i(\omega t - K_x x - K_z z)}$$

$$E(x,z) = \left(A^{+} e^{iK_z z} + A^{-} e^{-iK_z z}\right) e^{i(\omega t - K_x x)} \quad — (7)$$

For simplification, let us assume →

$$U^{+}(K_{zj}, z) = A^{+} e^{iK_z z}$$

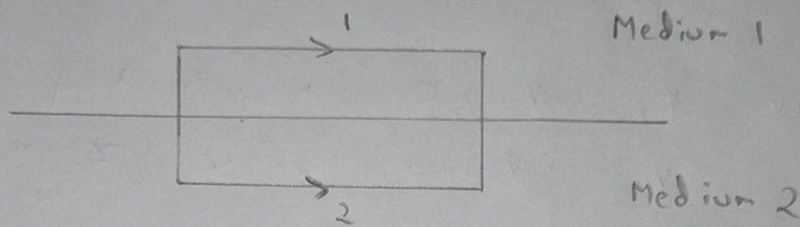
$$U^{-}(K_{zj}, z) = A^{-} e^{-iK_z z}$$

Thus eqn. (7) can be written as →

$$E(x,z) = \left(U^{+}(K_j, z) + U^{-}(K_j, z)\right) e^{i(\omega t - K_x x)} \quad — (7.1)$$

Now, if we look at the boundary of 2 mediums, for an infinitesemal small part of junction, we can assume the electric / magnetic field to be uniform.

So we consider a loop at this boundary to get the tangential boundary conditions.



According to the 3rd Equation of Maxwell →

$$\oint \vec{E} . dl = -\frac{\partial}{\partial t} \int_s \vec{B} . \vec{ds}$$

But, to get the field at the boundary, we consider the loop to be a line, i.e it has 0 area.

$$\therefore \oint \vec{E} . dl = 0 \qquad (\because B . \vec{ds} = 0)$$

$$\Rightarrow \quad E_1 . l = E_2 . l$$

$$\Rightarrow \quad E_1 = E_2 \quad — \quad (8)$$

Thus we can say, that the tangential electric field in medium 1 is equal to the tangential electric field in medium 2.

Also, eqn (8) remains true irrespective of the materials properties.

Using this eqn. (8) of continuity in x direction, we can write →

$$(U^+(K_j) + U^-(-K_j))\, e^{i(\omega t - K_x x)} = (U^+(K_{j+1}) + U^-(K_{j+1}))\, e^{i(\omega t - K_x x)}$$

↑ For jth medium ↑ For j+1th medium

The above is the equation of continuity at the boundary of 2 mediums.
It can be further simplified as →

$$U^+(K_j) + U^-(-K_j) = U^+(K_{j+1}) + U^-(-K_{j+1}) \quad \text{— (9)}$$

For eqn. (9) to be continous, its first derivative should also be conserved.

Thus taking 1st derivative of Eqn. (9) →

$$\Rightarrow K_j[U^+(K_j) - U^-(-K_j)] = K_{j+1}[U^+(K_{j+1}) - U^+(-K_{j+1})] \quad \text{— (10)}$$

Multiplying eqn. (9) with K_j and adding it to eqn. (10) →

$$\Rightarrow 2K_j U^+(K_j) = K_j + K_{j+1}(U^+(K_{j+1})) + K_j - K_{j+1}(U^-(K_{j+1})) \quad \text{— (11)}$$

Multiplying eqn. (9) with K_{j+1} and substracting it from eqn. (10) →

$$\Rightarrow 2K_j U^-(K_j) = K_j - K_{j+1}(U^+(K_{j+1})) + K_j + K_{j+1}(U^-(K_{j+1})) \quad \text{— (12)}$$

Rewriting eqn. (11) & (12) →

$$U^+(K_j) = \frac{K_j + K_{j+1}}{2K_j}(U^+(K_{j+1})) + \frac{K_j - K_{j+1}}{2K_j}(U^-(K_{j+1})) \quad \text{— (11.1)}$$

$$U^-(K_j) = \frac{K_j - K_{j+1}}{2K_j}(U^+(K_{j+1})) + \frac{K_j + K_{j+1}}{2K_j}(U^-(K_{j+1})) \quad \text{— (12.1)}$$

Writing the above eqns. in the matrix form →

$$\begin{bmatrix} U^+(K_j) \\ U^-(K_j) \end{bmatrix} = \begin{bmatrix} K_j + K_{j+1}/2K_j & K_j - K_{j+1}/2K_j \\ K_j - K_{j+1}/2K_j & K_j + K_{j+1}/2K_j \end{bmatrix} \begin{bmatrix} U^+(K_{j+1}) \\ U^-(K_{j+1}) \end{bmatrix} \quad (13)$$

Let $\dfrac{K_j + K_{j+1}}{2K_j} = p$ & $\dfrac{K_j - K_{j+1}}{2K_j} = m$

Substituting p & m in eqn (13) →

$$\begin{bmatrix} U^+(K_j) \\ U^-(K_j) \end{bmatrix} = \begin{bmatrix} p & m \\ m & p \end{bmatrix} \begin{bmatrix} U^+(K_{j+1}) \\ U^-(K_{j+1}) \end{bmatrix} \quad -(14)$$

Since this matrix equation gives us the relation between the electric field from one medium (j^{th}) to another medium ($j+1^{th}$), the matrix $\begin{bmatrix} p & m \\ m & p \end{bmatrix}$ is called the refraction matrix.

However, if the EM wave is travelling in a single medium, then for 'h' distance travelled, the electric field can be written as →

$$U^+(K_j, z+h) = U^+(K_j)\, e^{iK_{z,j}h} \quad -(15)$$

$$U^-(K_j, z+h) = U^-(K_j)\, e^{-iK_{z,j}h} \quad -(16)$$

Eqn. (15) & (16) can be re-written as →

$$U^+(K_j) = U^+(K_j, z+h)\, e^{-iK_{z,j}h} \quad -(15.1)$$

$$U^-(K_j) = U^-(K_j, z+h)\, e^{iK_{z,j}h} \quad -(16.1)$$

Writing the above equations in the matrix form :-

$$\begin{bmatrix} U^+(K_j) \\ U^-(K_j) \end{bmatrix} = \begin{bmatrix} e^{-ik_{z,j}h} & 0 \\ 0 & e^{ik_{z,j}h} \end{bmatrix} \begin{bmatrix} U^+(K_j, z+h) \\ U^-(K_j, z+h) \end{bmatrix} \quad \text{— (17)}$$

Since this matrix equation gives us the relation of electric field passing in one medium only, thus $\begin{bmatrix} e^{-ik_{z,j}h} & 0 \\ 0 & e^{ik_{z,j}h} \end{bmatrix}$ is called translation matrix.

Therefore for a multilayer specimen, we take a combination of the translation & refraction matrix, starting from the first interface until we reach the substrate.

$$\begin{bmatrix} U^+(K_0) \\ U^-(K_0) \end{bmatrix} = R_{01} T_1 R_{12} T_2 \dots \begin{bmatrix} U^+(K_s) \\ U^-(K_s) \end{bmatrix} \quad \text{— (18)}$$

where $R_{01} T_1 R_{12} T_2 \dots = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$

This matrix is known as the transfer matrix.

Substituting the transfer matrix in eqn (18), we get :-

$$\begin{bmatrix} U^+(K_0) \\ U^-(K_0) \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} U^+(K_s) \\ U^-(K_s) \end{bmatrix} \quad \text{— (19)}$$

Since reflectivity (r) is defined as $\rightarrow \dfrac{\text{reflected elec. field}}{\text{incident elec. field}}$

$$r = \frac{U^+(K_0)}{U^-(K_0)}$$

Using the eqn (19) we can write $\Rightarrow$

$$\begin{bmatrix} U^+(K_0) \\ U^-(K_0) \end{bmatrix} = \begin{bmatrix} M_{11}\, U^+(K_s) + M_{12}\, U^-(K_s) \\ M_{21}\, U^+(K_s) + M_{22}\, U^-(K_s) \end{bmatrix}$$

$$\therefore \quad r = \frac{M_{11}\, U^+(K_s) + M_{12}\, U^-(K_s)}{M_{21}\, U^+(K_s) + M_{22}\, U^-(K_s)}$$

But since X-Rays can penetrate only over a few microns, we can assume that no reflection occurs at the substrate;

$$\therefore \quad U^+(K_s) = 0$$

$$\Rightarrow \quad r = \frac{M_{12}\, U^-(K_s)}{M_{22}\, U^-(K_s)}$$

$$\Rightarrow \quad r = \frac{M_{12}}{M_{22}} \quad \text{—— (20)}$$

This calculation of reflectivity using the elements of a matrix is known as the matrix technique.

It is suitable for specimens with multiple layers and is valid for any EM wave.

1.10 Verifying Matrix method approach for a single layer-

★ Finding Reflectivity for a single flat surface →

Transfer matrix $= R_{01} = \begin{bmatrix} p & m \\ m & p \end{bmatrix}$

$$\therefore \quad r = \frac{M_{12}}{M_{22}} = \frac{m}{p} = \frac{K_0 - K_s / 2K_0}{K_0 + K_s / 2K_0}$$

$$r = \frac{K_0 - K_s}{K_0 + K_s}$$ ← same reflectivity as calculated by using Fresnels relationship.

★ Finding Reflectivity for a specimen, with single layer on substrate →

$$\text{Transfer matrix} = R_{01}\, T_1\, R_{0s} = \begin{bmatrix} p_1 & m_1 \\ m_1 & p_1 \end{bmatrix} \begin{bmatrix} e^{-ik_{z,j}h} & 0 \\ 0 & e^{ik_{z,j}h} \end{bmatrix} \begin{bmatrix} p_2 & m_2 \\ m_2 & p_2 \end{bmatrix}$$

$$T = \begin{bmatrix} p_1 e^{-ik_{z,j}h} & m_1 e^{ik_{z,j}h} \\ m_1 e^{-ik_{z,j}h} & p_1 e^{ik_{z,j}h} \end{bmatrix} \begin{bmatrix} p_2 & m_2 \\ m_2 & p_2 \end{bmatrix}$$

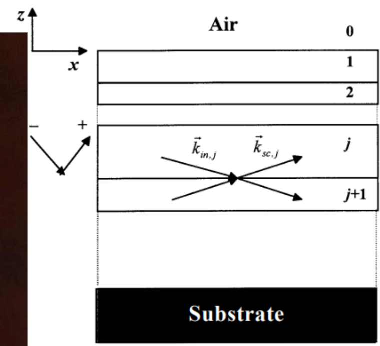
$$= \begin{bmatrix} p_1 p_2 e^{-ik_{z,j}h} + m_1 m_2 e^{ik_{z,j}h} & p_1 m_2 e^{-ik_{z,j}h} + m_1 p_2 e^{ik_{z,j}h} \\ m_1 p_2 e^{-ik_{z,j}h} + p_1 m_2 e^{ik_{z,j}h} & m_1 m_2 e^{-ik_{z,j}h} + p_1 p_2 e^{ik_{z,j}h} \end{bmatrix}$$

$$\therefore \quad r = \frac{M_{12}}{M_{22}} = \frac{p_1 m_2 e^{-ik_{z,j}h} + m_1 p_2 e^{ik_{z,j}h}}{m_1 m_2 e^{-ik_{z,j}h} + p_1 p_2 e^{ik_{z,j}h}} \quad \text{— (1)}$$

