

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

**DEVELOPMENT AND APPLICATION OF IMAGING ELLIPSOMETRY FOR
OPTICAL CHARACTERIZATION AND DEFECT ANALYSIS OF ADVANCED
THIN FILMS**



M.Sc. THESIS

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Physics Engineering Programme

JUNE 2025

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

**GELİŞMİŞ İNCE FİLMLERİN OPTİK KARAKTERİZASYONU VE KUSUR
ANALİZİ İÇİN GÖRÜNTÜLEME ELİPSOMETRİSİNİN GELİŞTİRİLMESİ
VE UYGULANMASI**

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To my family and friends,



FOREWORD

The current thesis has been thoroughly developed over a long span of time and finally arrived at this point with the contributions made by many notable individuals as well as organizations. Therefore, it is appropriate for this introduction to clarify the importance and context behind the work undertaken, along with expressing appreciation to all those who assisted me in my research work.

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ABBREVIATIONS

AlN	: Aluminum Nitride
SiC	: Silicon Carbide
STM	: Scanning Tunneling Microscope
UV	: Ultra-Violet
Hz	: Hertz
LCP	: Left Circular Polarization
RCP	: Right Circular Polarization
LP	: Linear Polarization
EP	: Elliptically Polarization
UL	: Unpolarized Light
PEM	: Photo Elastic Modulator
CCD	: Charge Couple Device
Si	: Silicon
EMA	: Effective Medium Approximation
EMAMG	: Effective Medium Approximation and Maxwell-Garnett
SSC	: Sen, Scala & Cohen
EMPIR	: European Metrology Programme for Innovation and Research
CSC	: The Compound Semiconductor Centre
AFM	: Atomic Force Microscope
BFP	: Back Focal Plane
NA	: Numerical Aperture
MOCVD	: Metal-Organic Chemical Vapor Deposition
HEMT	: High Electron Mobility Transistor
PSMA	: Phase-modulated ellipsometry
SiO₂	: Silicon Dioxide



SYMBOLS

ρ	: Complex reflectance ratio
Ψ	: Amplitude ratio
Δ	: Phase difference ratio
r_s	: Reflection coefficient for s-polarized light
r_p	: Reflection coefficient for p-polarized light
$\vec{E}$	: Electric field vector
$\vec{B}$	: Magnetic field vector
μ	: Magnetic permeability
c	: Speed of light
ε	: Dielectric constant
v	: The propagation speed of an electromagnetic wave in a medium
$\vec{r}$	: Location vector
t	: Time
$\tilde{n}$	: Complex refractive index
λ	: Wavelength
ω	: Angular frequency
$\vec{E}_0$	: Electric field amplitude
θ_g	: Angle of incident light with the surface
θ_y	: Angle of refracted light with the surface
δ_s	: s-Polarized phase shift
δ_p	: p-Polarized phase shift
d	: Thickness of the compensator
J	: Jones vector
I_0	: Initial light intensity
S_0, S_1, S_2, S_3	: Stokes parameters
I_a, I_b	: Light intensities in different analyzer directions
$I_{\pi/4}, I_{-\pi/4}$	: Light intensities in $\pi/4$ and $-\pi/4$ direction
I_R, I_L	: Right hand and left hand circular polarized light intensity



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DEVELOPMENT AND APPLICATION OF IMAGING ELLIPSOMETRY FOR OPTICAL CHARACTERIZATION AND DEFECT ANALYSIS OF ADVANCED THIN FILMS

SUMMARY

This study is based on research conducted under the title of " Development and Application of Imaging Ellipsometry for Optical Characterization and Defect Analysis of Advanced Thin Films ". The research covers substrate materials such as GaN and SiC, which are critical in power electronics within the scope of the PowerElec project, and varied materials in the ATMOC project. The main purpose of the study is to perform both defect analysis and determination of optical constants of these materials and to contribute to these processes with measurements in the visible and infrared (IR) bands.

Classical ellipsometry methods have various limitations, especially in terms of defect analysis. The disadvantages of these systems, such as low spatial resolution, narrow angular measurement range and complex sample preparation, have led to significant deficiencies in studies conducted in this field in literature. Against this background, instead of assuming that Imaging Ellipsometry implies a totally new principle, the current thesis puts its essential ideas to work to correct particular inadequacies found in traditional ellipsometry. Though traditional ellipsometry has already served, at one time or other, as a highly effective and precise technique for measuring optical constants and thin-film thicknesses, it necessarily supplies a macroscopic average of reflected light, consequently restricting its usefulness in surface investigation when lateral inhomogeneities or microscale structure attributes are concerned. To overcome this limitation, Imaging Ellipsometry has proven to be a highly effective auxiliary technique, allowing for spatially resolved surface and thin-film characterization. Here, unlike in usual dual-arm imaging ellipsometry systems, a small but easy-to-operate imaging ellipsometry instrument has been conceived and put in place. This tool unites optical microscopy principles and ellipsometric measurement, seeking to improve usability while, at the same time, maintaining high spatial resolution and clear imagery. Accordingly, it holds much potential for microscale surface defects analysis, besides surface and bulk substance characterization. The system consists of optical components such as a single wavelength tunable laser source (633 nm, 612 nm, 604 nm, 594 nm and 543 nm), and other light sources, motorized compensator and analyzer units, high NA (0.75) Nikon Plan Fluorite objective, a beam splitter on the light path and a Retiga-R6 CCD camera.

The data of the optical system is processed with a high-performance analysis infrastructure. In this context, CUDA-based software was developed to increase the parallel processing capacity and obtain faster analysis results. In the software development process, C++ programming language was used to optimize both system control and data analysis processes. This choice provided a performance-oriented and efficient infrastructure.

Empirical analysis has proven that the Imaging Ellipsometer system can be optimally applied for defect analysis and for determining optical constants for materials like GaN, SiC, and others. Moreover, this system has proven to offer higher accuracy and resolution compared to conventional ellipsometry methods described in published work elsewhere.

The study provides significant contributions in areas like material science and power electronics in terms of creating an innovative Imaging Ellipsometer. This research presents itself as a relevant resource for researchers, teachers, and professionals who encourage a wide-ranging use of technology in processes that evaluate material quality.



GELİŞMİŞ İNCE FİLMLERİN OPTİK KARAKTERİZASYONU VE KUSUR ANALİZİ İÇİN GÖRÜNTÜLEME ELİPSOMETRİSİNİN GELİŞTİRİLMESİ VE UYGULANMASI

ÖZET

Bu çalışma, "Gelişmiş İnce Filmlerin Optik Karakterizasyonu ve Kusur Analizi için Görüntüleme Elipsometresinin Geliştirilmesi ve Uygulanması" başlığı altında yürütülen disiplinler arası bir araştırma faaliyetinin sonuçlarını içermektedir. Bu kapsamda, malzeme bilimi, optik metroloji, yazılım mühendisliği ve güç elektroniği alanlarını bir araya getiren bütüncül bir yaklaşım benimsenmiştir. Çalışma, Avrupa Birliği tarafından desteklenen PowerElec ve ATMOC projeleri çerçevesinde gerçekleştirilmiş olup, özellikle güç elektroniğinde sıkça karşılaşılan SiC (Silisyum Karbür) ve GaN (Galyum Nitrür) gibi ileri teknoloji alt tabaka malzemelerinin karakterizasyonuna odaklanmaktadır. Aynı zamanda, ATMOC projesi kapsamında optik metroloji alanında değerlendirilen farklı malzemeler de çalışmanın odağına alınmıştır.

Bu tez çalışmasının temel amacı, hedeflenen malzemelerin yüzey kalitesi, kusur yoğunluğu ve optik sabitleri gibi kritik parametrelerinin hem görünür hem de kızılötesi (IR) bantlarda yüksek doğrulukla belirlenmesini sağlamaktır. Bu amaç doğrultusunda, özellikle yarı iletken, dielektrik ve metalik tabakalar gibi geniş bir malzeme yelpazesi üzerinde gerçekleştirilmesi gereken analizlerin hassasiyetini ve güvenilirliğini artırmak hedeflenmiştir. Bu bağlamda, mevcut literatürde sıklıkla karşılaşılan yöntemsel sınırlamaların üstesinden gelinmesi önemli bir motivasyon kaynağı olmuştur.

Geleneksel elipsometre teknikleri, özellikle geniş yüzey alanlarına sahip, heterojen yapılar barındıran ya da yüzey kusurları içeren malzemelerin analizinde yetersiz kalmaktadır. Bu yöntemlerde kullanılan optik sistemlerin sınırlı mekânsal çözünürlüğü, küçük ölçekli kusurların tespiti açısından ciddi bir dezavantaj oluşturmaktadır. Ayrıca, dar açısal ölçüm aralığı nedeniyle özellikle çok katmanlı yapılar veya kompleks optik davranış sergileyen malzemeler için yeterli veri elde edilememekte, bu da modelleme ve veriyle en iyi uyumun sağlanması süreçlerinde çeşitli belirsizlikler ortaya çıkmaktadır.

Bunun yanı sıra, klasik sistemlerin numune hazırlık süreçleri genellikle zaman alıcı ve kullanıcıya bağımlıdır. Örneğin, bazı sistemlerde ölçüm yapılabilmesi için malzeme yüzeyinin yüksek derecede pürüzsüz olması ya da belirli bir konfigürasyonda kesilmiş olması gerekmektedir. Bu tür sınırlamalar, hızlı ve tekrarlanabilir ölçümler yapılmasını zorlaştırmakta ve üretim sürecine entegre optik metroloji sistemlerinin geliştirilmesini engellemektedir. Özellikle endüstriyel uygulamalarda, yüksek hacimli üretim süreçlerinde hızlı ve güvenilir kalite kontrol sistemlerine ihtiyaç duyulurken, mevcut elipsometre sistemlerinin bu ihtiyaca cevap vermekte zorlandığı görülmektedir.

Bu nedenlerle, çalışmada geliştirilen Görüntüleme Elipsometresi sistemi, yalnızca bu sınırlamaları ortadan kaldırmakla kalmayıp aynı zamanda daha yüksek çözünürlük, geniş açısal aralık ve kullanıcı dostu bir ölçüm deneyimi sunacak şekilde tasarlanmıştır. Böylece hem akademik araştırmalarda hem de endüstriyel uygulamalarda kullanılabilecek esnek ve güçlü bir karakterizasyon aracı oluşturulması hedeflenmiştir.

Bu ihtiyaçlar doğrultusunda, tez kapsamında yenilikçi bir Görüntüleme Elipsometresi sistemi tasarlanmış ve deneysel olarak uygulanmıştır. Geliştirilen sistem, klasik elipsometrelerin sınırlamalarını aşmak amacıyla özel olarak yapılandırılmıştır. Sistem, kullanıcıya yüksek mekânsal çözünürlükte ve geniş spektral aralıkta ölçüm yapabilme imkânı tanımaktadır. Optik yapı, çeşitli dalga boylarında çalışan tek modlu ayarlanabilir lazer kaynakları (633 nm, 612 nm, 604 nm, 594 nm ve 543 nm), hassas hareket kabiliyetine sahip motorize kompensatör ve analizör birimleri, yüksek sayısal açıklığa sahip (NA = 0.75) Nikon Plan Florit objektif, ışığın yönlendirilmesi için kullanılan bir ışın bölücü ve yüksek çözünürlüklü Retiga-R6 CCD kamera gibi gelişmiş optik bileşenlerden oluşmaktadır.

Bu optik donanım, yazılım altyapısıyla entegre bir şekilde çalışacak şekilde tasarlanmıştır. Ölçüm sisteminin kontrolü ve elde edilen verilerin işlenmesi amacıyla yüksek performanslı bir yazılım platformu geliştirilmiştir. Özellikle yüksek çözünürlüklü verilerin hızlı ve verimli şekilde işlenmesi amacıyla, CUDA tabanlı paralel işlem algoritmaları kullanılmıştır. Bu sayede, geleneksel tek iş parçacıklı analiz süreçlerine kıyasla daha kısa sürede daha yüksek doğrulukta sonuçlar elde edilmiştir. Yazılım geliştirme sürecinde tercih edilen C++ programlama dili, sistem performansını artırmak ve donanımla doğrudan uyum sağlamak amacıyla seçilmiştir. Bu yazılım sayesinde hem sistem kontrolü hem de veri analizi süreçleri etkin bir şekilde yönetilebilmektedir.

Gerçekleştirilen deneysel çalışmalar, sistemin farklı örnekler üzerinde etkinliğini ortaya koymuştur. GaN ve SiC gibi endüstride kritik öneme sahip malzemeler üzerinde yapılan kusur analizleri, yüzey morfolojisinin yüksek çözünürlükte ortaya konmasını sağlamıştır. Ayrıca, geliştirilen sistemle elde edilen Ψ ve Δ spektrumları, geleneksel elipsometrelerle karşılaştırıldığında daha stabil ve yüksek hassasiyetli olarak ölçülmüştür. Optik sabitlerin (kırılma indisi ve sönüm katsayısı) belirlenmesinde kullanılan modelleme ve fit etme süreçleri, sistemin hem doğruluğunu hem de tekrarlanabilirliğini kanıtlamıştır. Ölçüm sonuçlarının, literatürdeki ileri düzey elipsometre sistemleriyle karşılaştırıldığında, benzer veya daha yüksek performans gösterdiği görülmüştür.

Bu tez çalışması, yalnızca teknik bir yenilik sunmakla kalmayıp, aynı zamanda ileri düzey malzeme karakterizasyonu için potansiyel uygulama alanlarını da genişletmektedir. Özellikle güç elektroniği, yarı iletken üretimi, fotonik cihaz geliştirme ve hassas metroloji gibi alanlarda kullanılabilecek bir ölçüm sistemi sunmaktadır. Ayrıca, geliştirilen Görüntüleme Elipsometresi sistemi, üniversitelerde araştırma-geliştirme süreçlerinde veya endüstriyel kalite kontrol uygulamalarında rahatlıkla adapte edilebilecek bir yapıya sahiptir. Bu yönüyle, akademik dünyada hem lisansüstü araştırmalar hem de sanayi uygulamaları için referans bir platform niteliği taşımaktadır.