Let $\dfrac{m_1}{p_1} = r_1$ & $\dfrac{m_2}{p_2} = r_2$ and substituting them in eqn (1) → after dividing by $p_1 p_2 e^{ik_z h}$ →

$$r = \frac{r_2 e^{-2ik_{z,j}h} + r_1}{r_1 r_2 e^{-2ik_{z,j}h} + 1}$$

1.11 Utilising the advantage of transfer matrix method for computational needs -

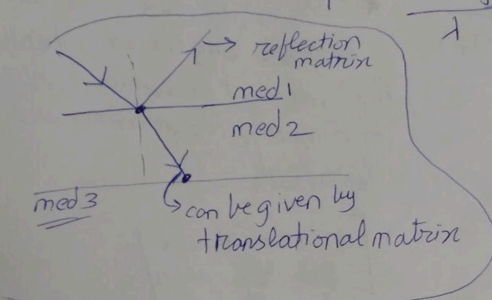


consider layer j

$$n_j = 1 - \delta_j - i\beta_j$$

$$k_{z,j} = k_j \sin\theta = k\sqrt{\theta^2 - 2\delta_j - 2i\beta_j}$$

$$k = \frac{2\pi n_j}{\lambda}$$



$$R = \begin{bmatrix} p_{j,j+1} & m_{j,j+1} \\ m_{j,j+1} & p_{j,j+1} \end{bmatrix}$$

$$p_{j,j+1} = \frac{k_{z,j} + k_{z,j+1}}{2k_{z,j}}$$

$$m_{j,j+1} = \frac{k_{z,j} - k_{z,j+1}}{2k_{z,j}}$$

$$T = \begin{bmatrix} e^{-ik_{z,\cancel{j}} * h} & 0 \\ 0 & e^{-ik_{z,j} * h} \end{bmatrix}$$

$k_{z,j}$ j medium in which ray is travelling.

h = thickness of medium or layer

$$M = R_{01} \times T_1 \times R_{1,2} \ldots R_{sub-1,\, sub}$$

↳ transfer matrix $= \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}$

$$r = \frac{M_{12}}{M_{22}}$$

fresnal refraction coeffecient

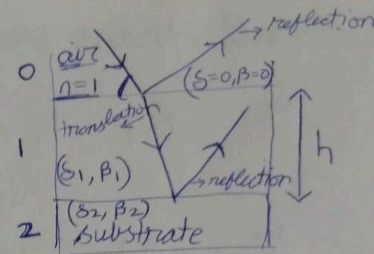
Reflectivity $= |r|^2$

absolute

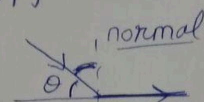
example $\boxed{\text{1 layer system}}$

→ consider a given 'θ' ←

$K_{z,j} = K\sqrt{\theta^2 - 2\delta_j - 2i\beta_j}$



$K_{z,0} = K \cancel{\cos\theta} \sin\theta$



$\left(K = \frac{2\pi}{\lambda}\right)$ $(\theta < \theta_c)$

$K_{z,1} = \underset{\downarrow \frac{2\pi n_1}{\lambda}}{K}\sqrt{\theta^2 - 2\delta_1 - 2i\beta_1}$

$\delta_1 = \frac{r_e}{2\pi}\lambda^2 \underset{\downarrow}{\rho_1}$ electron density of med 1

$K_{z,2} = \underset{\downarrow \frac{2\pi n_2}{\lambda}}{K}\sqrt{\theta^2 - 2\delta_2 - 2i\beta_2}$

$\beta_1 = \frac{\lambda}{4\pi}\mu$ → linear mass absorption coefficient.

$$\begin{bmatrix} n_1 = 1 - \delta_1 - i\beta_1 \\ n_2 = 1 - \delta_2 - i\beta_2 \end{bmatrix}$$

$R_{0,1}$ = reflection of light from air to layer 1

$$R_{0,1} = \begin{bmatrix} \frac{K_{z,0} + K_{z,1}}{2K_{z,0}} & \frac{K_{z,0} - K_{z,1}}{2K_{z,0}} \\ \frac{K_{z,0} - K_{z,1}}{2K_{z,0}} & \frac{K_{z,0} + K_{z,1}}{2K_{z,0}} \end{bmatrix}$$

T_1 = translation of ray ~~from~~ within layer 1

$$= \begin{bmatrix} e^{-iK_{z,1}h} & 0 \\ 0 & e^{-iK_{z,1}h} \end{bmatrix}$$

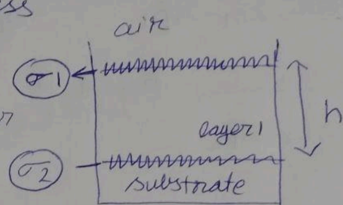
$$R_{1,2} = \begin{bmatrix} \frac{K_{z,1} + K_{z,2}}{2K_{z,1}} & \frac{K_{z,1} - K_{z,2}}{2K_{z,1}} \\ \frac{K_{z,1} - K_{z,2}}{2K_{z,1}} & \frac{K_{z,1} + K_{z,2}}{2K_{z,1}} \end{bmatrix}$$

overall transfer matrix

$$M = R_{01} \cdot T_1 \cdot R_{12} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

$$r = \frac{M_{12}}{M_{22}} \quad , \quad \text{reflectivity} = |r|^2$$

considering roughness in same case



σ_1 = roughness b/w air & layer 1

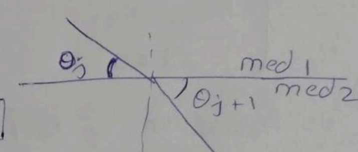
σ_2 = roughness b/w layer 1 and substrate

$$q = \frac{4\pi}{\lambda} \sin\theta = \frac{4\pi}{\lambda}\theta \quad (\theta \text{ is small})$$

$$q_{z,j} = \frac{4\pi\theta_j}{\lambda} \qquad \theta_j - \text{angle of incidence.}$$

$$n_j \cos\theta_j = n_{j+1} \cos\theta_{j+1}$$

$$\boxed{n_j \cos\theta_j = n_{j+1} \cos\theta_{j+1}}$$



$$\text{roughness term} = e^{-q_{z,j} * q_{z,j+1} * \sigma_{j+1}^2 / 2}$$

this term is multiplied with $m_{j,j+1}$ of R = reflection matrix.

$$R = \begin{bmatrix} p_{j,j+1} & m_{j,j+1} * R_T \\ m_{j,j+1} * R_T & p_{j,j+1} \end{bmatrix}$$

consider $R_{0,1}$

~~$R_{01} = k_{z0}$~~

~~$R_{201} = k_{z,0} \pm k$~~

$$R_{0,1} = \begin{bmatrix} \dfrac{k_{z,0} + k_{z,1}}{2k_{z,0}} & \dfrac{k_{z,0} + k_{z,1}}{2k_{z,0}} * e^{-\frac{q_{z,0} * q_{z,1} \sigma_1^2}{2}} \\ \dfrac{k_{z,0} - k_{z,1}}{2k_{z,0}} * e^{-\frac{q_{z,0} * q_{z,1} \sigma_1^2}{2}} & \dfrac{k_{z,0} + k_{z,1}}{2k_{z,0}} \end{bmatrix}$$

no change in translational matrix.

$$T_1 = \begin{bmatrix} e^{-ik_{z,1}h} & 0 \\ 0 & e^{-ik_{z,1}h} \end{bmatrix}$$

$$R_{1,2} = \begin{bmatrix} \dfrac{k_{z,1} + k_{z,2}}{2k_{z,1}} & \dfrac{k_{z,1} - k_{z,2}}{2k_{z,1}} * e^{-\frac{q_{z,1} * q_{z,2} \sigma_2^2}{2}} \\ \dfrac{k_{z,1} - k_{z,2}}{2k_{z,2}} * e^{-\frac{q_{z,1} * q_{z,2} \sigma_2^2}{2}} & \dfrac{k_{z,1} + k_{z,2}}{2k_{z,1}} \end{bmatrix}$$

overall, transfer matrix.

$$M = R_{0,1} * T_1 * R_{1,2} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$$

$$r = \frac{M_{12}}{M_{22}}$$

reflectivity $R = |r|^2$

$$n_1 \cos\theta_1 = n_2 \cos\theta_2$$

$$\cos^{-1}\left(\frac{n_1}{n_2}\cos\theta_1\right) = \theta_2$$

$$q_1 = \cancel{\frac{4\pi}{\lambda}\theta_1} \quad \frac{4\pi}{\lambda}\sin\theta = \frac{4\pi}{\lambda}\theta_1$$

$$q_1 = \frac{4\pi}{\lambda}\theta_1$$

$$q_2 = \frac{4\pi}{\lambda}\theta_2 = \frac{4\pi}{\lambda}\cos^{-1}\left(\frac{n_1}{n_2}\cos\theta_1\right)$$

$$q_2 = \frac{4\pi}{\lambda}\cos^{-1}\left(\frac{n_1}{n_2}\cos\theta_1\right)$$

and we always know θ_1 i.e angle of incidence.
θ_1 is an input by us/code.