Sonuç olarak, bu çalışma, Görüntüleme Elipsometresi alanında literatüre önemli bir katkı sunarken, aynı zamanda geliştirilen sistemin gelecekteki versiyonları için de bir temel oluşturmaktadır. Yapılabilecek olası geliştirmeler arasında çoklu açılı ölçüm

imkânı, otomatik odaklama sistemleri, daha geniş spektral aralıkta çalışan kaynakların entegrasyonu ve yapay zekâ destekli analiz yazılımlarının geliştirilmesi yer almaktadır. Bu kapsamda, tez çalışması yalnızca mevcut gereksinimlere yanıt vermekle kalmamış, aynı zamanda ileriye dönük yeni araştırma alanlarına da kapı aralamıştır.





1. INTRODUCTION

Scientific improvements were often made possible via the development of a new measurement technique in general. Scientific facts are called experimental knowledge unless they are supported with scientific evidence. In other words, scientific improvements in fields were often made via various measurements to prove scientific evidence. Many characterization techniques have been developed in the last 50 years and progress in a scientific field largely depended upon development of measurement techniques. STM is one example of development of measurement techniques that revolutionized surface science and contributed much to the fast pace at which scientific field has grown [1]. On the other hand, even though the fundamentals of ellipsometry were developed more than a century ago, ellipsometry was thought of as an "secondary tool" until recently. Situation completely reversed in the mid-1990s since fast advance in computer technology enabled automation in ellipsometry instruments and data analysis [2].

Ellipsometry became one of the widely used techniques spanning from semiconductors to organic material research areas since the commercialization of spectroscopic ellipsometry instruments in the mid-1990s. Recent advances in spectroscopic ellipsometry have allowed the possibility of real-time characterization during film growth and assessing optical anisotropy. In this respect, spectroscopic ellipsometry is actually among the very few precise optical characterization techniques, and as such, its application is becoming quite common even at university and industrial levels.

Ellipsometry as an optical diagnostics method has been used for a long time starting from Null-ellipsometers not requiring complex electronics. With the increasing computing speeds and fast detectors, popularity of the Ellipsometry for both ex-situ and in-situ analysis of materials is rising constantly. Although the principles of ellipsometry seems trivial, application of the technique and development of such systems are quite complicated. The method uses polarized light as optical probing, and its measurand (ψ , Δ) as ellipsometric quantities may not mean much to people

who are not familiar with the method itself. Data analysis procedures in ellipsometry are different from those used in other optical measurement techniques. Thus, it is the purpose of this thesis to present the basic principles of spectroscopic ellipsometry to those researchers who are familiar with optical techniques but who has not involved in ellipsometric measurement and analysis yet.

Although certain points may be complicated, the principles of ellipsometry are never difficult if one learns about it systematically. From this purpose, general explanations concerning measurements and data analysis procedures executed in spectroscopic ellipsometry are given. Several figures are provided to help readers better understand the content. In this text, complex and long formulas concerning electromagnetism and quantum mechanics were avoided for simplicity, whilst key formula derivations performed in spectroscopic ellipsometry are shown.

In this theses an innovative and an alternative approach for imaging ellipsometry technique has been investigated with particular focus on determination of surface defects.

1.1 General Objectives of the Research

The primary objective of this research is to investigate spectroscopic ellipsometry as a metrology tool from both optical and dimensional nanometrology aspect through gaining deep understanding of the physics and technology behind it. This objective is used in studying the principles of the technique by using such commercial devices as well as developing bench measurement systems where new aspects needed to be investigated. These studies led me to work on new imaging system to answer limitations of defect detection using classical measurement systems.

In accordance with the above background, the specific focus of the research would relate to:

- Improvement of the analysis of defects in terms of exact defect detection and characterization at the surface and interface of SiC materials.
- Advancing measurement precision: application of high-resolution and extremely sensitive imaging ellipsometry technique in material characterization.

- Contributing to Material Sciences: providing a tool reliably for the quality assessment of SiC both industrially and scientifically.
- Integration of Advanced Optical Techniques: application of the concept of imaging ellipsometry to overcome particular shortcomings in traditional ellipsometry techniques.
- Experimental methodology development: extending a holistic structure regarding the implementation and testing of a proposed ellipsometry system.

Given this, the current study will help further develop optical characterization techniques with practical solutions for certain challenges in defect analysis within materials science.

1.2 Importance and Justification of the Study

Silicon Carbide is a very important material used in advanced technology applications because of its unique mechanical, thermal, and electronic properties [3]. Silicon Carbide finds its application in various high-performance industries, namely, semiconductors, power electronics, and aerospace. Ensuring quality and reliability of SiC materials demands accurate and in-depth defect analysis since very small defects may have significant effects on performance and lifetime.

The traditional characterization techniques, while helpful in many aspects, suffer from serious limitations in the detection and appropriate analysis of complex surface and interface SiC material defects. These drawbacks, therefore, signal the urgent need to develop advanced measurement techniques offering high resolution, non-destructive, and precise evaluation.

Imaging ellipsometry is, therefore, one of the solutions by bridging the gap between conventional ellipsometry and high-resolution imaging. It allows detailed analysis of material surfaces, offering insight into heterogeneities, thickness variations, and optical anisotropy that are not easily measured using traditional methods.

The rationale behind this research work is based on the following reasons:

- Improve Characterization Techniques: Address the limitations of existing methods by developing a robust imaging ellipsometry system tailored for SiC defect analysis.

- Support for industrial and scientific applications, which will provide a stable tool for quality control during industrial production and basic investigations of the properties of materials.
- Imaging ellipsometry becoming a promising tool for defect metrology on surfaces and interfaces of thin films.
- To contribute to the understanding of advanced material technology, the research will enable detailed investigation of the structural and optical properties of SiC and other advanced materials.

By addressing these needs, the study not only advances the field of optical characterization but also supports broader technological developments reliant on high-quality SiC materials [4].

1.3 Structure and Objectives of the Thesis

The construction of this thesis has been done in such a way that the development, implementation, and testing of the ellipsometric imaging system will be addressed for defect analysis in the materials such as SiC for a comprehensive basis in principles, methodologies, and applications concerning the innovative optical characterization technique.

This thesis systematically approaches the development, implementation, and evaluation of an imaging ellipsometry system with the aim of defect analysis in SiC materials. It, therefore, gives a wide framework for understanding the principles, methodologies, and applications involved in this innovative optical characterization technique. The structure of the thesis begins with an introductory chapter that presents the motivation, objectives, and significance of the study, along with a general overview of the ellipsometry technique. Further, it discusses the principles of ellipsometry wherein the physical and mathematical backgrounds have been discussed in some detail. In addition, it reviews ellipsometry system configurations and technologies, giving a signal on the advantages and shortcomings of each configuration. Next follows the development of a rotating compensator ellipsometry system, its construction, experimental setup, data acquisition, and interpretation. Further, it shows the limitations of traditional spectroscopic ellipsometry systems in defect analysis, indicating the utility of imaging ellipsometry to overcome these limitations. The last

few sections give a summary of the results, performance evaluation of the system, and further work that may be carried out.

The main objectives of the thesis are the elaboration of a new imaging ellipsometry system with superior performance in detecting and analyzing defects in SiC material, enriching optical characterization methods concerning the improvement of measurement precision and resolution, and experimental tests confirming the performance of the developed system in such respects as reliability and effectiveness. In this work, it will be possible to further develop material science, contributing to knowledge about the optical and structural properties of SiC. Further, this will lay a foundation for further research in imaging ellipsometry and its application within material characterization. With this logical flow, the thesis would contribute to a worthy contribution within optical metrology and material science.

2. ELLIPSOMETRY AND BASIC PRINCIPLES

2.1 Ellipsometry: Principles, Measured Parameters and Application Limits

Ellipsometry has evolved a great deal from the late 19th century [5], especially during the last few decades, with the development of computers and automation. Such leaps in technology have converted ellipsometry into a prerequisite technique to be used in various fields such as semiconductors, opto-electronics, photovoltaics, chemistry, and metallurgy [6].

It works by sending polarized light onto the surface of a material and determining how the polarization state changes upon its reflection or transmission. Changes are then studied with the use of mathematical models to extract thorough optical and structural information from the material. The polarized nature of light is what makes ellipsometry particularly sensitive to the subtlety of change in properties of either a surface or a film.

The main strengths of ellipsometry are speed, precision, non-invasiveness, and wide applicability. It can be of particular use in assessing semiconductor quality, optimizing the manufacturing process, efficiency in photovoltaic cells, studies concerning chemical material surface properties, and investigations into metallurgical surfaces.

By following this logical advancement, the thesis will make a meaningful methodological contribution to optical metrology and materials science.

2.1.1 What Do We Measure?

Ellipsometry measures the change in the polarization state of a light beam caused by reflection at, or transmission through, the sample surface. The quantities measured are called ellipsometric angles: Ψ and Δ . Those are related to the ratio of complex Fresnel reflection coefficients, r_s and r_p , respectively. Herein, r_s denotes the reflection coefficient for light polarized perpendicular to the plane of incidence and r_p represents the coefficient for light polarized parallel to the plane of incidence. The dependence

of the ellipsometric angles from r_s and r_p is expressed via the basic ellipsometric equation.

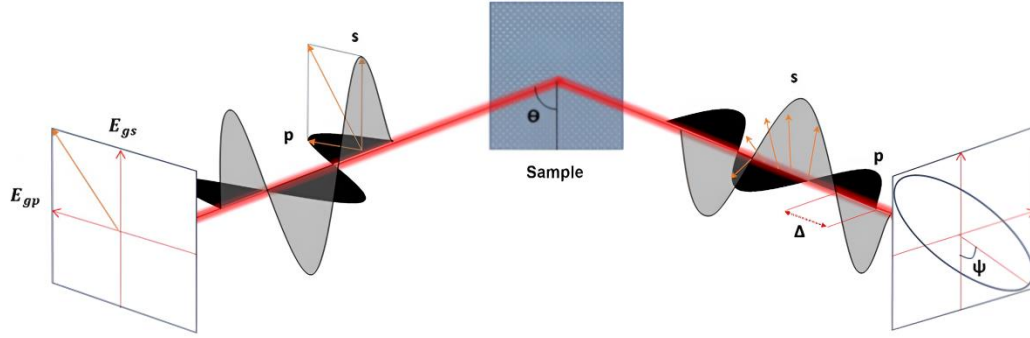


Figure 2.1 : Ellipsometry measurement principle demonstration

$$\rho = \frac{r_p}{r_s} = \tan \Psi e^{i\Delta} = \frac{\left(\frac{E_{rp}}{E_{gp}}\right)}{\left(\frac{E_{rs}}{E_{gs}}\right)} \quad (2.1)$$

Utilizing measured parameters Ψ and Δ , besides adequate modeling, the optical and structural properties of the samples can be precisely determined. Among such sample characteristics are the following:

- Optical constants in the near-UV, visible, and near-infrared wavelength ranges
- Thickness of single or multiple layers
- Thickness of layers within superconducting structures
- Surface and interface roughness
- Anisotropy
- Gradients in optical constants within single layers

Ellipsometry is a very sensitive and precise metrology technique because, besides the measurement of light intensity, the phase shift caused by the change in polarization state is gauged. Indeed, this distinctive capability of the technique allows great detail in material property characterization within a wide range of applications.

2.1.2 Major Limiting Factors in Ellipsometry

A major limitation intrinsic to ellipsometry relates to the quality of the surface of the sample. Owing to the fact that ellipsometry eliminates all scattering phenomena and is focused solely on specular reflection, it is crucial that surface roughness and interfacial roughness between two media be less than that of the incident wavelength. Not satisfying this requirement gives way to light scattering, which in turn causes the depolarization of the reflected beam. In addition, if the thickness of the film shows a small variation in the region around the light spot, then it is impossible to fulfill the requirement for nominally flat interfaces. Finally, achieving maximum smoothness of the surface is an essential requirement, making surface treatment an unavoidable process that should never be neglected.

Based on the postulated hypothesis for an ideal optical surface, the lower limit for measurement accuracy in minimum film thickness is dictated by the measurement device's sensitivity, subsequently enabling sub-monolayer increments in assessment. The maximum observable film thickness for films is usually bounded either by spectral resolution or wavelength range of the instrument available [7]. Typically films of thicknesses up to several tens of micrometers can be measured precisely.

2.2 Electromagnetic Waves According to Maxwell's Equations

The general definition of an electromagnetic wave is that it's a transverse wave. It has an electric field vector and a magnetic field vector whose magnitudes vary with both position and time. Vectors are always perpendicular to each other and to the direction of propagation, too.

The electric field vector is the most important quantity characterizing the wave nature of light. On the other hand, a magnetic field vector is usually neglected as the magnetization induced in materials can't follow these fast optical oscillations due to the rather slow dynamics of magnetic moments of both electrons and nuclei.

Maxwell's equations describe the behaviors of the electromagnetic fields, showing the overall view of how the fields propagate and interact with materials [8]. For an infinite medium with no sources, these can be written in differential form as,

$$\vec{\nabla} \cdot \vec{E} = 0 \quad (2.2)$$

$$\vec{\nabla} \cdot \vec{B} = 0 \quad (2.3)$$

$$\vec{\nabla} \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0 \quad (2.4)$$

$$\vec{\nabla} \times \vec{B} - \frac{\mu\epsilon}{c} \frac{\partial \vec{E}}{\partial t} = 0 \quad (2.5)$$

Here, $\vec{E}$ and $\vec{B}$ represent the electric and magnetic fields, c denotes the speed of light, μ represents permeability, and ϵ refers to the dielectric function.