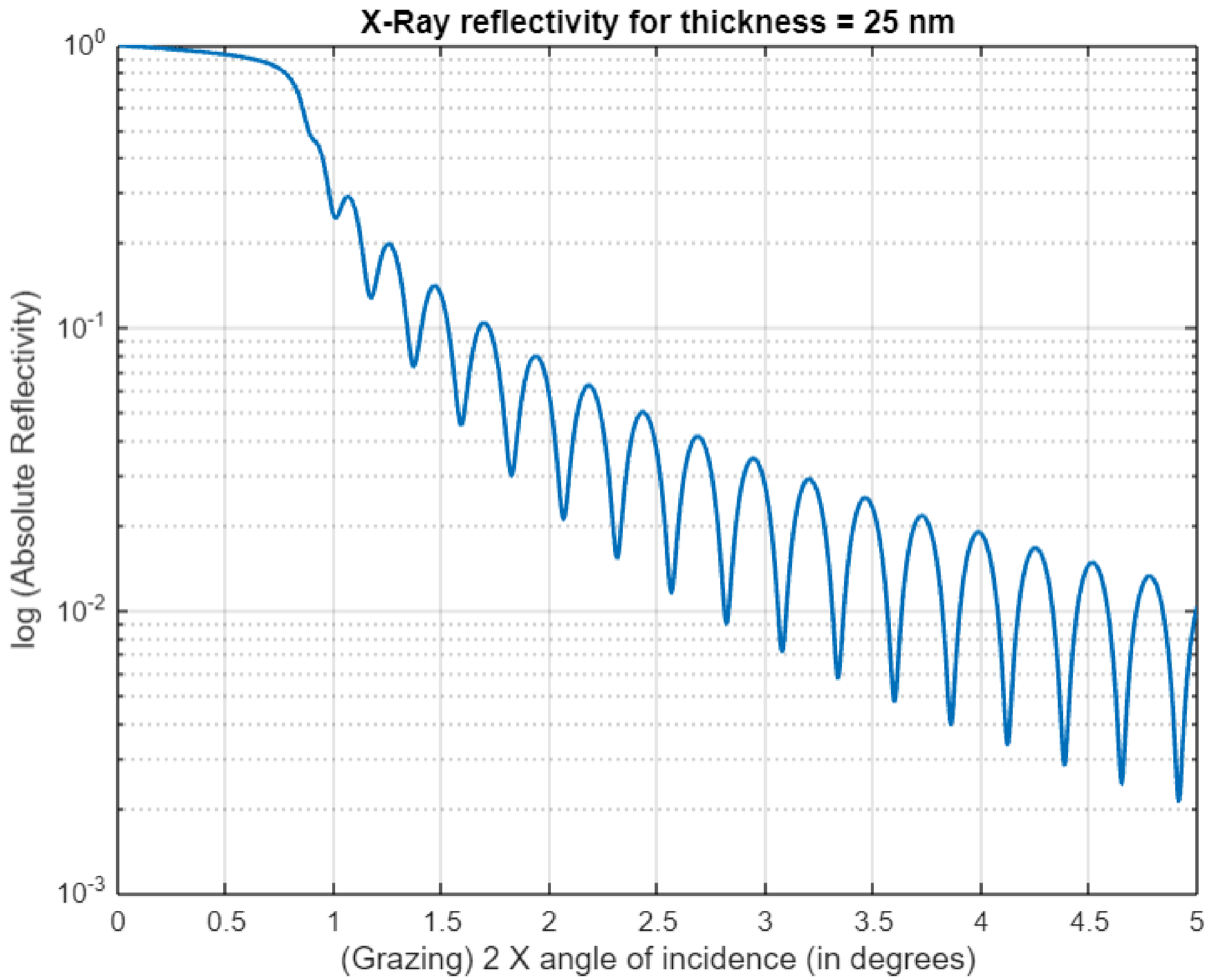
1.12 MATLAB IMPLEMENTATION OF PRESENTED FORMULAS -

For a 2-Layer system -

```
function R1_1layer

   %----Initialising values------%
   lambda = 1.54e-10;                % wavelength of X-ray in cm (1.54 Angstroms)
   theeta = linspace(0,pi/36,500);   % incident angles in radians
   a=(2*theta-pi)*180/pi;
   h_1=25e-9;                        %thickness of layer.
   s1= 20e-10;                       %surface roughness of uppermost layer.
   s2= 15e-10;                       %surface roughness between 2 layers.


   %----Calculating refractive index------%
   beta_1 = 0.000004839430707;
   delta_1= 0.000046517164;
   beta_2 = 0.00000017678661;
   delta_2= 0.000007667635;
   n0=1;                             %refractive index of air
   n1 = 1 - delta_1 - 1i*beta_1;     %refractive index of first layer
   n2 = 1 - delta_2 - 1i*beta_2;     %refractive index of second layer


   %-----applying Snell's law---------%
   theta1=asin((n0 /n1)*sin(theta*180/pi));
   theta2=asin((n0 /n2)*sin(theta*180/pi));


   %------Finding Wave vectors----------%
   k = (2 * pi) / lambda;            % wave number
   kz_0 = k*sin(theta*180/pi);       % Wave vector in layer 0.
   kz_1 = k*n1 * sqrt(sin(theta1).^2  - 2 * delta_1 - 2 * 1i * beta_1) ;
% Wave vector in layer 1.
   kz_2 = k*n2 * sqrt(sin(theta2).^2 - 2 * delta_2 - 2 * 1i * beta_2) ;
% Wave vector in layer 0.

   %-------Defining Fresnals Coefficients------%
   P0_1 = (kz_0 + kz_1) ./ (2 * kz_0);
   P1_2 = (kz_1 + kz_2) ./ (2 * kz_1);
   m0_1 = (kz_0 - kz_1) ./ (2 * kz_0);
   m1_2 = (kz_1 - kz_2) ./ (2 * kz_1);


   %-----Building Transfer Matrix------%
   Ref = zeros(size(theta));         %initialising a matrix of size theeta
```

```
   p = zeros(size(theta));          %initialising a matrix of size theeta

   % Loop over all incident angles
   for i = 1:length(theta)
        q = (4 * pi * sin( theta(i))) / lambda;
        Rough01 = exp(-(q)^2 * s1^2); %calculating roughness.
        Rough12 = exp(-(q)^2 * s2^2);

       % Construct transfer matrices
       R0_1 = [P0_1(i), m0_1(i)*Rough01; m0_1(i)*Rough01, P0_1(i)];

       T_1 = [exp(-1i * kz_1(i) * h_1), 0; 0, exp(1i * kz_1(i) * h_1)];

       R1_2 = [P1_2(i), m1_2(i)*Rough12; m1_2(i)*Rough12, P1_2(i)];

       % R0_1 - Reflectivity matrix due to reflection between layer 0 and
       % layer 1.
       % R1_2 - Reflectivity matrix due to reflection between layer 0 and
       % layer 1.
       % T_1 - Translational matrix due to translation of ray in layer 1.

       % Calculate total transfer matrix
       M = R0_1 * T_1 * R1_2;
       % Calculate reflection coefficient
       r = M(1,2) / M(2, 2);       % r- reflectivity coefficient.

       % Calculate reflectivity
       Ref(i) = abs(r);            % abs(r) gives reflectivity.
        p(i) = q;
   end
   b = Ref;                  %storing reflectivity for each theeta to plot later.

%----Plotting Reflectivity as a function of theeta----------%
grid on;              % to show grid in plot
xlabel ('(Grazing) 2 X angle of incidence (in degrees)'); % X-axis nameing.
ylabel ('log(Absolute Reflectivity)');                    % Y-axis naming.
title(['X-Ray Reflectivity for thickness =']);            % Title of graph.
figure;
semilogy((theta*36/pi)*180*4,Ref,'LineWidth',1.5); % semilogy function allows us to
take log.
grid on;
xlabel ('(Grazing) 2 X angle of incidence (in degrees)');
ylabel ('log (Absolute Reflectivity)');
title(['X-Ray reflectivity for thickness = 25 nm']);
end
%----Thank you--------%
```

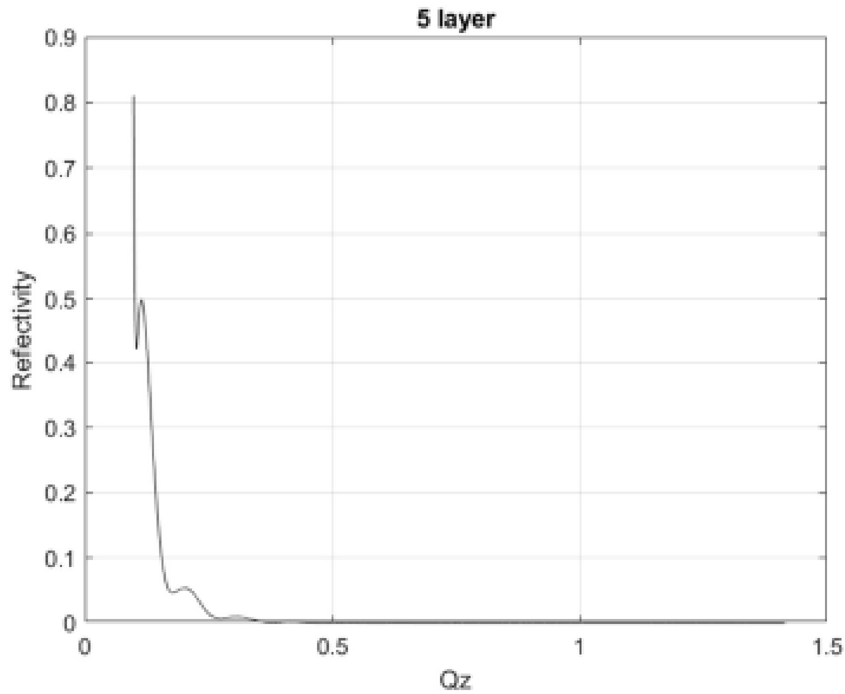
RESULT -



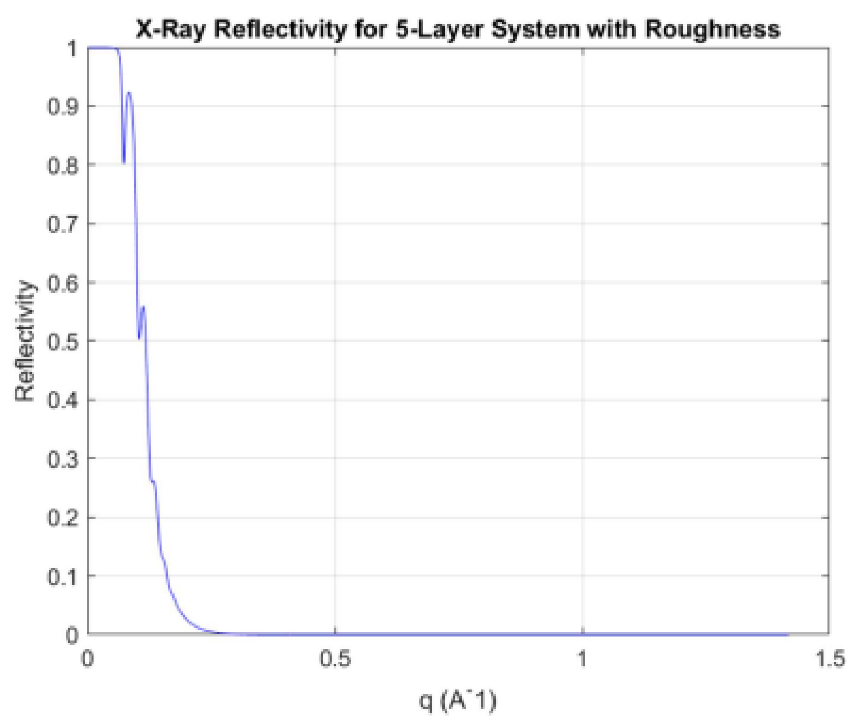
X-Ray reflectivity for thickness = 25 nm
log (Absolute Reflectivity)
10^0
10^-1
10^-2
10^-3
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
(Grazing) 2 X angle of incidence (in degrees)