The integration of these equations results in the formulation of the electric field wave equation as follows:

$$\vec{\nabla}^2 \vec{E} - \frac{1}{v^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad (2.6)$$

The phase velocity v of the electromagnetic wave in the medium is given by:

$$v = \frac{c}{\sqrt{\mu\epsilon}} \quad (2.7)$$

A general solution to this wave equation is a monochromatic plane wave propagating in a given direction. The electric field of such a wave can be written as:

$$\vec{E}(\vec{r}, t) = \vec{E}_0 \exp[i(\vec{k} \cdot \vec{r} - \omega t)] \quad (2.8)$$

In this equation: $\vec{r}$ represents the position vector in the direction of propagation, t denotes time, and ω is the angular frequency of the wave. The vector $\vec{E}_0$ is a complex amplitude that defines both the magnitude and the polarization state of the electric field. The wave vector $\vec{k}$ describes the direction of propagation and spatial frequency of the wave and is defined as $\vec{k} = \frac{2\pi}{\lambda} \cdot \tilde{n} \vec{q}$, where λ is the wavelength in vacuum, $\tilde{n}$ is the complex refractive index of the medium, and $\vec{q}$ is the unit vector in the propagation

direction. In the special case where the wave propagates along the z-axis, the equation simplifies to,

$$\vec{E}(z, t) = \vec{E}_0 \exp[i(k_z z - \omega t)] \quad (2.9)$$

with, $k_z = \frac{2\pi}{\lambda} \tilde{n}$ representing the component of the wave vector along the z-direction. This formulation is commonly used to describe plane electromagnetic waves in layered media and is particularly useful in optical modeling and ellipsometry.

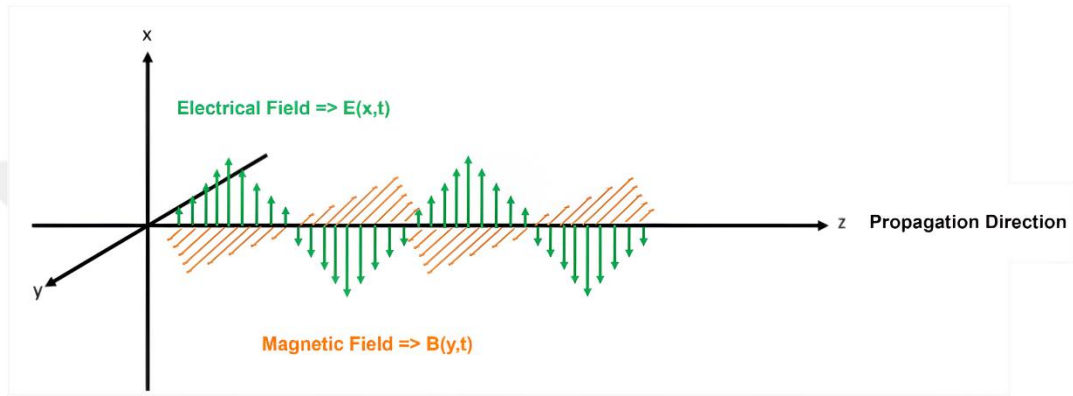


Figure 2.2 : Linearly polarized plane wave propagating along the z-axis

2.3 Fundamental Optical Concepts

2.3.1 Optical Behaviour of Materials

Actually, optical behavior refers to the very basic principle by which light interacts with the material. This includes how a material affects incident light that goes through the processes of reflection, refraction, and absorption while passing through it. These three different ways of interaction define the optical behavior of the material. Knowledge about such behavior is crucial in a wide range of applications, including materials science, semiconductor technology, optoelectronic devices, and optical design.

Understanding these basic principles of optical behavior forms the basis for appreciating how a material interacts with light and determining its optical properties. The succeeding discussion now considers the basic principles of optical behavior, the factors that determine the optical properties of a material, and some basic terms involved in the analysis of light-matter interaction. Such an understanding will provide

the basic framework for material characterization by ellipsometric measurements and other optical analysis methods.

2.3.1.1 Reflection and Refraction of Light

The law of reflection is a fundamental concept that describes light's behavior when it rebounds off a given surface. The law creates an essential relationship defining the geometric arrangement relevant to reflection as a phenomenon. Under the principle of reflection, the angle of reflection (θ_y) is assumed to relate in direct manner to the angle of incidence (θ_g).

$$\theta_y = \theta_g \quad (2.10)$$

The mathematical formalism explains the phenomenon of reflection that occurs when light impinges upon a surface. The Fresnel equations and corresponding theories offer further insight into the use of the concept in more complex systems. The law of reflection is a basic principle needed for understanding light behavior while being reflected from a material surface, enabling optical measurement and material property characterization.

This principle forms the basis for several measurement and characterization optical methods, including ellipsometry. The principle that describes bending as light moves from one medium into another is referred to as the law of refraction. Often called Snell's Law or the Snell-Descartes Law [9], this law stipulates that the change in direction, which occurs when light moves from one medium into another, is dependent upon the difference in their respective indices of refraction and the angle of incidence. This can be expressed mathematically as:

$$\tilde{n}_0 \sin \theta_g = \tilde{n}_1 \sin \theta_y \quad (2.11)$$

In this equation, $\tilde{n}_0$ and $\tilde{n}_1$, represent the refractive indices of the first and second media, respectively, while θ_g denotes the angle of incidence of the incoming light, and θ_y represents the angle of refraction of the transmitted light. Both principles form the foundation of optical characterization, playing a critical role in material analysis and measurements.

2.3.2 Polarization

Polarization refers to the time-dependent behavior of the electric field vector observed at a fixed point in space.

2.3.2.1 Linearly Polarized Light

Linearly polarized light has an electric vector that always remains transverse in nature and varies in magnitude and polarity with time, and this aspect is referred to as linearly polarized light [10]. The transverse direction can be along the x-direction, the y-direction, or any direction perpendicular to the direction of propagation (z). More generally, any case of linearly polarized light may be considered as a mixture of x-polarized and y-polarized light. Though these may differ in magnitude, their phases are equal.

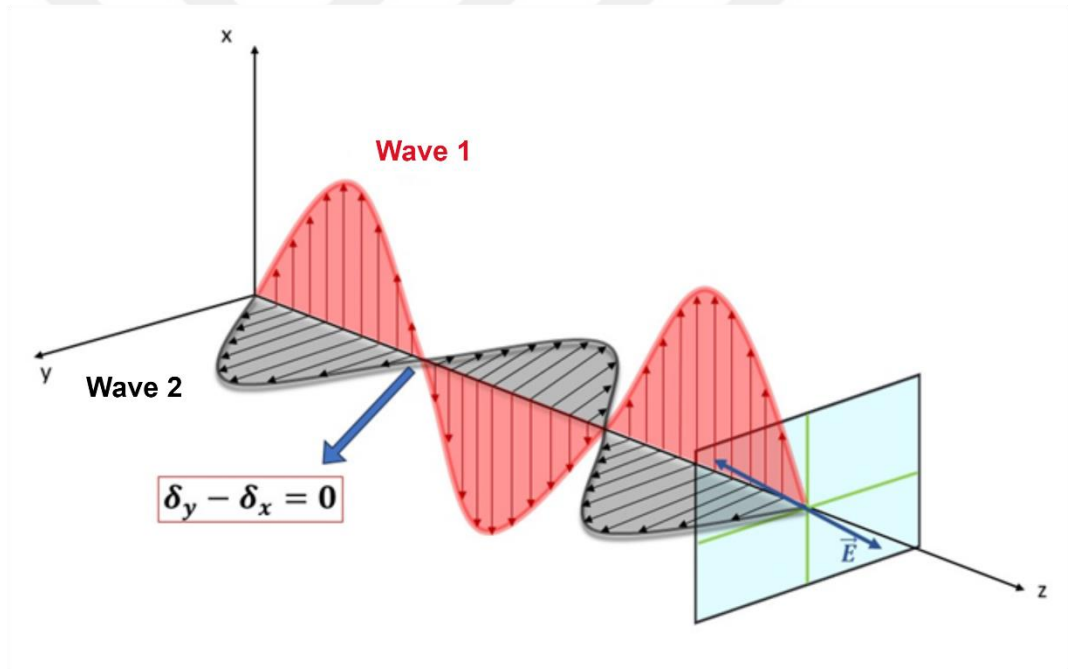


Figure 2.3 : Linear polarization vector space representation

2.3.2.2 Circularly Polarized Light

If the two perpendicular components of a light wave have equal amplitudes with a phase difference between them, then light undergoes circular polarization when its two perpendicular components have equal amplitudes and a phase difference of $\pi/2$ [11].

Right-handed circular polarization takes place when, looking in the direction of wave propagation, the electric field vector seems to rotate clockwise. This occurs for a phase difference of $-\pi/2 + 2m\pi$, where $m = 0, \pm 1, \pm 2, \dots$

A phase difference of $+\pi/2 + 2m\pi$ corresponds to left-handed polarization whereby the electric field vector will rotate counterclockwise for the same conditions of observation.

The rotation imposed on the electric field vector determines the handedness of the circular polarization of the light.

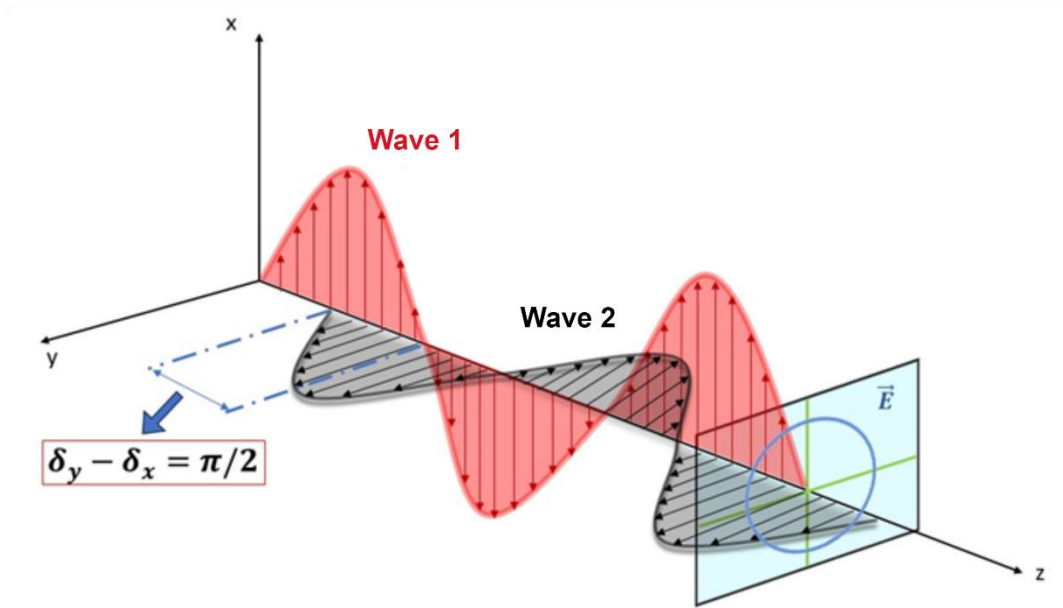


Figure 2.4 : Circular polarization vector space representation

2.3.2.3 Elliptically Polarized Light

In general, if a light wave consists of two components with different amplitudes and a varying phase difference, the result is elliptically polarized light. The tip of the electric field vector traces an ellipse in the x-y plane. To describe the state of polarization, the components along the x- and y-axes are typically used. However, in a broader sense, any two orthogonal polarization states can be employed to explain the polarization of light. For instance, two oppositely polarized circular waves can also be used.

Elliptically polarized light can be generated, for example, when linearly polarized light reflects off a surface. As a result, in ellipsometry, linearly polarized incoming light often transforms into elliptically polarized light upon reflection, which is then observed by the detector.

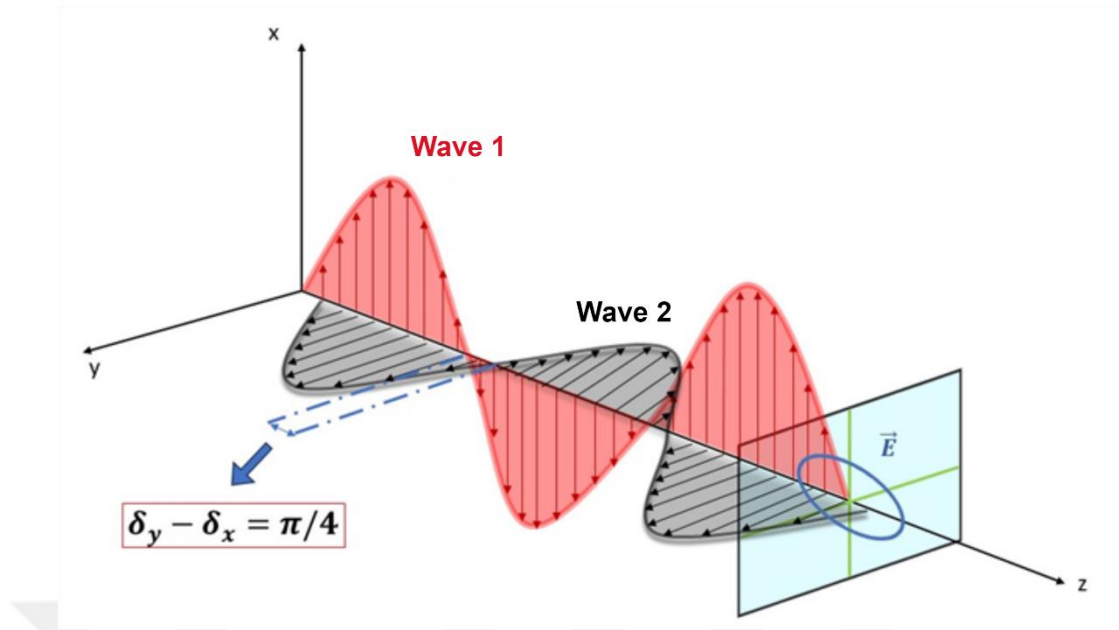


Figure 2.5 : Elliptical polarization vector space representation

2.3.2.4 Partially Polarized Light

Directions of electric fields of photons emitted from a light source are in all possible directions so that the characteristic of light is called unpolarized. Most often, electric field is neither totally random nor completely organized and thus called partially polarized light.