1.13 FOR 5 LAYERS -

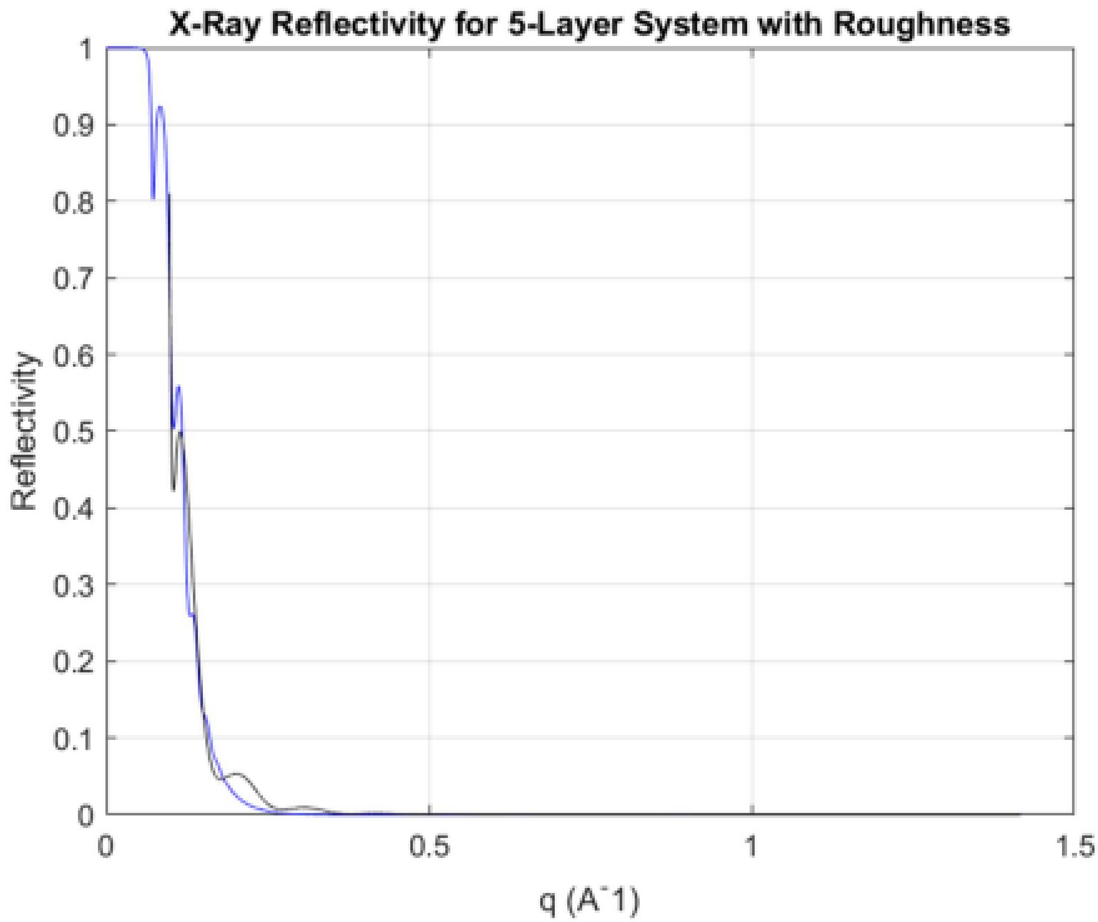
GRAPH FROM EXPERIMENT



GRAPH FROM CALCULATION



1.14 CURVE FITTING ANALYSIS



LAYER 1 - **AlN**

LAYER 2 - **GaN**

LAYER 2 - **AlN**

LAYER 2 - **InN0.180 AlN0.820**

LAYER 2 - **GaN**

SUBSTRATE - **SiC**

Through the curve fitting we get the results of the thickness and roughness of all the 5 layers and the substrate to be newRX2_5layer(80e-7,1705e-7,0.75e-7,7e-7,1.6e-7,9.56e+23,1.67e+24,9.56e+23,1.1e+24,1.67e+24,9.63e+23,0.1,0.25,0.1,0.2,0.25,0.2,1.35e-7,1.6e-7,0.6e-7,1.2e-7,0.7e-7,1.5e-7)

h_1 - 80e-7

h_2 - 1705e-7

h_3 - 0.75e-7

h_4 - 7e-7

h_5 - 1.6e-7

e_density1 - 9.56E+23

e_density2 - 1.67e+24

e_density3 - 9.56E+23

e_density4 - 1.1e+24

e_density5 - 1.67e+24

e_density6 - 9.63e+23

abs_coeff1 - 0.1

abs_coeff2 - 0.25

abs_coeff3 - 0.1

abs_coeff4 - 0.2

abs_coeff5 - 0.25

abs_coeff6 - 0.2

s1 -1.35e-7

s2 - 1.6e-7

s3 - 0.6e-7

s4 - 1.2e-7

s5 - 0.7e-7

s6 - 1.5e-7

MATLAB CODE

newRX2_5layer(80e-7,1705e-7,0.75e-7,7e-7,1.6e-7,9.56e+23,1.67e+24,9.56e+23,1.1e+24,1.67e+24,9.63e+23,0.1,0.25,0.1,0.2,0.25,0.2,1.35e-7,1.6e-7,0.6e-7,1.2e-7,0.7e-7,1.5e-7)

```
function newRX2_5layer(h_1, h_2, h_3, h_4, h_5, e_density1, e_density2, e_density3,
e_density4, e_density5, e_density6, abs_coeff1, abs_coeff2, abs_coeff3, abs_coeff4,
abs_coeff5, abs_coeff6, s1, s2, s3, s4, s5, s6)
   % Constants
   theta = linspace(0, pi/18, 10000);  % incident angle range in radians (adjusted
to a smaller range)
   re = 2.8179403227e-13;  % classical electron radius (cm)
   lambda = 1.54e-8;  % X-ray wavelength (cm)

   % Calculate delta and beta for each layer
   delta = re * lambda^2 .* [e_density1, e_density2, e_density3, e_density4,
e_density5, e_density6] / (2 * pi);
   beta = [abs_coeff1, abs_coeff2, abs_coeff3, abs_coeff4, abs_coeff5, abs_coeff6]
* lambda / (4 * pi);
   % Refractive indices
   n = 1 - delta - 1i * beta;
   % Wave vectors
   k = 2 * pi / lambda;
   kz_0 = k * sin(theta);
   kz = sqrt(k^2 * (n.').^2 - kz_0.^2);  % Ensure n is column vector
   % Fresnel coefficients and roughness
   P = @(kz1, kz2) (kz1 + kz2) ./ (2 * kz1);
   m = @(kz1, kz2) (kz1 - kz2) ./ (2 * kz1);
   Rough = @(q, s) exp(-q^2 * s^2);
   % Initialize reflectivity array
   Ref = zeros(size(theta));
   p = zeros(size(theta));
   % Calculate reflectivity for each theta
   for i = 1:length(theta)
       % Construct 2x2 matrices for the current theta
       q = 4 * pi * sin(theta(i)) / lambda;
       Roughness = arrayfun(@(s) Rough(q, s), [s1, s2, s3, s4, s5, s6]);
       R = arrayfun(@(j) [P(kz_0(i), kz(j, i)), m(kz_0(i), kz(j, i)) *
Roughness(j); m(kz_0(i), kz(j, i)) * Roughness(j), P(kz_0(i), kz(j, i))], 1:5,
'UniformOutput', false);
       T = arrayfun(@(j, h) [exp(-1i * kz(j, i) * h), 0; 0, exp(1i * kz(j, i) *
h)], 1:5, [h_1, h_2, h_3, h_4, h_5], 'UniformOutput', false);
       % Perform the matrix multiplication
       M = R{1} * T{1} * R{2} * T{2} * R{3} * T{3} * R{4} * T{4} * R{5} * T{5} *
[P(kz(5, i), kz(6, i)), m(kz(5, i), kz(6, i)) * Roughness(6); m(kz(5, i), kz(6, i))
* Roughness(6), P(kz(5, i), kz(6, i))];
```

```
        % Extract the reflection coefficient
        r = M(1, 2) / M(2, 2);
        Ref(i) = abs(r)^2;
        p(i) = q;
    end
    % Apply a smoothing filter
    %Ref_smoothed = smooth(Ref, 0.01, 'rloess');
  %  filename = 'C:\Users\Mageshan\Downloads\Xr.xlsx'; % Replace with your actual
filename
    % Read the data from the Excel file
  %  data = readtable(filename);
% Extract wavelength and reflectance columns
  %  q = data{:, 5}; % Assuming the first column is wavelength
  %  reflectivity = data{:, 3}; % Assuming the second column is reflectance
    % Plot the reflectivity as a function of incident angle
    figure;
    plot(p * 1e-8, Ref , 'Color','b');
   % hold on ;
  %  plot(q, reflectivity, 'k'); % Plot with line and markers
    xlabel('q (A^-1)');
    ylabel('Reflectivity');
    title('X-Ray Reflectivity for 5-Layer System with Roughness');
    hold off;
    grid on;
end
```

1.15 CONCLUSION

X-ray reflectometry is now widely used for the analysis of surfaces and interfaces. Its main advantage is that it allows one to determine the surface and interface roughness and the structural arrangement of complex architectures.

Since measurements are made at small angles of incidence, it is not necessary for the analysed materials to be crystallised which is also an advantage of the technique over classical diffraction methods.

In this experiment we discussed the technique of specular X-ray reflectivity and illustrated with experimental results obtained on different kinds of thin films and surfaces. After a short introduction on the Fresnel reflectivity, the matrix technique is developed and discussed how it can be used to determine the electron density and the roughness of the interfaces.

In particular we also discussed that the roughness of the interfaces is of crucial importance for many technological applications and it is a parameter which must be determined to appreciate the quality of the interfaces.

CHAPTER 2 : FTIR

1.1 ABSTRACT:

Recently there has been a great deal of interest in silicon carbide due to its applicability for power electronic devices.In order to characterise the electrical and thickness uniformity of the epi-wafers during the device process, that is to know how the thickness, doping concentration and mobility are dis-tributed over the SiC epi-layers, it is necessary to develop the characterization method that can perform the determinations of thickness and electrical properties simultaneously in a nondestructive and noncontact way.

We will be using 4H-SiC as our sample which has p-type Al doped epilayer and n-type N doped substrate and will be finding the carrier concentration and mobility of both the epilayer and the substrate. Interference fringes from the epi-films are observed in the reflectance spectra and we will be using it to accurately determine the thickness of these epi-films.

With this Nondestructive and contactless characterization method we find the thickness and electrical properties in homo-epitaxially grown SiC epilayers using Infrared Reflectance Spectroscopy.

1.2 INTRODUCTION:

FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY

Fourier Transform Infrared (FTIR) spectroscopy is a technique used to obtain the infrared spectrum of absorption, emission, or photoconductivity of a solid, liquid, or gas. The FTIR spectrum typically ranges from:

Far-Infrared (FIR): 400 cm^{-1} to 10 cm^{-1} (25 µm to 1000 µm)
Mid-Infrared (MIR): 4000 cm^{-1} to 400 cm^{-1} (2.5 µm to 25 µm)
Near-Infrared (NIR): 14000 cm^{-1} to 4000 cm^{-1} (0.8 µm to 2.5 µm)

The most commonly used range in FTIR spectroscopy is the mid-infrared region, as it provides detailed information about the molecular vibrations and functional groups in a sample. The typical FTIR instrument covers a spectral range from about 4000 cm^{-1} to 400 cm^{-1}.We have also used the same for our experiment and through Non-dispersive way , we obtained IR spectra in a whole range of wave number simultaneously.

WORKING PRINCIPLE :

The Michelson Interferometer is used in the FTIR apparatus.