This partial polarization can be quantified by the so-called degree of polarization, which essentially quantifies the amount of the light that has the same polarization state. This arises when the electric field has fluctuations in one direction in an irregular manner, thus forming a mixture of polarized and non-polarized components.

2.3.3 s- and p- Polarized Light and Fresnel Equations

Figure 2.6 indicates that to see how s- and p-polarized light waves reflect from a surface, we must examine how they travel in relation to the plane upon which they strike. These oscillation directions are critical for interpreting the reflection and refraction phenomena governed by the Fresnel equations.

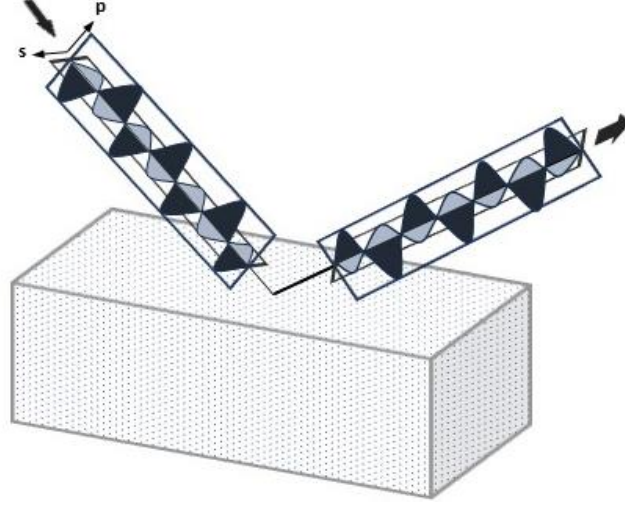


Figure 2.6 : Reflection of p and s polarized light waves

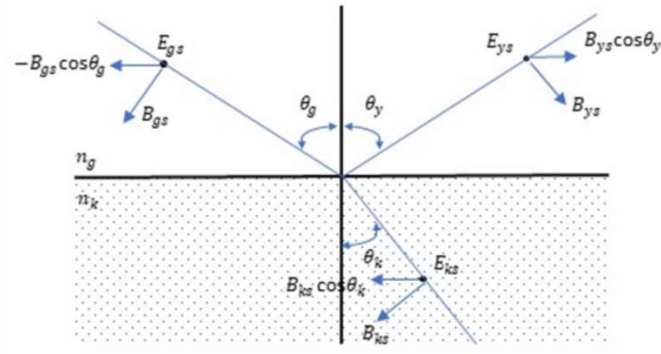
Light incident at an angle upon a sample splits into two polarization types known as p- and s-polarized waves. This varies according to the direction in which the electric field travels, with each type having a different behavior [12]. In p-polarization, the electric fields of the incident and reflected light remain in one plane, called the plane of incidence.

In this context, Fresnel equations for s- and p-polarized light are used to describe the reflection and transmission properties of light in these two polarization states.

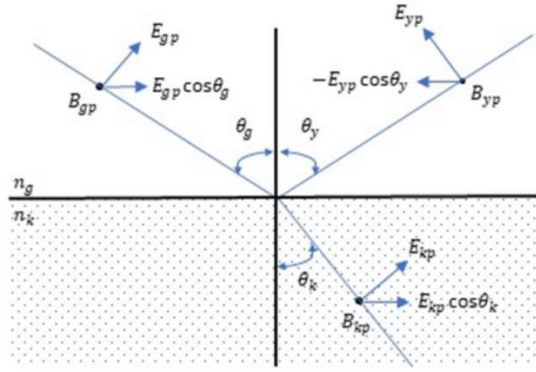
We can also consider how p-polarized and s-polarized waves reflect and transmit, depicted in Figure 2.7, by applying equations 2.12, 2.13, and by means of the following Fresnel equations.

$$r_{p,s} = \frac{E_{yp,ys}}{E_{gp,gs}} = \frac{n_{k,g} \cos \theta_g - n_{g,k} \cos \theta_k}{n_{k,g} \cos \theta_g + n_{g,k} \cos \theta_k} \quad (2.12)$$

$$t_{p,s} = \frac{E_{kp,ks}}{E_{gp,gs}} = \frac{2n_g \cos \theta_g}{n_{k,g} \cos \theta_g + n_{g,k} \cos \theta_k} \quad (2.13)$$



(a) s - polarization



(b) p - polarization

Figure 2.7 : Electric field and magnetic induction vector representation for (a) p-polarization and (b) s-polarization [2]

$$r_p = \frac{E_{yp}}{E_{gp}} = |r_p| \exp(i\delta_p) \quad (2.14)$$

$$r_s = \frac{E_{ys}}{E_{gs}} = |r_s| \exp(i\delta_s) \quad (2.15)$$

$$\rho = \frac{r_p}{r_s} = \tan \Psi e^{i\Delta} \quad (2.16)$$

$$\frac{|r_p|}{|r_s|} = \tan \Psi e^{i\Delta} \quad (2.17)$$

$$\Delta = \delta_p - \delta_s \quad (2.18)$$

These equations describe the reflection and transmission behavior of light within the plane of incidence, linking these characteristics to the properties of the material. Consequently, studying the interaction between p- and s-polarized light wavelengths and the material surface is a critical focus in the fields of optical characterization and materials science.

2.4 Optical Components Used in Ellipsometry Systems

2.4.1 Polarizer (Analyzer)

Polarizer is an optical filter that will allow light polarized in a single direction to pass and will never allow light polarized in the orthogonal direction to pass [13]. Certain materials, like Polaroid, for instance, give transmission of light in one direction and not in the orthogonal direction. This is done in order to permit the electric field absorbs in one direction and not in the other direction, thereby managing the polarization of light.

Polarizers serve extremely important functions in most optical experiments and measurements for maintaining and creating a predetermined polarization state of light. Through their function of managing the polarization state of light in a precise way, polarizers have an extremely important role in precision optical arrangements and ellipsometric studies.

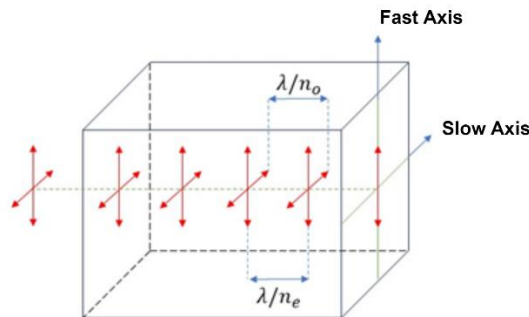


Figure 2.8 : Distribution of light wave in calcite crystal [2]

Polarizers are utilized in producing a polarized beam of light in ellipsometry measurements and in enabling analysis of measured signals. This enhances sensitivity and allows precise control in ellipsometric measurement of a material's optical properties. Polarizers allow for measurement under known polarization states, which allows the optical response of the material to be more fully characterized. Polarizers are thus essential optical hardware to study basic optical principles and to conduct detailed materials science studies for ellipsometry and other optics experiments.

2.4.2 Compensator

A compensator is usually placed either behind a polarizer or in front of an analyzer, and its major application is usually associated with converting linear polarization into circular polarization or vice versa. Figure 2.9 illustrates how light traverses a compensator. Particularly, this diagram illustrates how linear polarization at a 45° can be changed into circular polarization by using a compensator, which creates a phase shift and aligns the perpendicular components of the wave of light in a structure favorable to circular polarization. Light travelling along the fast axis here has a higher velocity than that travelling along the slow axis, leading to a phase difference causing a change in polarization state of the light [14]. Thus, the compensator introduces a phase difference between the electric field vectors E_x and E_y , which is essential in changing linear polarization into circular polarization by shifting the relative phases of these orthogonal components [15]. The phase difference such as:

$$\delta = 2\pi \cdot \frac{|n_e - n_o| \cdot d}{\lambda} \quad (2.19)$$

Here, d represents the thickness of the compensator. As can be seen from Equation (2.19), δ varies depending on λ . In Figure 2.9, the phase difference created by the compensator is $\delta = \pi/2$.

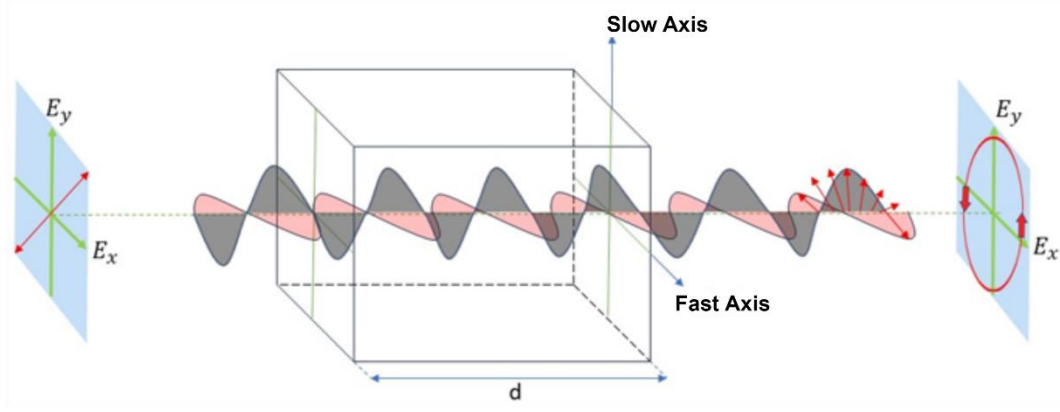


Figure 2.9 : Illustration of the distribution of the light wave in the compensator

In addition, when the retarder in Figure 2.9 is rotated in the x-y plane, phase control can be achieved by changing the phase difference. In this case, it is referred to as a rotating compensator. This configuration provides the opportunity for modulation in ellipsometry setups. Recently, such a rotating compensator has found extensive applications in spectroscopic ellipsometry.

2.5 Mathematical Framework of the Ellipsometry

The mathematical framework for ellipsometry is constructed to systematically solve an optical configuration with the aim of deducing sample optical and dimensional properties. Jones matrix and Mueller matrix methods are the primary mathematical tools describing the optical system configuration. This methods helps extracting sample information from the ellipsometric system and thus able to analyze data obtained to evaluate sample properties.

Ellipsometry is able to analyze the reflected light with various polarization states; therefore, it allows determination of material properties like thickness, dielectric constant, and surface structure by means of mathematical tools. Hence, the mathematical foundation of the ellipsometer allows analysis of the optical measurement data and extraction of material properties.

2.5.1 Jones Matrix and Vector

Jones matrix is a 2x2 matrix, as illustrated in Equation 2.20, that is utilized for explaining the propagation of the polarization state of light by an optical component. The two components (x and y) of the electric field vector are represented by this matrix and contain the amplitude and phase information of the polarization state of the light.

In addition, the Jones matrix representation of a few of the optical components is also given in Table 2.1.

$$J = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} \quad (2.20)$$

The Jones vector is a two-dimensional vector that represents the polarization state of light. This vector includes the two components (x and y) of the electric field vector and describes the amplitude and phase of the light's polarization state. Similarly, examples of various Jones vectors are presented in Table 2.1.

To calculate how the polarization state of light changes as it passes through an optical element using the Jones matrix, follow these steps:

- 1- Construct the Jones matrix for the optical element.
- 2- Form the Jones vector that represents the polarization state of the incident light.
- 3- Calculate the output polarization state by multiplying the Jones vector with the Jones matrix of the each optical element.

This process allows us to determine how the light's polarization state is altered by the optical element.

2.5.2 Stokes Parameters and Mueller Matrix

Stokes parameters are a group of four quantitative values describing the polarization state of an incident beam. These parameters give a complete account of polarization-related qualities. In theory, three different sets of real quantitative values can describe different polarization modes, e.g., partial polarization. Adding the total intensity, four particular measurable values are obtained. This leads to defining the Stokes vector, including Stokes parameters S_0, S_1, S_2, S_3 :

$$\vec{S} = \begin{bmatrix} S_0 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix} = \begin{bmatrix} I_0 \\ I_a - I_b \\ I_{\pi/4} - I_{-\pi/4} \\ I_R - I_L \end{bmatrix} \quad (2.21)$$

As seen in equation 2.21, I_0 represents the total light intensity, while I_a and I_b denote the intensities of light passing through a linear polarizer oriented at 0° and 90° ,

respectively. Similarly, $I_{\pi/4}$ and $I_{-\pi/4}$ correspond to the intensities of light passing through a linear polarizer oriented at 45° and -45° . Additionally, I_R and I_L represent the intensities of light passing through right circular and left circular polarizers, respectively. These parameters are used to measure the light intensity based on different polarization states [16]. Examples of Stokes vectors for specific polarization states are provided in Table 2.1.

An alternative approach to systematic formalism in polarization state transfer through a group of optical components is by use of a 4x4 Mueller matrix. This approach gives a full description of polarization state interactions with optical components in terms of polarization state modifications.

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} \\ M_{21} & M_{22} & M_{23} & M_{24} \\ M_{31} & M_{32} & M_{33} & M_{34} \\ M_{41} & M_{42} & M_{43} & M_{44} \end{bmatrix} \quad (2.22)$$

The Mueller matrices of some common optical elements are also given in Table 2.

Within ellipsometry, a choice concerning a matrix representation depends upon a particular system being explored as well as polarization modes to be measured. The use of the Jones matrix applies for more straightforward situations while Mueller's matrix applies more for complex and broad systems. In applied situations, accurate modeling and interpretation often require experimental conditions along with properties of the material being inspected. For purposes of this thesis, mathematical modeling will be carried out using Jones matrices.

Table 2.1: Representation of polarization states with Jones and Stokes vectors [2]

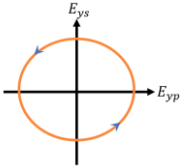
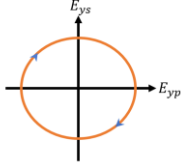
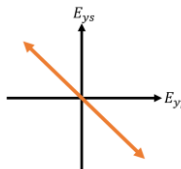
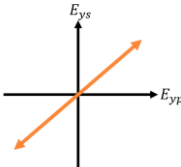
Polarization	Polarization State	Jones Vector	Stokes Vector
LCP		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix}$
RCP		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$
LP (-45°)		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}$
LP (45°)		$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$

Table 2.1 (Continue) : Representation of polarization states with Jones and Stokes vectors [2]

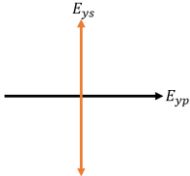
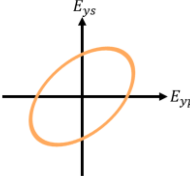
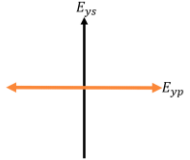
Polarization	Polarization State	Jones Vector	Stokes Vector
LP (parallel to the y-axis)		$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}$
EP		$\begin{bmatrix} \sin\psi \exp(i\Delta) \\ \cos\psi \end{bmatrix}$	$\begin{bmatrix} 1 \\ -\cos 2\psi \\ \sin 2\psi \cos \Delta \\ -\sin 2\psi \sin \Delta \end{bmatrix}$
UL	—	—	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$
LP (parallel to x-axis)		$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$

Table 2.2 : Representation of optical elements with Jones and Mueller matrix [2]

Optical Element	Jones Matrix	Mueller Matrix
Compensator (K)	$\begin{bmatrix} 1 & 0 \\ 0 & \exp(-i\delta) \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\delta & \sin\delta \\ 0 & 0 & -\sin\delta & \cos\delta \end{bmatrix}$
PM (P)	$\begin{bmatrix} 1 & 0 \\ 0 & \exp(i\delta) \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\delta & -\sin\delta \\ 0 & 0 & \sin\delta & \cos\delta \end{bmatrix}$
Coordinate Rotation (R)	$\begin{bmatrix} \cos a & \sin a \\ -\sin a & \cos a \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2a & \sin 2a & 0 \\ 0 & -\sin 2a & \cos 2a & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Sample (O)	$\begin{bmatrix} \sin\psi \exp(i\Delta) & 0 \\ 0 & \cos\psi \end{bmatrix}$	$\begin{bmatrix} 1 & -\cos 2\psi & 0 & 0 \\ -\cos 2\psi & 1 & 0 & 0 \\ 0 & 0 & \sin 2\psi \cos \Delta & \sin 2\psi \sin \Delta \\ 0 & 0 & -\sin 2\psi \sin \Delta & \sin 2\psi \cos \Delta \end{bmatrix}$
Polarizer (P)	$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$	$\frac{1}{2} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

3. ELLIPSOMETRY SYSTEMS

As discussed in previous sections, ellipsometry systems represent important investigation tools for the characterization of the optical properties and thickness of surface layers. All kinds of ellipsometry techniques and their modifications are concerned. An overview of these systems was provided in this section, and further details on these techniques will now be discussed.

3.1 Null Ellipsometry

Historically, null ellipsometry was the basis for the original ellipsometry instruments and is generally thought to have first been developed by Drude; however, no specific proof of this exists in literature [17]. The term "ellipsometry," nonetheless, had been coined by Alexandre Rothen in 1945 in his paper entitled "The Ellipsometer, an Apparatus to Measure Thicknesses of Thin Films."

At that time, determining the null position of the analyzer, a critical aspect of ellipsometry measurements, was performed using the human eye. Figure 3.1 shows one example of null ellipsometry. In the null ellipsometry method, polarizer and analyzer are mechanically rotated so that the intensity of detected light is null (zero) and (ψ, δ) is obtained from the rotation angles of polarizer and analyzer. Consequently, when light intensity is assessed visually, the measurement can be carried out without the use of electrical equipment.

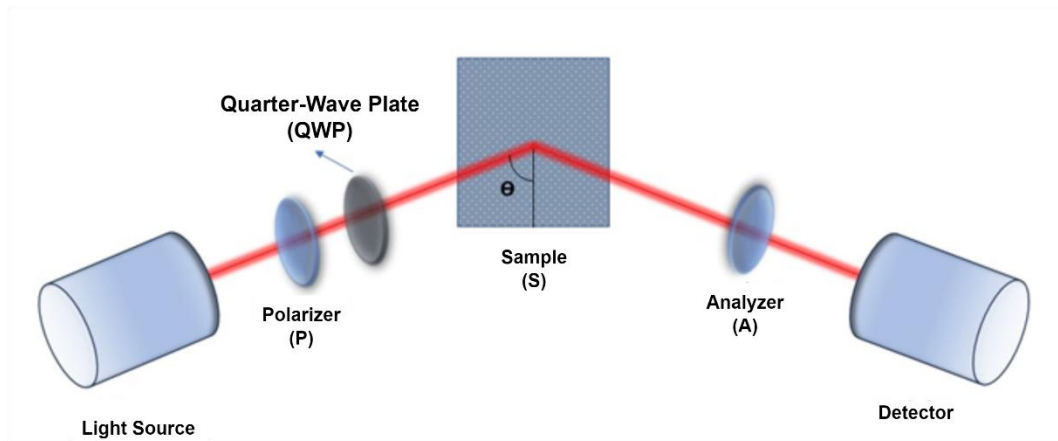


Figure 3.1 : Schematic diagram of null ellipsometry [2]

3.2 Modern Ellipsometry Technologies

3.2.1 Spectroscopic Ellipsometry

Modern ellipsometry began in the 1970s when automated ellipsometers were developed, for example by D. E. Aspnes [18], P. S. Hauge [19], and others [20]. These automated devices made use of rotating optical elements, typically polarizers, analyzers, or compensators, to provide the modulation of the phase of light-the so-called PEM. Rotating compensators, such as Berek-type compensators [21], also became popular in the following years. The application of dual rotating compensators or PEMs showed considerable advantages, especially for the case of depolarized incident light; one is able to measure the complete Mueller matrix.

The technological development made the ellipsometry system to be more automated, fast, and less prone to measurement errors. One huge development is spectroscopic ellipsometry-the powerful technique to study the material optical properties over a wide wavelength range. Spectroscopic ellipsometry became one of the most important techniques for the characterization of thin-film materials and devices, as it identifies the complex dielectric function of the material using multiple wavelengths. This enables the detailed description of the optical properties, namely the refractive index n and extinction coefficient k .

Spectroscopic ellipsometry does more than just analyze the surface that any other ellipsometer would provide; instead, it probes into multilayer structures. For the thin films, it would be able to deliver information on thickness, composition, and optical

properties. Because it employs variable wavelengths to make a measurement, spectroscopic ellipsometry provides information on how the optical properties of materials change with wavelength. Accordingly, it finds important applications in a very wide range of fields, from photovoltaics to semiconductor development and optoelectronic design. Its detailed and precise optical data are important in material design and manufacturing processes.

3.2.1.1 Analyzer-Modulated Ellipsometry Configuration

Modulator-analyzer ellipsometry is a case of spectroscopic ellipsometry where, by introducing modulation in the analyzer, high precision with an improved signal-to-noise ratio can be achieved in measurement. The applications with particular incidence for the setup were found dealing with thin-film characterization and studies in material surface optical properties where this setup result is quite successfully applied. Modulation usage in the analyzer plane brings enhanced variation of the measured signal. An example typical of such a setup is presented in Figure 3.2.

This technique operates at a modulation frequency range of roughly 10-300 Hz where the parameters $\tan\Psi$ and $\cos\Delta$ are measured characterizing material properties. Such systems are relatively easy to implement, calibration is simple, and operation over a large spectral range without optics at each wavelength is possible. Other salient features are that a CCD detection system integration is possible, and hence the configuration is rather versatile.

Some of the disadvantages are: There is a loss of some accuracy when Δ is close to 0° or even 180° . Residual polarization errors might affect measurement quality. Mechanical errors can also be possible, quite easily in fact, and since there are a large number of moving parts, it translates to increased mechanical complexity with increased maintenance costs.

Yet, along with such possible disadvantages, the analyzer-modulated ellipsometry due to its simplicity, broad spectral range, and delivery of important optical data about material characterization, it has been, nevertheless, a simple and practical technique that is widely used.

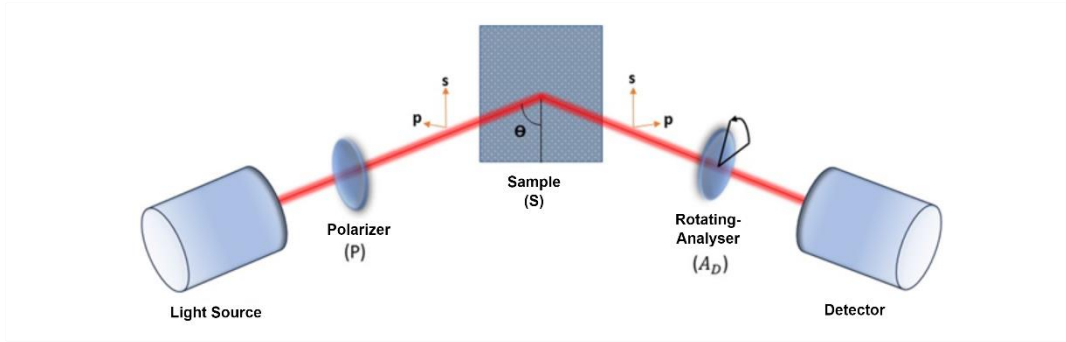


Figure 3.2 : Analyzer modulated ellipsometry (PSA_D) [2]

3.2.1.2 Compensator-Assisted Analyzer-Modulated Ellipsometry Configuration

One of the variants of spectroscopic ellipsometry is the compensator-assisted analyzer-modulated ellipsometry configuration, whereby enhancement in the precision of measurement was done. It involves the use of a compensator combined with analyzer modulation, where more control and correction in the measurement processes are allowed. It finds its application in the characterization of thin-film layers and determination of material surface optical properties in so many areas.

Here, the modulation system of the analyzer includes a compensator. Some of its major tasks are to suppress noise, cancel system error signals, and improve system measurement precision. This is highly applicable to carrying out complicated optical property analyses on the material surface; thus, it is able to provide more accurate and reliable results. A sample configuration is shown in Figure 3.3.

The operating modulation frequency is within the range of 15-320 Hz. The setting allows for measurement of $\tan\Psi$ and $\cos\Delta$ amongst others. The set-up also has its good and bad points. The major advantage of this set-up is the precision it gives, majorly on transparent thin films whose Δ is near 0° or 180° .

This setup is also beset with some drawbacks on the other side. For one, calibration is quite tedious and may require expertise to even extremely high levels for some very demanding applications. Other than that, the said setup is not conducive to detection systems using CCD, and it entails limited application in quite a number of applications. Mechanical components in the system cause the presence of mechanical errors and complicate the requirements in its maintenance. Despite all its advantages, this renders the compensator-assisted analyzer-modulated ellipsometry setup relatively unwanted and thus mainly limited to applications that demand high accuracy-particularly in

analyzing very thin transparent film properties. This being a very precise system is, however, complicated, CCD camera-hostile, and moving-part-based.

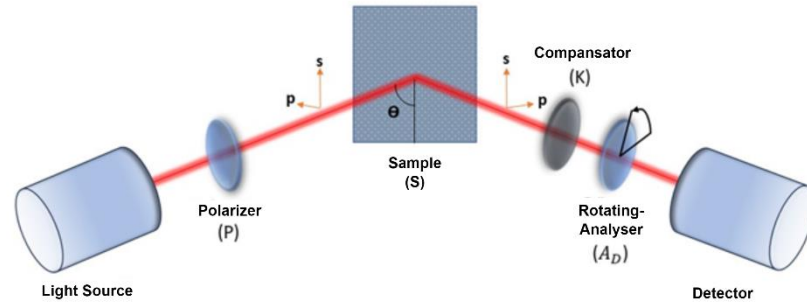


Figure 3.3 : Analyzer modulated ellipsometry optical configuration with compensator ($PSCA_D$) [2]

3.2.1.3 Rotating Compensator Modulated Ellipsometry Configuration

The rotating compensator ellipsometer modulated design is a suitable alternative to spectroscopic ellipsometry, with higher measurement precision, removal of systematic error, and even simplicity of measurement across a broad spectral range of wavelengths [22]. By including the rotating compensator in the design, the highest control and versatility in ellipsometric measurements are attained. The rotating compensator changes the state of polarization of the incoming light and hence makes precise determination of measurements in the predetermined spectral range of wavelengths. In addition, it reduces noise effects and makes corrections on different wavelengths to produce more reliable results. This technique is widely utilized in order to attain more detailed characterization of material surfaces as well as better accuracy of measurements as can be seen in Figure 3.4.

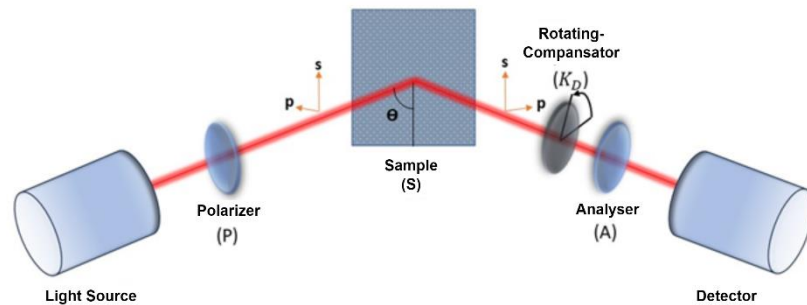


Figure 3.4 : Compensator modulated ellipsometry optical configuration (*PSC_DA*)

[2]

Operating at the modulation frequency range of 10–300 Hz, this approach measures parameters $\tan\Psi$ and $\cos\Delta$ and hence allows for an evaluation of the material's optical properties. The technique has many advantages in terms of its ability to record the full range of Ψ and Δ and hence for the characterization of a vast number of materials [23]. In addition to this, the setup allows for the examination of depolarization spectra, enabling detailed examination of the material's polarization properties.