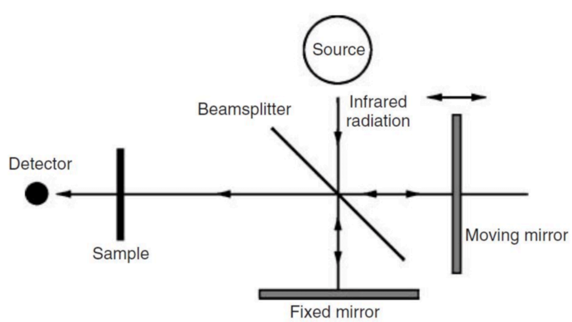


Figure showing the pathway covered by the incident beam from the source

Interferogram

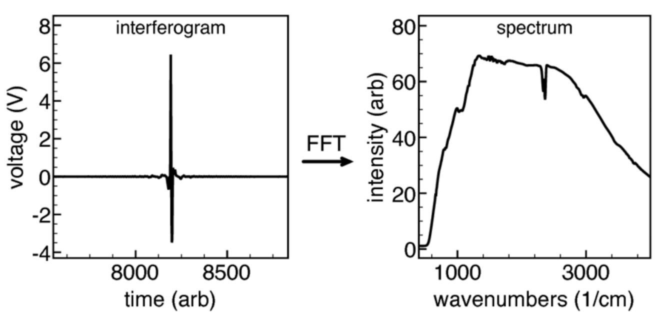
The interferogram is a raw data output of an FTIR spectrometer. It is a complex signal generated by the interferometer that contains all the spectral information of the sample.

Fourier Transform

The Fourier Transform is a mathematical process that converts the interferogram into a readable IR spectrum.

Process

Interferogram to Spectrum: The interferogram, which is a time-domain signal, is transformed into a frequency-domain spectrum using the Fourier Transform.



IR Source :

The IR source in an FTIR spectrometer emits broad-spectrum infrared radiation, which is necessary for the analysis.

Nernst Glower: Composed of rare earth oxides (zirconium oxide), it also provides a broad IR spectrum.

The beam splitter :

Material: Typically made from KBr (potassium bromide)

Directs one part of the IR beam towards a fixed mirror and the other part towards a movable mirror. After reflecting off these mirrors, the beams are recombined, creating an interference pattern that forms the interferogram.

Detector :

The detector converts the incoming IR radiation into an electrical signal. This signal corresponds to the intensity of the IR radiation at different wavelengths and is processed to produce the final IR spectrum.

MCT (Mercury Cadmium Telluride): A photoconductive detector with high sensitivity and fast response, suitable for mid to far IR regions.

1.3 CHARACTERIZATION METHOD OF THE ELECTRICAL PROPERTIES IN SIC SUBSTRATE USING IR REFLECTANCE SPECTROSCOPY

Method of obtaining carrier concentration and mobility from IR reflectance spectroscopy.

In the case of wide bandgap semiconductors with an overdamped plasmon system like SiC, the reflectance spectrum is, however, strongly dependent on LO-phonon damping because the plasmon is overdamped and the LO phonon frequency is much higher than the plasma frequency except for heavily doped cases. For these reasons, we have chosen to use the modified classical dielectric function (MDF) model taking into account the contribution of the TO phonon damping constant and the LO phonon damping constant.

$$\varepsilon(\omega)=\varepsilon_{\infty}\left(\frac{\omega_L{}^2-\omega^2-i\Gamma_L\,\omega}{\omega_T{}^2-\omega^2-i\Gamma_T\omega}-\frac{\omega_p{}^2}{\omega^2+i\gamma_p\omega}\right)$$

Classical theory

$D = \epsilon_0 \epsilon(\omega) E$

$\epsilon(\omega)$ - Dielectric function
ϵ_0 - permittivity
E - Electric field

Under external electric field, the Equation of motion of an electron

$$m\frac{d^2x}{dt^2} + m\gamma\frac{dx}{dt} + m\omega_0^2 x = -eE_0 e^{-i\omega t}$$

$E_0 e^{-i\omega t}$ - applied E. Field

assuming $x = x_0 e^{-i\omega t}$ and substituting

$$-m\omega^2 x_0 e^{-i\omega t} - im\gamma\omega x_0 e^{-i\omega t} + m\omega_0^2 x_0 e^{-i\omega t} = -eE_0 e^{-i\omega t}$$

simplifying we get

$$x_0(\omega_0^2 - \omega^2 - i\gamma\omega) = \frac{eE_0}{m}$$

$$x_0 = \frac{eE_0}{m(\omega_0^2 - \omega^2 - i\gamma\omega)}$$

$P = +Nex$ N - density of electrons

$P = \epsilon_0 \chi_e(\omega) E \rightarrow ①$ $x = x_0 e^{-i\omega t}$

$$P = +Nex_0 e^{-i\omega t} = +Ne\frac{eE_0 e^{-i\omega t}}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} \rightarrow ②$$

comparing ① + ②

$$\chi_e(\omega) = +\frac{Ne^2}{\epsilon_0 m(\omega_0^2 - \omega^2 - i\gamma\omega)}$$

Dielectric function: $\epsilon(\omega) = 1 + \chi_e(\omega)$

$$\epsilon(\omega) = 1 + \frac{Ne^2}{\epsilon_0 m \left(\omega_0^2 - \omega^2 - i\gamma\omega\right)}$$

in terms of Phonon Frequency

strength of phonon contribution : $\frac{Ne^2}{\epsilon_0 m} = \omega_L^2 - \omega_T^2$

Through Drude's model :

plasmon contribution from oscillation of free electron

$$\epsilon_{plasmon} = - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$$

$$\epsilon(\omega) = \epsilon_\infty \left(1 + \frac{\omega_L^2 - \omega_T^2}{\omega_T^2 - \omega^2 - i\gamma\omega} - \frac{\omega_p^2}{\omega(\omega + i\gamma)} \right)$$

where ε_∞ is the high frequency dielectric constant, ω_T and ω_L are the TO- and LO-phonon frequencies, respectively, Γ_T and Γ_l are the TO- and LO-phonon damping constants, respectively, γ_p is the free-carrier damping constant, and ω_p is the plasma frequency of the free carriers, which is given by

$$\omega_p = \sqrt{\frac{Ne^2}{m^* \varepsilon_\infty}}$$

where N, e, and m* are the free carrier concentration, electron charge, and effective mass, respectively. The free-carrier damping constant γ_p is the inverse of the scattering time τ and therefore the free-carrier mobility can be derived using the following relation

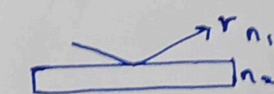
$$\mu = \frac{e}{m^* \gamma_p}$$

Assuming that the wafers are uniformed in the depth direction, we used the normal incidence reflectance of a semi-infinite medium R, which is expressed as

$$R(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

where n and k are the optical constants, derived from ε/ε0=(n–ik) ^2 .

Fresnel reflectance coefficient



$$r = \frac{n_2 - n_1}{n_2 + n_1}$$

n_1 - air

n_2 - 4H - SiC (n type substrate) $\Rightarrow$ $n_2 = n + ik$

Reflectance (normal) $= r r^* = \left[\frac{(n-1) + ik}{(n+1) + ik} \times \frac{(n-1) - ik}{(n+1) - ik} \right]$

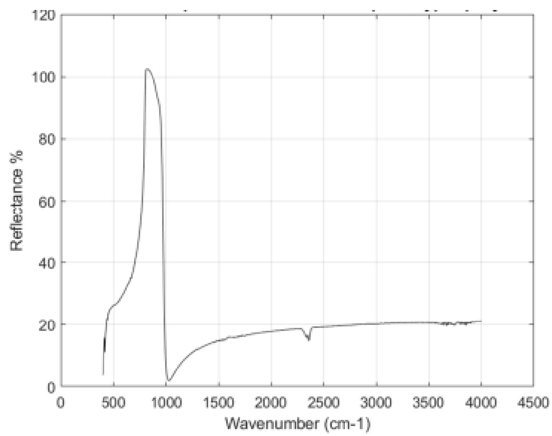
$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

The carrier concentration and mobility can be determined by fitting the experimental infrared reflectance spectrum with calculated ones with ωp , γp , and ΓL as adjustable parameters.

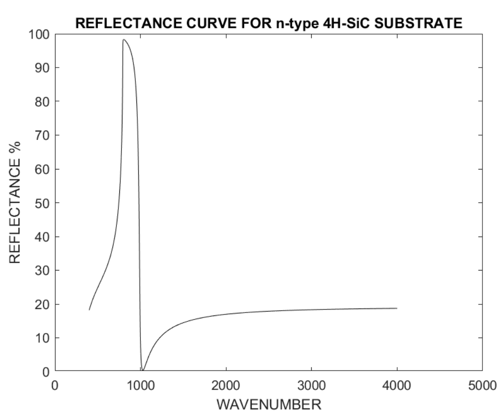
1.4 Measurements of IR reflectance spectra of SiC wafers and estimation of electrical properties

The measurements were performed for 4H-SiC wafers at nearly normal incidence.

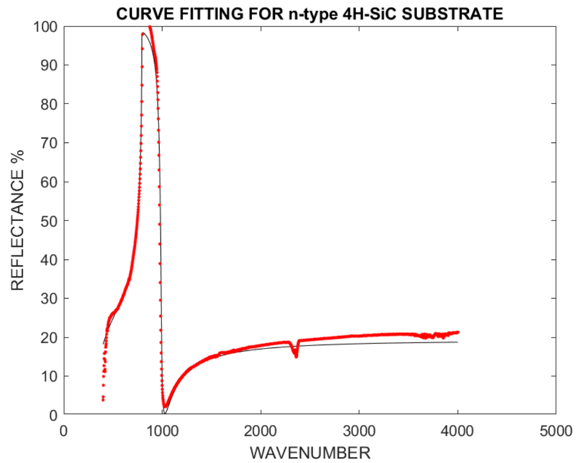
❖ **Graph of n-type SiC substrate from the experiment**



❖ **Graph of n-type SiC substrate from the calculation**



❖ **Curve fitting analysis**



INPUT PARAMETERS :

Constants are ωl= 970 cm-1 and ωt = 793 cm-1 .And through the curve fitting analysis by changing the oscillator parameters we obtained the carrier concentration value to be **1.1583e+17 cm-3** and the mobility value to be 21.70.

The refractive index of the substrate is found to be 2.6741.