The system setup is not without drawback. The optical design is more complex than the design of simpler systems, such as rotating analyzer setups, which may make it more difficult to manage. The system's capability of having chromatic characteristics also causes issues, such as color image artifacts at specific red and blue wavelengths. The system is also fairly technology-intensive, with training needed for use. The calibration procedure is not simple and its improper execution can result in a lack of accuracy in the measurements acquired. Furthermore, the moving parts introduce some degree of susceptibility to mechanical breakdown, thus requiring frequent maintenance. These drawbacks notwithstanding, the rotating compensator modulated ellipsometry setup is an exceedingly powerful tool for highly accurate and detailed optical characterization.

3.2.1.4 Phase-Modulated Ellipsometry Configuration

PEM is an ellipsometry configuration based on its capability of light-phase modulation [24]. Basically, this is applied to the precise characterization of optical properties in the thin-film layers. Different from the traditional mechanically modulated ellipsometry, the phase modulation of light in this is achieved electronically using an electronic system without the involvement of a mechanical system [25]. Therefore, it provides fast and accurate measurements, hence quite efficient in determining the major parameters like thickness, alignment, and optical characteristics of surface layers. It can further provide much higher measurement speed and better precision compared to those given by general ellipsometry systems [26].

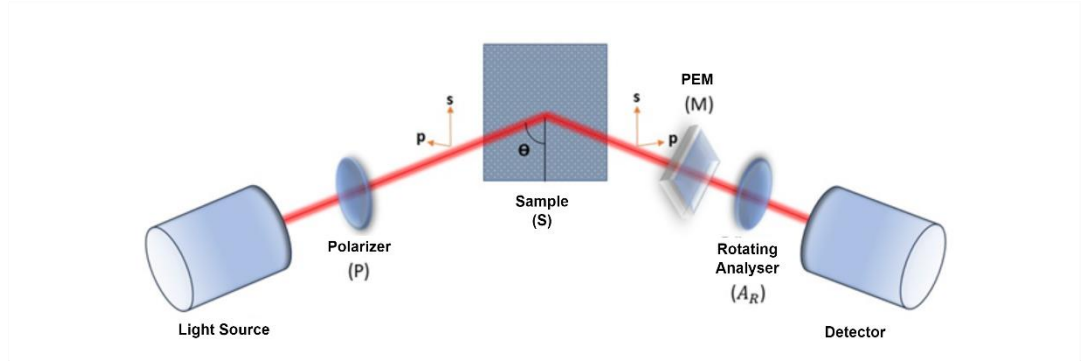


Figure 3.5 : Phase-modulated ellipsometry optical configuration (PSMA) [2]

As illustrated in Figure 3.5, PEM operates at modulation frequencies of about 51 kHz and hence allows for fast measurements [27]. This setup studies the optical constants of materials from parameters like $\sin 2\Psi - \cos \Delta$ and $\sin 2\Psi - \sin \Delta \cos 2\Psi$. The major characteristics of this technique are the capability of fast measurement and real-time infrared spectroscopy it provides, which allows a close investigation into dynamic optical constants of materials. Besides that, the other capability of PEM is the analysis of depolarization spectra, which provides full information about material polarization characteristics [28].

In turn, this creates further limitations. Only a single measurement cannot estimate either S_1 or S_2 , but this could not be restraining. The errors during measurement increase around some places from Ψ and Δ [29]. In particular, color imaging artefacts may result through a series of defined particular wavelengths for a chromatic type of instrument such as PEM. Technologically complex, this thus requires good training for proper implementation. Even then, calibration becomes complex. Very poor calibration sometimes contributes to a bigger error. However, there still remains an element of restrictions especially when used by CCD detection systems.

Despite these two problems, phase-modulated ellipsometry has a capability of fast measurement and real-time spectroscopy, which gives this technique a particular position in conducting dynamic and fine optical characterization of materials.

3.2.2 Imaging ellipsometry

Imaging ellipsometry is a high-level optical characterization technique that can be applied to quantify and visualize the lateral thickness distribution of thin transparent films on solid substrates [30]. It goes beyond traditional ellipsometry techniques in terms of performing simultaneous and high-resolution measurements across the entire surface. These techniques very often combine null and off-null ellipsometry close to the pseudo-Brewster angle, taking advantage of a high-refractive-index substrate, normally made up of silicon [31].

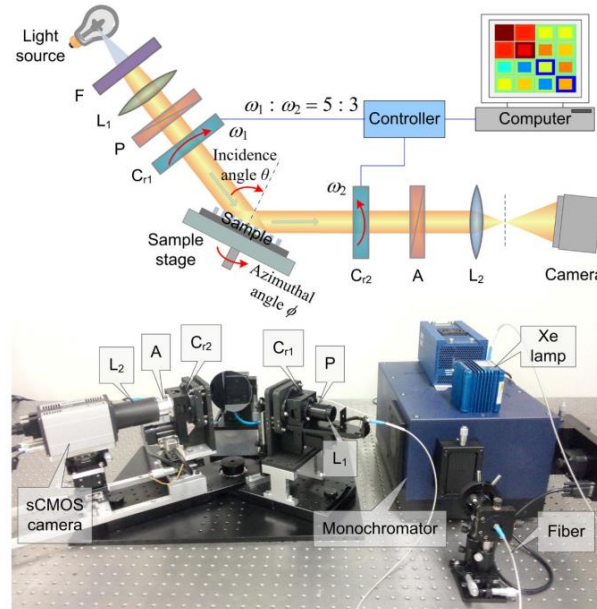


Figure 3.6 : Schematic (top) and prototype (bottom) of a Mueller matrix imaging ellipsometer with dual rotary compensator: L1 and L2 - collimating lens and imaging lens, F - filter or monochromator, P and A-polarizer and analyzer, Cr1 and Cr2 -1st and 2nd rotary compensators

Here, in Figure 3.6 below, some of the key components of the experimental setup include a xenon lamp, a collimator, and a wavelength-selective filter creating the collimated probe beam, while the key measuring system contains a polarizer, a compensator, and an analyzer. Often, in imaging data format, it can be presented as a 4×4 Mueller matrix, from which it tries to extract information about the structural properties of the sample.

Imaging ellipsometry therefore provides a high-throughput, nondestructive means for the precise characterization of nanostructures in the nanometer range, besides furnishing important information for both research and industrial use. These have been applied with great success in nanotechnology for the precise characterization of isolated nanostructures, such as Käseberg, Tim, et al. [32], whereas analysis of Mueller matrix data makes this technique very effective in nanostructure metrology, as can be seen from Liu, Shiyuan, et al. [33].

3.2.3 Comparisons and Configuration Selection

The compensator-assisted rotating analyzer modulation ellipsometry configuration is instrumental, cost-effective, and simple in operation; hence, the major reasons it has been chosen. By doing so, the approach will be able to offer improved control and correction during the analysis process hence better measurements. Besides, the setup has presented cost-effectiveness compared with other configurations, thus more suitable for laboratories on a stringent budget [34]. The design also assures user-friendliness and easiness in calibration; hence, this enhances further efficiency in the laboratory.

This setup provides enormous advantages in taking exact measurements of thin transparent films, mostly within the ranges of $\Delta \approx 0^\circ$ or 180° . Hence, this device is enormously capable of precisely characterizing the complicating optical properties pertinent to material surfaces. Considering this technique, one has to mention problems such as complex calibration procedures and the usage of CCD detection systems. Having the above-mentioned limitations, this setup works very well for applications such as the characterization of thin-film layers and determination of optical properties of material surfaces. The big measuring range, combined with high precision, at affordable costs, contributes much to laboratory research.

3.3 Construction and Outputs of the Rotating Analyzer System

Under this title, how the ellipsometry system with a rotary-analyzer configuration is designed using the Jones matrix and how the raw data obtained from the modulation is analyzed will be examined in detail. First, the steps performed on the raw data set resulting from the modulation will be explained step by step and how the obtained

results are converted to basic ellipsometry parameters such as Ψ and Delta Δ will be explained in detail. Then, the equations utilized in calculating thin film thickness, and the process of data fitting included in such equations, will be highlighted. These steps will constitute a thorough outline of the comprehension of the structure of the rotary analyzer system, among other arrangements, and the analysis of the resultant outputs. The primary purpose of explaining the design of ellipsometry under this setup and the application of Jones matrices should be considered as a starting point for moving forward with the Mueller matrix approach, which demands a more involved and difficult mode of analysis. This constitutes a step that is needed to comprehend ellipsometry instruments, particularly when factoring in the complexity and work involved in the analytical process.

3.4 Investigation of Rotary Analyzer System with Jones matrix

The design of the ellipsometry system must be carefully planned to obtain accurate measurements and reliable results. In this section, the solution of the rotating analyzer system with Jones vector will be shown. Using the Jones matrix abbreviations of the optical elements in Table 2.1, the ellipsometry device with the POA_D configuration can be shown as:

$$L_C = AR(A)ROR(-P)PL_G \quad (3.1)$$

In Equation 3.1, L_C represents the Jones vector representation of the light detected by the detector, L_G represents the Jones vector representation of the incident light. According to Equation 3.1, we can show the matrix representation of the system as follows:

$$\begin{aligned} \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} \sin \psi \cdot e^{i\Delta} & 0 \\ 0 & \cos \psi \end{bmatrix} \\ &\times \begin{bmatrix} \cos P & \sin P \\ -\sin P & \cos P \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix}^G \end{aligned} \quad (3.2)$$

To solve this matrix more easily, we can convert the sample (O) matrix in Equation 3.1 into the matrix $\begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix}$ from the equation $\rho = \frac{r_p}{r_s} = \tan \psi e^{i\Delta} = \frac{\sin \psi \cdot e^{i\Delta}}{\cos \psi}$ [35] and update the calculation 3.2 to:

$$\begin{aligned}
\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \\
&\times \begin{bmatrix} \cos P & \sin P \\ -\sin P & \cos P \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \end{bmatrix}^G
\end{aligned} \tag{3.3}$$

Continuing with the matrix solution, if we perform matrix multiplication from left to right:

$$\begin{aligned}
\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \\
&\times \begin{bmatrix} \cos P & \sin P \\ -\sin P & \cos P \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} E_x
\end{aligned} \tag{3.4}$$

$$\begin{aligned}
\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \\
&\times \begin{bmatrix} \cos P & \sin P \\ -\sin P & \cos P \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} E_x
\end{aligned} \tag{3.5}$$

$$\begin{aligned}
\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \\
&\times \begin{bmatrix} \cos P \\ \sin P \end{bmatrix} E_x
\end{aligned} \tag{3.6}$$

For simplicity, let's proceed without taking the polarizer angle into account when continuing the matrix multiplication, that is:

$$\begin{bmatrix} r_p & 0 \\ 0 & r_s \end{bmatrix} \begin{bmatrix} \cos P & \sin P \\ -\sin P & \cos P \end{bmatrix} \Rightarrow \begin{bmatrix} r_p \cos P \\ r_s \sin P \end{bmatrix} = \begin{bmatrix} r'_p \\ r'_s \end{bmatrix} \tag{3.7}$$

The terms r'_p and r'_s in Equation 3.7 express the new values of the reflection coefficients when the angle of the polarizer (P) is taken into account. r'_p represents the new value obtained when we multiply the r_p value by the angle P. Similarly, r'_s represents the new value obtained when we multiply the r_s value by the angle P. Continuing the matrix multiplication in this light:

$$\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A & \sin A \\ -\sin A & \cos A \end{bmatrix} \begin{bmatrix} r'_p \\ r'_s \end{bmatrix} E_x \tag{3.8}$$

$$\Rightarrow \begin{bmatrix} E'_x \\ E'_y \end{bmatrix}^C = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos A \cdot r'_p + \sin A \cdot r'_s \\ -\sin A \cdot r'_p + \cos A \cdot r'_s \end{bmatrix} E_x \quad (3.9)$$

$$E'_x = (\cos A \cdot r'_p + \sin A \cdot r'_s) E_x \quad (3.10)$$

In the real configuration, the data received from the detector represents the light intensity [10]. The relationship between the light intensity and the electric field can be expressed as in Equation 3.11:

$$I = |E|^2 \quad (3.11)$$

If we continue the analysis with this information:

$$\Rightarrow I = |E'_x|^2 = (\cos A \cdot r'_p + \sin A \cdot r'_s) \cdot (\cos A \cdot (r'_p)^* + \sin A \cdot (r'_s)^*) \cdot |E_x|^2 \quad (3.12)$$

$$\begin{aligned} \Rightarrow I_D = |r'_p|^2 \cdot \cos^2 A + |r'_s|^2 \cdot \sin^2 A + r'_p \cdot (r'_s)^* \cdot \sin A \cdot \cos A \\ + r'_s \cdot (r'_p)^* \cdot \sin A \cdot \cos A \end{aligned} \quad (3.13)$$

The expression $|E_x|^2$ in Equation 3.12 represents the proportional constant of the intensity of the reflected light and is denoted by I_0 .

$$\cos^2 A = \frac{1 + \cos 2A}{2} \quad (3.14)$$

$$\sin^2 A = \frac{1 - \cos 2A}{2} \quad (3.15)$$

$$\sin A \cdot \cos A = \frac{1}{2} \sin 2A \quad (3.16)$$

When the expressions in 3.14 - 3.16 are used for the analyzer angle terms in Equation 3.13, 3.17 is obtained:

$$\begin{aligned} \Rightarrow I_D = \frac{I_0}{2} \{ |r'_p|^2 + |r'_s|^2 + [|r'_p|^2 - |r'_s|^2] \cdot \cos 2A \\ + [r'_p \cdot (r'_s)^* + r'_s \cdot (r'_p)^*] \cdot \sin 2A \} \end{aligned} \quad (3.17)$$

The r_p and r_s values in the curly brackets in equation 3.17 correspond to the Stokes parameters in equation 2.21. These are shown in equations 3.18 - 3.20 below.

$$S_0' = |r_p'|^2 + |r_s'|^2 \quad (3.18)$$

$$S_1' = |r_p'|^2 - |r_s'|^2 \quad (3.19)$$

$$S_2' = 2\text{Re}((r_p')^* r_s') = r_p' \cdot (r_s')^* + r_s' \cdot (r_p')^* \quad (3.20)$$

An important note is that the reason why unpolarized light is not used in the rotary analyzer configuration is that the S_3 element of the Stokes parameter is missing in equation 3.17 and the depolarization equation is shown as seen in equation 3.21 [36].

$$S_0'^2 \geq S_1'^2 + S_2'^2 + S_3'^2 \leftrightarrow \text{depolarization} \quad (3.21)$$

$$\Rightarrow I_D = \frac{I_0}{2} \{S_0' + S_1' \cdot \cos 2A + S_2' \cdot \sin 2A\} \quad (3.22)$$

The reflected light passes through a rotating analyzer before reaching the detector. The reflected light is monitored for 360° at each rotation, which produces a similar sinusoidal signal at each rotation. A modulation representation of the analyzer is shown in Figure 3.7.