1.5 MATLAB CODE FOR REFLECTANCE SPECTRA OF SUBSTRATE:

INPUT : Reflectance_substrate(970 , 793 , 340 , 0.0001 , 15.63 , 1.03)

```
function Reflectance_substrate(LO_freq , TO_freq , S_plasma_freq , S_gamma_p ,
S_LO_dampconst , S_TO_dampconst)
wavenumber = 400 :4000 ; % Wavenumber of the input rays
c = 3e10 ;               % speed of light in (cm/s)
m_e= 9.31e-31;           % mass of electron in kg
e_charge= 1.6e-19;       % charge of an electron
S_m_eff = 0.42 * m_e ;   % effective mass of the electron in the substrate
epsilon_infinite = 6.56; % permittivity
% Equations for carrier concentration and mobility
N_conc = (S_plasma_freq.^2 * S_m_eff * epsilon_infinite ) ./ ( e_charge.^2) ;
Mobility = (e_charge ./(2* pi * c *S_m_eff * S_gamma_p));
% Expression for the epsilon function as derived
S_epsilon_func = epsilon_infinite *(((LO_freq.^2 - wavenumber.^2 -
1i*S_LO_dampconst*wavenumber) ./ (TO_freq^2 - wavenumber.^2 -
1i*S_TO_dampconst*wavenumber)) - ((S_plasma_freq^2) ./ (wavenumber.^2 +
1i*S_gamma_p*wavenumber)));
S_epsilon_real = real(S_epsilon_func) ;
S_epsilon_imaginary= imag(S_epsilon_func);
% n2 and k2 are the real and imaginary part of refractive index of substrate
n2 =sqrt((S_epsilon_real + sqrt(S_epsilon_real.^2 + S_epsilon_imaginary.^2)) ./ 2);
k2 =S_epsilon_imaginary ./ (2 * n2);
% Reflectance formula for normal incidence
R = ((n2-1).^2 + k2.^2)./((n2+1).^2 + k2.^2);
R_percent = R;
% Specify the filename
filename = '21-may-sic n-doped ref.xlsx'; % Replace with your actual filename
% Reading the data from the Excel file
data = readtable(filename);
% Extracting wavelength and reflectance columns
wavelength1 = data{:, 1}; % Assuming the first column is wavelength
reflectance2 = data{:, 3}; % Assuming the second column is reflectance
% graph
figure;
plot(wavenumber, R_percent * 100,'k');
hold on ;
plot(wavelength1, reflectance2, '.', 'Color','r');
xlabel('WAVENUMBER');
ylabel('REFLECTANCE %');
title('REFLECTANCE CURVE FOR n-type 4H-SiC SUBSTRATE');
hold off  ;
axis([0 5000 0 100]);
end
```

1.6 CHARACTERIZATION METHOD OF THE ELECTRICAL PROPERTIES AND THICKNESS OF EPILAYERS USING IR REFLECTANCE SPECTROSCOPY

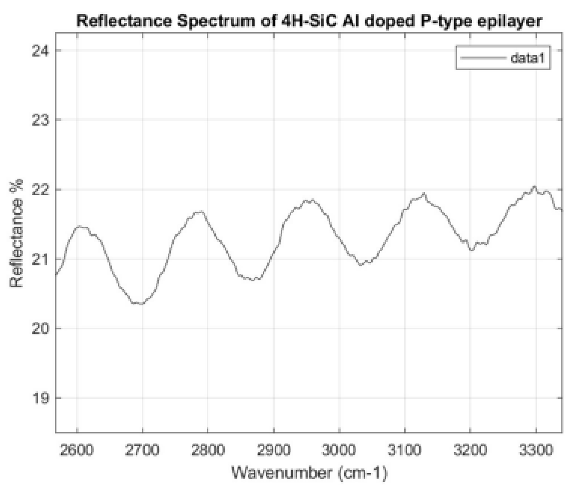
Measurements of IR reflectance spectra and derivation thickness of SiC epi-layer

From this fringing effect we can calculate the thickness of the film using the following equation;

b = 1/2n x N / (υ1 - υ2)

where; b = film thickness and n = refractive index of sample N = number of fringes within a given spectral region υ1 , υ2 = start and end point in the spectrum in cm-1.

- **Graph**



- **Calculations and Result**

υ1 = 3297.6   υ2 = 2605.36 ;

N = 4 ; n = 2.7143 (average value from Dielectric function)

D = 10.644 micrometre

Method of obtaining the carrier concentration, mobility, and thickness of epilayers

The reflectance R from an air/ epilayer/substrate structure at normal incidence is given by

$$R = \left| \frac{r_1 + r_2 e^{-2i\delta}}{1 + r_1 r_2 e^{-2i\delta}} \right|^2, \quad where \quad \delta = \frac{2\pi n d}{\lambda}$$

where r1 and r2 are the Fresnel reflection coefficients at the air/epilayer and the epilayer/ substrate interface, respectively, and δ is the phase shift of light in the epilayer, n and d are the refractive index and the thickness of epilayer, respectively, and λ is wavelength.

Reflectivity from single layer + a substrate

Transfer matrix = $R_{01} T_1 R_{12}$

$$= \begin{bmatrix} p_1 & m_1 \\ m_1 & p_1 \end{bmatrix} \begin{bmatrix} e^{-ik_2h} & 0 \\ 0 & e^{+ik_2h} \end{bmatrix} \begin{bmatrix} p_2 & m_2 \\ m_2 & p_2 \end{bmatrix}$$

$$= \begin{bmatrix} p_1 e^{-ik_2h} & m_1 e^{ik_2h} \\ m_1 e^{-ik_2h} & p_1 e^{ik_2h} \end{bmatrix} \begin{bmatrix} p_2 & m_2 \\ m_2 & p_2 \end{bmatrix}$$

$$= \begin{bmatrix} p_1 p_2 e^{-ik_2h} + m_1 m_2 e^{ik_2h} & p_1 m_2 e^{-ik_2h} + m_1 p_2 e^{ik_2h} \\ m_1 p_2 e^{-ik_2h} + p_1 m_2 e^{ik_2h} & m_1 m_2 e^{-ik_2h} + p_1 p_2 e^{ik_2h} \end{bmatrix}$$

$$r = \frac{M_{12}}{M_{22}} = \frac{p_1 m_2 e^{-ik_2h} + m_1 p_2 e^{ik_2h}}{m_1 m_2 e^{-ik_2h} + p_1 p_2 e^{ik_2h}}$$

$$r_1 = \frac{m_1}{p_1} \qquad r_2 = \frac{m_2}{p_2}$$

Or Simply in our case, we can write

$$r_1 = \frac{n_{layer} - 1}{n_{layer} + 1} \qquad r_2 = \frac{n_{substrate} - n_{layer}}{n_{substrate} + n_{layer}}$$

$$r = \frac{r_1 + r_2 e^{-2ik_2h}}{1 + r_1 r_2 e^{-2ik_2h}}$$

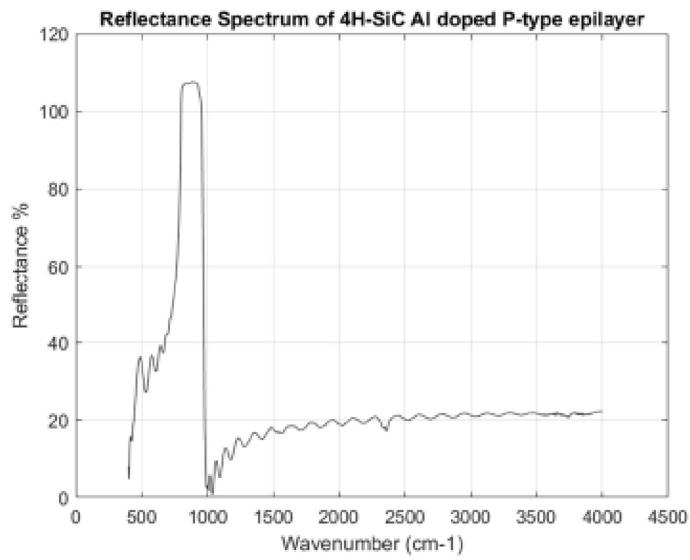
k_z in presence of medium nk

$h \rightarrow$ thickness

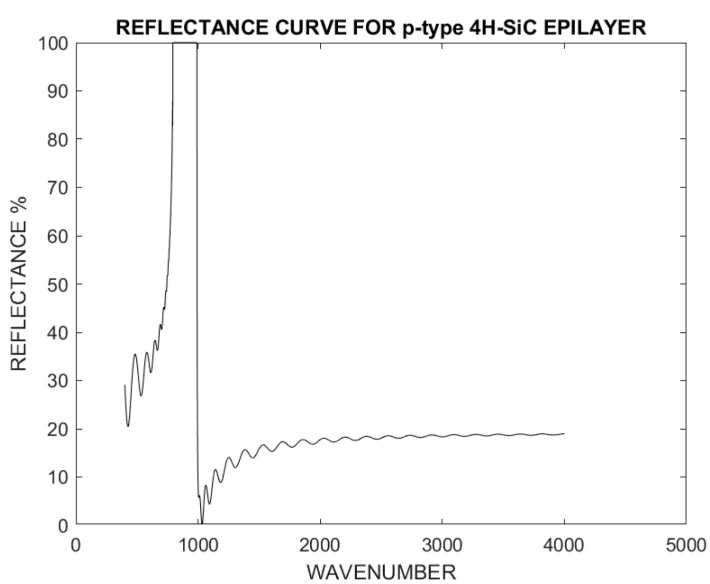
$$R = |r|^2 = \left| \frac{r_1 + r_2 e^{-2i\delta}}{1 + r_1 r_2 e^{-2i\delta}} \right|$$

$\delta = nkh = k_z h$

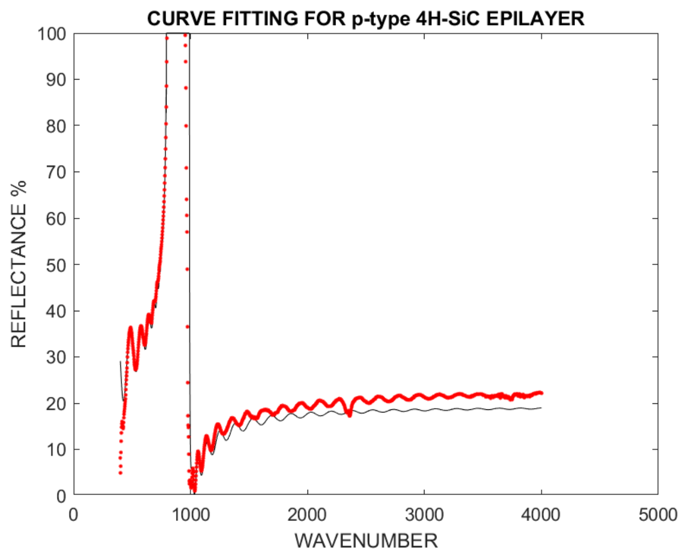
❖ **Graph of p-type SiC epilayer from the experiment**



❖ **Graph of p-type SiC epilayer from the calculation**



❖ Curve fitting analysis



INPUT PARAMETERS :

Constants are ωl= 970 cm-1 and ωt = 793 cm-1 .And through the curve fitting analysis by changing the oscillator parameters we obtained the carrier concentration value to be **7.5553e+16 cm-3** and the mobility value to be 139.6.

The refractive index of the substrate is found to be 2.7143.