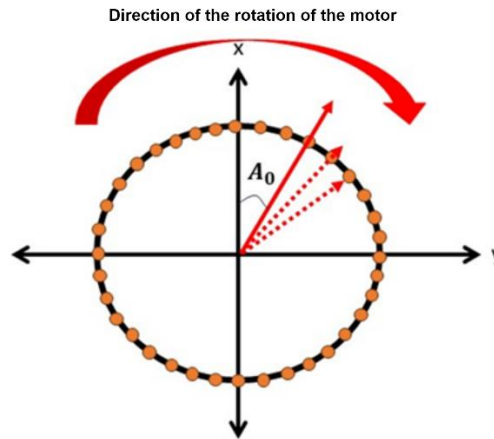


Figure 3.7 : Illustration of analyzer modulation

The frequency of the data received from this modulation can significantly affect the data processing speed of the system. For example, to obtain an array of 90 elements, we can digitize the signal every 4 degrees. A_0 in Equation 3.23 represents the angle that the analyzer makes with the plane of incidence, ω is the angular frequency, and t is the time.

$$A = \omega t \quad (3.23)$$

$$\Rightarrow I_D = \frac{I_0}{2} \{S_0' + S_1' \cdot \cos 2\omega t + S_2' \cdot \sin 2\omega t\} \quad (3.24)$$

$$\begin{aligned} S_0' &= |r_p'|^2 + |r_s'|^2 = \frac{|r_p|^2 + |r_s|^2}{2} + \frac{|r_p|^2 - |r_s|^2}{2} \cos 2P \\ &= \frac{S_0}{2} + \frac{S_1 \cdot \cos 2P}{2} = \frac{1}{2} - \frac{\cos 2\psi \cos 2P}{2} \end{aligned} \quad (3.25)$$

$$\begin{aligned} S_1' &= |r_p'|^2 - |r_s'|^2 = \frac{|r_p|^2 - |r_s|^2}{2} + \frac{|r_p|^2 + |r_s|^2}{2} \cos 2P \\ &= \frac{S_1}{2} + \frac{S_0 \cdot \cos 2P}{2} = \frac{\cos 2P - \cos 2\psi}{2} \end{aligned} \quad (3.26)$$

$$S_2' = 2\text{Re}(r_s' \cdot (r_p')^*) = \text{Re}(r_p^* r_s) \cdot 2\sin P \cdot \cos P = \frac{\sin 2P \cos \Delta \sin 2\psi}{2} \quad (3.27)$$

$$\begin{aligned} I_D &= \frac{I_0}{4} \{1 - \cos 2\psi \cos 2P + \cos 2\omega t (\cos 2P - \cos 2\psi) \\ &\quad + \sin 2\omega t (\sin 2P \cos \Delta \sin 2\psi)\} \end{aligned} \quad (3.28)$$

When we normalize equation 3.28 with the term $1 - \cos 2\psi \cos 2P$, we obtain the normalized Fourier coefficients (Ω, Λ) in 3.29:

$$\Lambda = \frac{\cos 2P - \cos 2\psi}{1 - \cos 2\psi \cos 2P} \quad \Omega = \frac{\sin 2P \cos \Delta \sin 2\psi}{1 - \cos 2\psi \cos 2P} \quad (3.29)$$

Using simple trigonometry, we can write the coefficients in 3.29 as follows:

$$\Lambda = \frac{\tan^2 \psi - \tan^2 P}{\tan^2 \psi + \tan^2 P} \quad \Omega = \frac{2 \tan \psi \tan P \cos \Delta}{\tan^2 \psi + \tan^2 P} \quad (3.30)$$

The ellipsometry parameters (ψ, Δ) calculated from the (Λ, Ω) coefficients are shown in equation 3.31:

$$\tan\psi = \sqrt{\frac{1+\Lambda}{1-\Lambda}} |\tan P| \qquad \cos\Delta = \frac{\Omega}{\sqrt{1-\Lambda^2}} \qquad (3.31)$$

One of the main advantages of this method and other methods is the ability to distinguish between linear, circular and elliptical polarization conditions. When choosing the Rotary Analyzer Configuration, it is important why the analyzer angle is selected as 45 degrees. This choice emphasizes the situation that especially in the case of 45-degree linear polarization, the light intensity is zero when the analyzer angle is 45 degrees and reaches a maximum at 135 degrees. This allows linear polarization to be observed clearly.

Choosing the analyzer angle as 45 degrees is a strategic choice in terms of correctly interpreting the obtained data and emphasizing linear polarization during the analysis. This choice ensures that the obtained results can be evaluated reliably.

The optical configuration refers to the arrangement and location of the optical components in the system. Ellipsometry systems with rotary analyzer configuration usually include a rotary analyzer. Correct configuration of the optical configuration is a critical factor that determines the sensitivity and reliability of the measurements. This configuration includes analyzer modulation and rotary analyzer modulation, which enables the system to measure with high accuracy.

3.4.1 Obtaining Ellipsometric Value from Pseudo-Data

In this section, we will generate pseudo-sinusoidal data for the rotary analyzer and obtain the Fourier coefficients in equation 3.24 from this data.

$$I_n = I_D + I_\Lambda \cdot \cos 2A_n + I_\Omega \cdot \sin 2A_n \qquad (3.32)$$

In Equation 3.32, I_D , I_Λ and I_Ω are the Fourier coefficients and A_n is the analyzer angle ($A_n = \frac{2\pi n}{N}$) between 0 and 2π . Now let's expand the I_n expression to the Fourier series to find these coefficients. The Fourier coefficients are found as follows:

The I_D value is obtained by taking the average of the analyzer rotation, and is shown with equation 3.32:

$$I_D = \frac{1}{N} \sum_{j=0}^{N-1} I_n \quad (3.33)$$

The values of I_Λ and I_Ω are derived from equations 3.33, respectively:

$$I_\Lambda = \frac{1}{\pi} \sum_{j=0}^{N-1} I_n \sin 2A_n \cdot \Delta A \quad I_\Omega = \frac{1}{\pi} \sum_{j=0}^{N-1} I_n \cos 2A_n \cdot \Delta A \quad (3.34)$$

where $\Delta A = 2\pi/N$.

After the C++ libraries associated with these equations were created in Figures A.1 and A.2, the pseudo-signal was created using equation 3.32 with the previously determined I_D , I_Λ and I_Ω coefficients together with the light intensity calculation program in Figure A.3. The coefficients were obtained from this fake signal with the equations 3.32 and 3.33 Fourier series at a certain noise tolerance. The outputs of the light intensity program are presented in Figure 3.8.

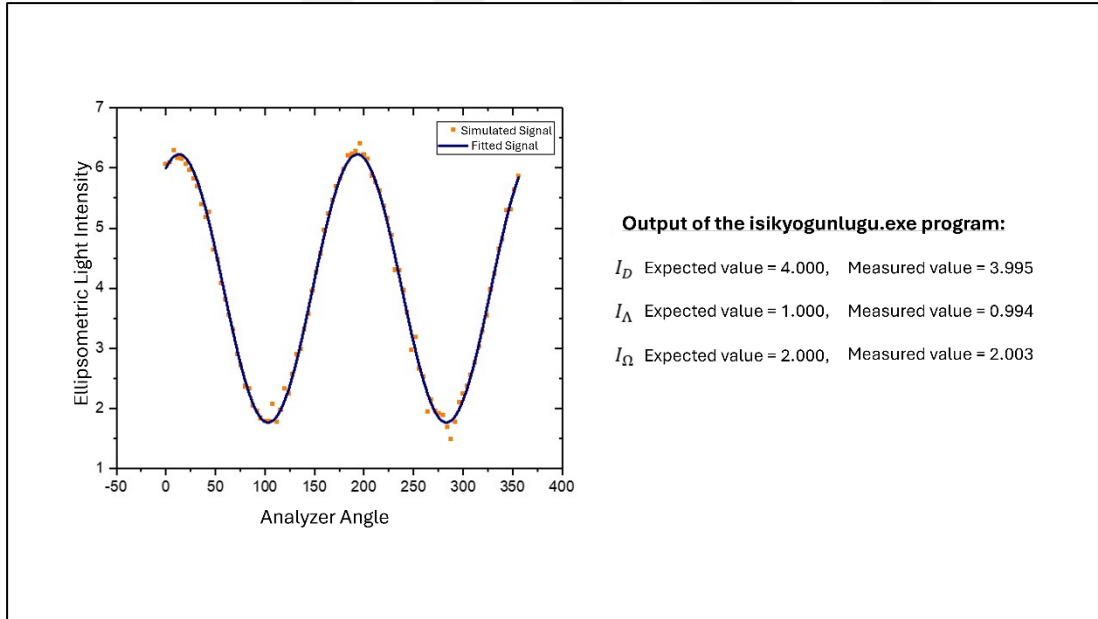


Figure 3.8 : Outputs of the light intensity program (Figure A.3)