1.7 MATLAB CODE FOR REFLECTANCE SPECTRA OF SUBSTRATE AND THE EPILAYER:

Reflectance_epilayer4(90 , 1.67e-5 , 55.6 , 1.6 , 970 , 793 , 340 , 0.0001 , 15.63 , 1.03)

```
function Reflectance_epilayer4( plasma_freq , gamma_p , LO_dampconst , TO_dampconst
, LO_freq , TO_freq , S_plasma_freq , S_gamma_p , S_LO_dampconst , S_TO_dampconst )
%constants
wavenumber = 400 :4000 ;  % Wavenumber of the input rays
c = 3e10 ;                % speed of light in (cm/s)
wavelength = 1 ./ wavenumber ; % conversion of wavenumber to wavelength
m_e= 9.1e-28;             % mass of electron in kg
e_charge= 1.6e-19;        % charge of an electron
m_eff = 0.4 * m_e;        % effective mass of the electron in the substrate
d = 10e-4 ;               % thickness
epsilon_infinite = 6.56;  % permittivity
% Equations for carrier concentration and mobility
N_conc = (plasma_freq.^2 * m_eff * epsilon_infinite ) ./ ( e_charge.^2)  ;
Mobility = (e_charge ./(2* pi * c *m_eff * gamma_p)) ;
% Expression for the epsilon function as derived
% for epilayer
epsilon_func = epsilon_infinite *(((LO_freq.^2 - wavenumber.^2 -
1i*LO_dampconst*wavenumber) ./ (TO_freq^2 - wavenumber.^2 -
1i*TO_dampconst*wavenumber)) - ((plasma_freq^2) ./ (wavenumber.^2 +
1i*gamma_p*wavenumber)));
epsilon_real = real(epsilon_func) ;
%for substrate
S_epsilon_func = epsilon_infinite *(((LO_freq.^2 - wavenumber.^2 -
1i*S_LO_dampconst*wavenumber) ./ (TO_freq^2 - wavenumber.^2 -
1i*S_TO_dampconst*wavenumber)) - ((S_plasma_freq^2) ./ (wavenumber.^2 +
1i*S_gamma_p*wavenumber)));
S_epsilon_real = real(S_epsilon_func) ;
epsilon_imaginary= imag(epsilon_func);
% n1 and k1 are the real and imaginary part of refractive index of epilayer
n1 =sqrt((epsilon_real + sqrt(epsilon_real.^2 + epsilon_imaginary.^2)) ./ 2);
k1 =epsilon_imaginary ./ (2 * n1);
% n2 and k2 are the real and imaginary part of refractive index of substrate
S_epsilon_imaginary= imag(S_epsilon_func);
n2 =sqrt((S_epsilon_real + sqrt(S_epsilon_real.^2 + S_epsilon_imaginary.^2)) ./ 2);
k2 =S_epsilon_imaginary ./ (2 * n2);
% refractive indices of both the substrate and the epilayer
n_epi = sqrt(epsilon_real) ;
n_sub = sqrt(S_epsilon_real);
% equation of fresnel coefficient
r1 = ( 1 - n_epi ) ./ ( 1 + n_epi);
r2 = (n_epi - n_sub) ./ (n_epi + n_sub) ;
% Equation for phase shift when the light penetrates the epilayer
```

```
phase_shift = (2 * pi * n_epi * d ) ./ wavelength ;
ratio_R = (r1 + r2 .* exp( (-2) * 1i * phase_shift)) ./ (1 + r1 .* r2 .* exp( (-2)
* 1i * phase_shift));
% Final formula for reflectivity
R_epi = abs(ratio_R).^2 ;
% Specify the filename
filename = 'C:\Users\mageshan\Downloads\21-may-sic n-doped ref.xlsx'; % Replace
with your actual filename
% Reading the data from the Excel file
data = readtable(filename);
% Extracting wavelength and reflectance columns
wavelength1 = data{:, 1}; % Assuming the first column is wavelength
reflectance1 = data{:, 2}; % Assuming the second column is reflectance
reflectance2 = data{:, 3}; % Assuming the second column is reflectance
% graph
figure;
plot(wavenumber, R_epi * 100,'k');
hold on ;
plot(wavelength1, reflectance1, '.', 'Color','r');
xlabel('WAVENUMBER');
ylabel('REFLECTANCE %');
title('IR REFLECTANCE FOR SiC');
hold off  ;
axis([0 5000 0 100]);
end
```

1.8 CONCLUSION

We proposed the method for estimating the electrical properties, such as, carrier concentra- tion and mobility of semiconductor wafers using IR reflectance spectroscopy. In the method, the observed spectra are fitted with the calculated ones, and the free carrier concentration and mobility are determined from the fitted parameters.

In the calculation, we used the modified dielectric function (MDF) model for the dispersion relation of dielectric constants. We demonstrated the estimations of carrier concentrations and mobilities of commercially produced 4H-SiC wafers from observed IR reflectance spectra in the frequency range of 400– 4000 cm−1.

Next, we applied this method to the simultaneous determination of the carrier concentra- tion, mobility and thickness of homo-epilayers, and the carrier concentration and mobility of substrates.

IR reflectance spectra with the frequency range of 400–4000 cm−1 were measured for **p-type 4H-SiC epilayer** on **n-type 4H-SiC substrate** .

We conclude that the electrical characteristics of SiC wafers and the electrical properties and thickness of SiC epilayers can be obtained simultaneously from the analyses of IR reflectance spectroscopy in nondestructive and contactless manner.

CHAPTER - 3

DETERMINATION OF EIGENSTATE ENERGIES OF A PARTICLE IN A FINITE POTENTIAL WELL

3.1 INTRODUCTION

Quantum mechanics is a fundamental theory in physics that describes the physical properties of nature at small scales, such as that of atomic and subatomic particles. One of the fundamental problems in quantum mechanics is understanding the behaviour of a particle in a potential well, which is a key concept in quantum mechanics used to model various physical systems where a particle is confined within a specific region of space due to the presence of a potential energy barrier.

The potential well describes a region where the potential energy of the particle is lower than in the surrounding regions. This confinement leads to quantized energy levels for the particle, meaning that the particle can only possess certain discrete energy values.

TYPES OF POTENTIAL WELLS

Infinite Potential Well : In this idealised model, the potential energy inside the well is zero, and it becomes infinitely large outside the well. This results in a particle being strictly confined within the well with no probability of being found outside. The energy levels are discrete.

Finite Potential Well : This model extends the concept of the potential well to cases where the potential energy outside the well is finite rather than infinite. The potential well has a finite depth Vo and width L. Inside the well, the potential is constant (usually taken as zero), while outside the well, the potential is a constant value V0.

- The finite potential well allows for a more realistic description of physical systems and leads to a different set of quantized energy levels.
- The energy levels in a finite potential well are calculated by solving the Schrödinger equation with appropriate boundary conditions at the edges of the well.

SIGNIFICANCE OF EIGENSTATE

The eigenstate energies, also known as eigenvalues, represent these discrete energy levels. Studying these energies helps in understanding how particles are confined in potential wells and how their energy levels are determined by the quantum constraints of the system.

3.2 OBJECTIVE

The objective of this report is to calculate and analyse the eigenstate energies of a particle in a finite potential well using numerical methods. MATLAB will be used for the implementation of these calculations.

3.3 NUMERICAL METHODS FOR SOLVING SCHRÖDINGER EQUATION

Finite Difference Method for Approximating Derivatives

The finite difference method is a numerical technique the derivative of a function based on the values of the function at discrete points.

The second derivative is often used in solving differential equations such as the Schrödinger equation.The finite difference approximation of this derivative is used to construct the kinetic energy operator matrix, which is then used to form the Hamiltonian matrix in numerical simulations.

Kinematic operator

In numerical simulations, the tridiagonal matrix represents the finite difference approximation for the kinetic energy operator.

Potential Energy Operator

Basis functions are chosen such that the potential energy operator only affects the diagonal elements of the matrix representation; the matrix for potential energy will be diagonal.

3.4 MATLAB Implementation

```
% Constants
hbar = 1.0545718e-34; % Planck's constant (Joule second)
m = 9.10938356e-31;   % Mass of electron (kg)
L = 2e-10;             % Half-width of the well (metres)
V0 = 75 * 1.60218e-19; % Depth of the well (10 eV converted to Joules)
% Number of points for spatial discretization
N = 1000;
x = linspace(-3*L, 3*L, N); % Extended range to better visualise the potential well
dx = x(2) - x(1);
% Potential well
V = V0 * (abs(x) >= L);
% Kinetic energy operator
T = - (hbar^2 / (2 * m * dx^2)) * (diag(ones(N-1,1),1) - 2*diag(ones(N,1)) +
diag(ones(N-1,1),-1));
% Hamiltonian
H = T + diag(V);
% Solve the eigenvalue problem
[eigenVectors, eigenValues] = eig(H);
% Extract the eigenvalues (energies)
eigenEnergies = diag(eigenValues);
% Convert energies to electron volts (eV)
eigenEnergies_eV = eigenEnergies / 1.60218e-19;
% Display the first few eigenenergies
disp('Eigenstate energies (eV):');
disp(eigenEnergies_eV(1:10));
% Plot the potential well and the first few eigenfunctions
figure;
plot(x, V / 1.60218e-19, 'k', 'LineWidth', 1.5); % Potential in eV
hold on;
for n = 1:5
   plot(x, eigenVectors(:,n) * 10 + eigenEnergies_eV(n), 'LineWidth', 1.5);
end
xlabel('Position (m)');
ylabel('Energy (eV)');
title('Potential well and first few eigenstates');
legend('Potential well', '1st eigenstate', '2nd eigenstate', '3rd eigenstate', '4th
eigenstate', '5th eigenstate');
grid on;
hold off;
```

3.5 RESULT

L = 2e-10 (**Half-width of the well (metres) Depth of the well in joules**)

V0 = 75 * 1.60218e-19 (**Depth of the well in joules**)

EIGENSTATE ENERGIES (EV) OBTAINED FROM THE CODE :

1.9067
7.6060
17.0281
30.0255
46.2816
64.8885

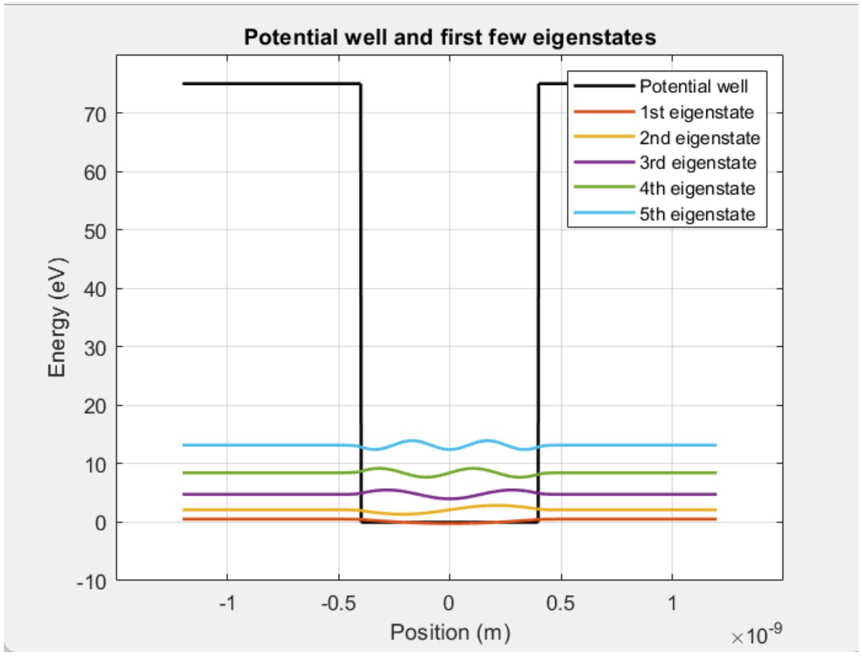
THEORETICAL RESULT FOR REFERENCE :

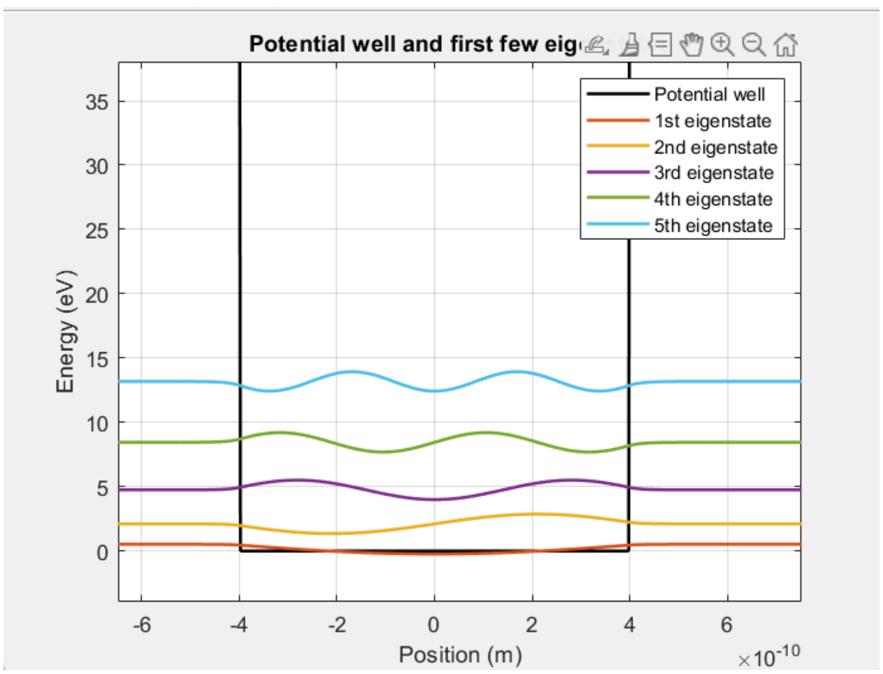
Table (1)
Eigen value from GM and IM
for PW 4 A^o and PD 75 eV.

n	Parity	Eigen value (eV) (GM) Ref [15]	Eigen Value (eV) (IM) Present Work
1	Even	1.9	1.901826
2	Odd	7.6	7.586675
3	Even	16.9	16.95550
4	Odd	29.9	29.95245
5	Even	46.1	46.17400
6	Odd	64.6	64.75384

3.6 VISUALISATION

Potential Well Plot





The potential well shows where the particle is confined, while the eigenfunctions illustrate how the particle behaves in each quantized state within the well.

3.7 CONCLUSION

This study provides a clear and practical approach to solving the eigenvalue problem for a particle in a finite potential well, offering valuable insights into quantum confinement effects and the quantization of energy levels. The use of numerical methods and MATLAB demonstrates a robust technique for analysing quantum systems. Future work could extend this study by varying well parameters, using more advanced numerical methods, exploring multi-dimensional potentials, and applying perturbation theory to further understand and refine quantum mechanical models.

REFERENCES

- **X-ray reflectivity and diffuse scattering**

  By - A. Gibaud* and S. Hazra.

  Université du Maine, Faculté des Sciences, UPRES-A 6087, 72085 Le Mans, Cedex 9, France.

- **X-ray thin film measurement techniques.**

  By - Miho Yasaka.

- **X-ray Diffraction of Solids and Semiconductors.**

  Universität Paderborn, Department Physik, Warburger Str. 100, 33098 Paderborn, Germany .

- **Nondestructive and Contactless Characterization Method for Spatial Mapping of the Thickness and Electrical Properties in Homo-Epitaxially Grown SiC Epilayers Using Infrared Reflectance Spectroscopy**.

  BY - Sadafumi Yoshida, Yasuto Hijikata and Hiroyuki Yaguchi.

  http://dx.doi.org/10.5772/50749

- **Thickness Determination of Low Doped SiC Epi-Films on Highly Doped SiC Substrates.**

  BY - M.F. MACMILLAN, A. HENRY, and E. JANZÉN.

  1—Department of Physics and Measurement Technology, Linköping University, S-58183 Linköping, Sweden. 2.—Also ABB Corporate Research, S-72178 Västerås, Sweden.

- **Methods for Thickness Determination of SiC Homoepilayers by Using Infrared Reflectance Spectroscopy.**

  BY - LI Zhi-Yun(李志云), SUN Ji-Wei(孙纪伟), ZHANG Yu-Ming(张玉明), ZHANG Yi-Men(张义门), TANG Xiao-Yan(汤晓燕).**

  Key Laboratory of Wide Band-Gap Semiconductor Materials and Devices, School of Microelectronics, Xidian University, Xi'an 710071.

  PACS: 81.05.Hd, 81.70.Fy DOI: 10.1088/0256-307X/27/6/068103.

- **Infrared reflectance study of 3C-SiC epilayers grown on silicon substrates.**

  BY - Lin Dong, Guosheng Sun, Liu Zheng, Xingfang Liu, Feng Zhang, Guoguo Yan, Wanshun Zhao, Lei Wang, Xiguang Li and Zhanguo Wang.

  Material Science Center, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, People's Republic of China.

  doi:10.1088/0022-3727/45/24/24510.

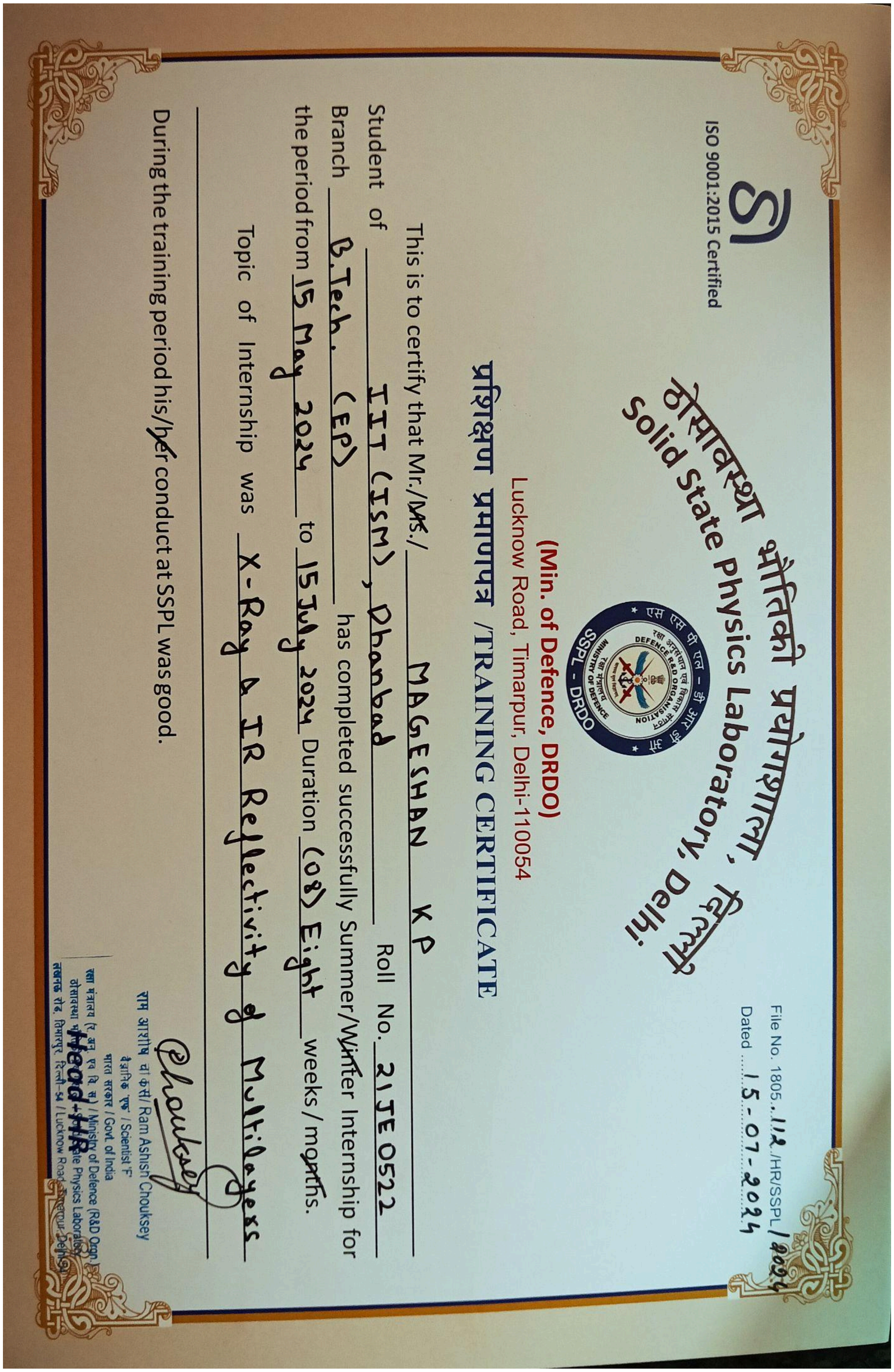
- **Solving Schrödinger Equation for Finite Potential Well Using the Iterative Method.**

  By - Laith A. Al-Ani and Russul K. Abid.

  Department of Physics, College of Science, Al-Nahrain University.

Thank You

CERTIFICATE ISSUED BY DRDO



ISO 9001:2015 Certified

ठोसावस्था भौतिकी प्रयोगशाला, दिल्ली

Solid State Physics Laboratory, Delhi

(Min. of Defence, DRDO)

Lucknow Road, Timarpur, Delhi-110054

File No. 1805..112../HR/SSPL/2024

Dated ..15-07-2024

प्रशिक्षण प्रमाणपत्र /TRAINING CERTIFICATE

This is to certify that Mr./~~Ms.~~/ MAGESHAN KP

Student of IIT (ISM), Dhanbad Roll No. 21JE0522

Branch B.Tech. (EP) has completed successfully Summer/~~Winter~~ Internship for the period from 15 May 2024 to 15 July 2024 Duration (08) Eight weeks/~~months~~.

Topic of Internship was X-Ray & IR Reflectivity of Multilayers

During the training period his/~~her~~ conduct at SSPL was good.

Chouksey

राम आशीष चौकसे / Ram Ashish Chouksey

वैज्ञानिक 'एफ' / Scientist 'F'

Head-HR

भारत सरकार / Govt. of India

रक्षा मंत्रालय (र. अ. एवं वि. सं.) / Ministry of Defence (R&D Organ.)

ठोसावस्था भौतिकी प्रयोगशाला / Solid State Physics Laboratory

लखनऊ रोड, तिमारपुर, दिल्ली-54 / Lucknow Road, Timarpur, Delhi-54