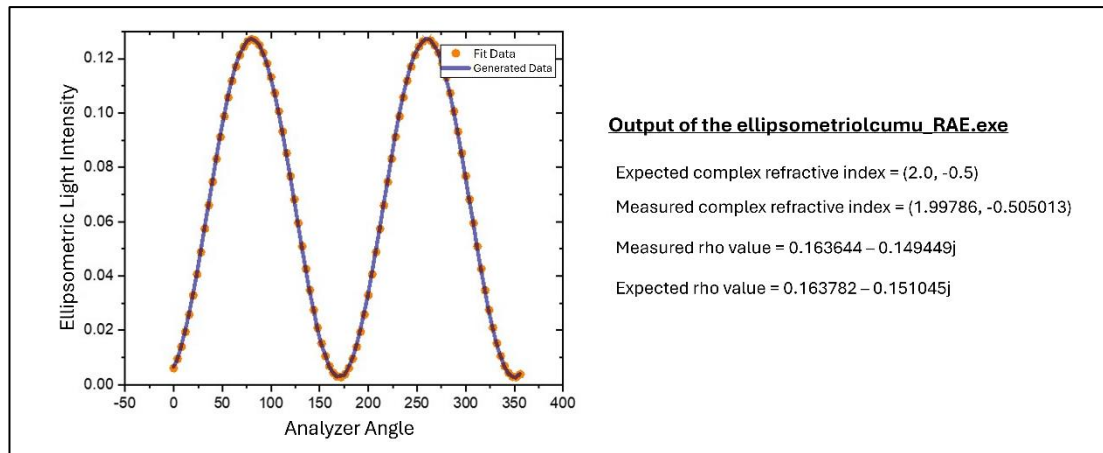


Figure 3.9 : Outputs of the rotary analyzer (Figure A.4) program

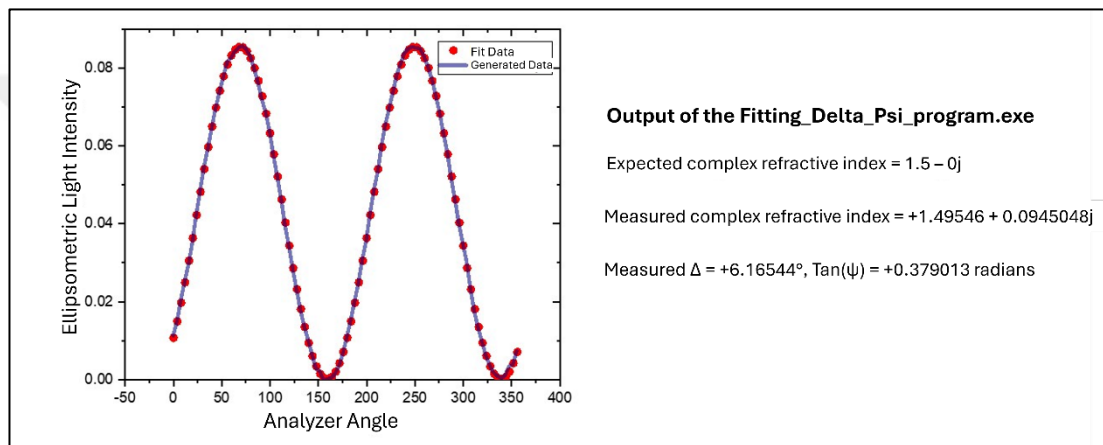


Figure 3.10 : Outputs of the fitting delta psi (Figure A.5) program

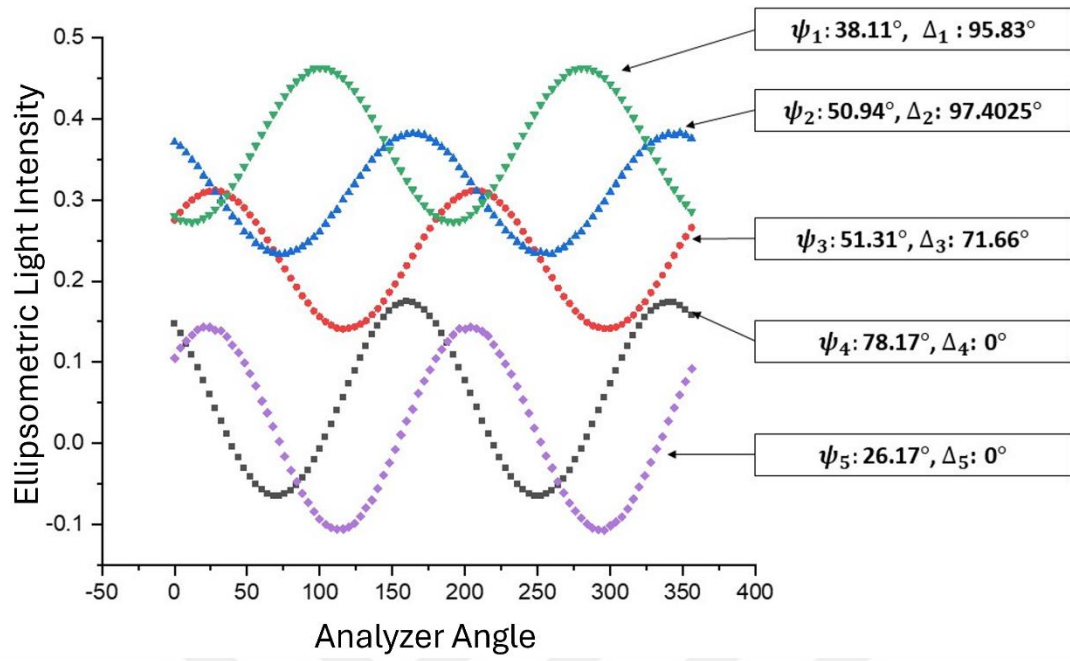


Figure 3.11 : Results of the polarization states of reflected lights

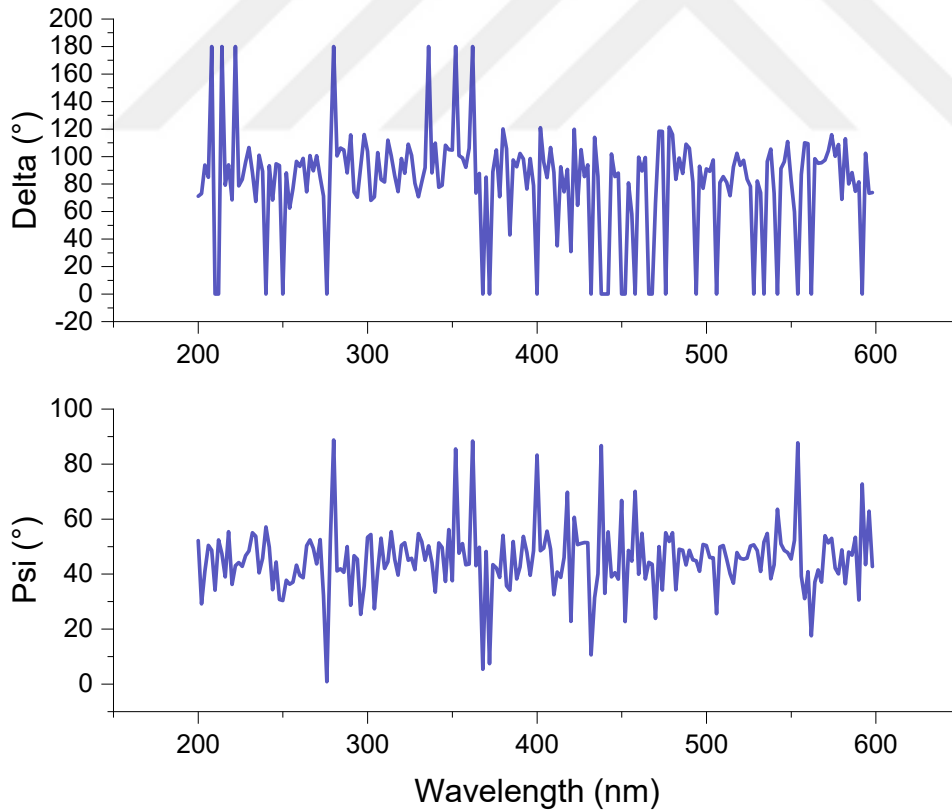


Figure 3.12 : Outputs of the delta&psi data generation (Figure A.6) program

4. OPTICAL CHARACTERIZATION OF SILICON-BASED THIN FILMS BY SPECTROSCOPIC ELLIPSOMETRY

In this section, we focus on the analysis of some SiC and Si-based thin films measured by Horiba Uvisel Spectroscopic Ellipsometry and Woolam Spectroscopic Ellipsometry.

4.1 Optical Methods for Material Characterization

These measurements provided input to establish dielectric functions and to identify related defect types and densities of such materials.

In this chapter, the measurement results were analyzed by considering material properties-thickness, defect type, and densities-with preliminary information from the sample manufacturer. Consequently, the following measurements and various discussions and researches about the spectroscopic ellipsometry instrumentation being used showed that it was not possible to do the defect type/shape analysis with this type of instrumentations; thus, the defect density determination was given special focus [37]. The analysis study to investigate the defects is based on the Effective Medium Analysis. The various techniques, such as Bruggeman's Effective Medium Approximation (EMA), Extended Maxwell-Garnett Approximation (EMAMG), Sen, Scala & Cohen model SSC, and Maxwell-Garnett model, are taken into consideration in analyzing the ellipsometric data. Besides these, material-specific parameters have been determined for GaN on SiC using reference GaN data with the Adachi-New Forouhi function [38].

The Horiba DP2 software uses above mentioned Effective Medium Models for data analysis. Brief description of models is given below.

4.1.1 Maxwell-Garnett model

This model is based on the Clausius-Mosotti relationship [39] which describes the dielectric function of a set of spheres that are at a certain distance to each other and homogeneously immersed in a host medium. This model defines the dielectric function ε of the effective medium according to the following formula:

$$\varepsilon = \varepsilon_0 \frac{\varepsilon_1(1 + 2f) + 2\varepsilon_0(1 - f)}{\varepsilon_1(1 - f) + \varepsilon_0(2 + f)} \quad (4.1)$$

with the dielectric constant of spherical particles ε_1 immersed in a host medium whose dielectric constant is ε_0 . f is the volume fraction of the spheres.

4.1.2 EMA-Bruggeman model

In Bruggeman EMA model, the different components of the mixture are treated equivalently, without preliminary assumption on the relative proportions [40]. It is self-consistent such that the mixture of the different materials forms the host medium, which means that the dielectric function of the host medium is the EMA-Bruggeman dielectric function. In this model the number of phases can exceed 2 [41]. The dielectric functions of the different materials are ε_i with $i = 1, 2, 3, \dots$ with corresponding volume fractions f_i . The dielectric function of the effective medium [42] fulfills the following equation:

$$\sum_i f_i \frac{\varepsilon_i - \varepsilon}{\varepsilon_i + 2\varepsilon} = 0 \quad (4.2)$$

In the DP2 software the number of components per layer is limited to three to avoid complicated calculations and eventual correlations between the different parameters. This model is very useful for modelling surface roughness consisting of 50% void and 50% material of the layer below.

4.1.3 EMAMG

Indeed, the so-called EMAMG model is one step ahead in the integration of two highly recognized theoretical ways of looking into the behavior of effective media, namely the Maxwell-Garnett model and the Bruggeman model [43]. The Maxwell-Garnett model, accordingly, usually provides for systems whose host medium has been embedded with inclusions of a secondary phase in case there is a clear distinction

among the matrix and inclusions. Such a model is highly suitable for systems of low concentration in which inclusions are sufficiently separated and their interactions negligible. In contrast to this, the Bruggeman model considers the symmetric treatment of the components under consideration of a more homogenized mixture in which no phase is privileged to act as a host. This could be the situation to be considered in the event of comparable volume fractions of the constituent phases or inclusions that are strongly interacting.

Combining these two approaches, the EMAMG model has as its goal grasping features of the two methodologies for an increasingly comprehensive and realistic description of the effective optical, electrical, or structural properties of such complex composite materials. It turns out to be very helpful in practice when the material system crosses the limits of Maxwell-Garnet and Bruggeman, including nanostructured or multi-phase systems where geometry, distribution, and interaction of inclusions change with scale.

Due to its flexibility, EMAMG allows bridging between these two traditional models in the development of a more robust theoretical tool that can analyze and predict properties for various advanced material applications in photonics, optoelectronics, and materials science.

4.1.4 SSC model

Sen & al presented a self-similar model based on the following equation:

$$\frac{\varepsilon - \varepsilon_0}{\varepsilon + 2\varepsilon_0} = f \frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_1 + 2\varepsilon_0} \quad (4.3)$$

The derivation provided by Sen & al results in:

$$\left(\frac{\varepsilon_1 - \varepsilon}{\varepsilon - \varepsilon_0} \right) \left(\frac{\varepsilon_0}{\varepsilon} \right)^{1/3} = \phi \quad (4.4)$$

with ϕ the proportion of the host medium

This model is applied to a fractal medium of infinitely wide particle size distribution.

4.2 Data Analysis Procedure in Ellipsometry Experiments

An ellipsometric experiment proceeds as schematically depicted in Figure 4.1, in the following way:

1. Ellipsometric measurements report the ellipsometric angles Ψ and Δ , and not the actual sample parameters, which are thickness and optical constants.
2. A model of the sample should be developed in order to understand its parameters.
3. After the model is constructed, the computed data have to be fitted to the experimental data, and some optimum match between the two sets has to be chosen.
4. The user must check the best-fit model for physical plausibility of the estimated model and uniqueness and no correlation among the various parameters.

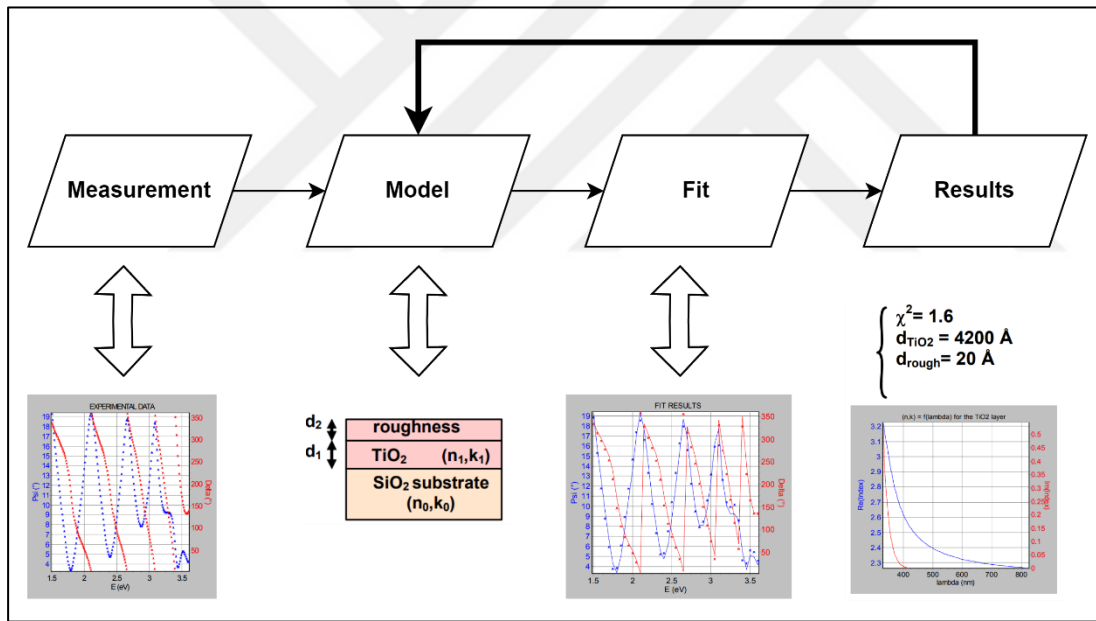


Figure 4.1 : Diagram of data analysis procedure

4.3 Optical Characterization of GaN on SiC Material

Sample 7971 is the GaN on SiC material provided by CSC and AXITRON within the scope of the EMPIR project named PowerElec. In this thesis, many pieces of these thin films were separated, and sample pieces named D5, E6, F7, G8 (these are same sample but were examined. Preliminary information on these pieces also was obtained by these suppliers. In the examination of these thin films, the optic parameters and the thicknesses are considered. In this thesis, defect analysis was performed with

spectroscopic ellipsometry measurement together with the methods given in the previous titles.

Sample number 7971 investigated in this thesis is a HEMT (High Electron Mobility Transistor) epitaxial layer with a GaN-on-SiC structure. This HEMT structures designed for high frequency wireless applications (X Band and K_a Band). The sample was grown on an AlN nucleation and bottom buffer layer and contains GaN:C and GaN channel layers. The total epitaxial layer thickness varies between approximately 1.8 and 1.9 μm . The layer structure is designed as 20 nm AlGaIn, 1 nm AlN, 200 nm GaN, 1.1 μm GaN:C, 400 nm GaN and 170 nm AlN, respectively. The sample was grown using the cassette-to-cassette wafer transport system with the AIX G5+ C MOCVD reactor module.

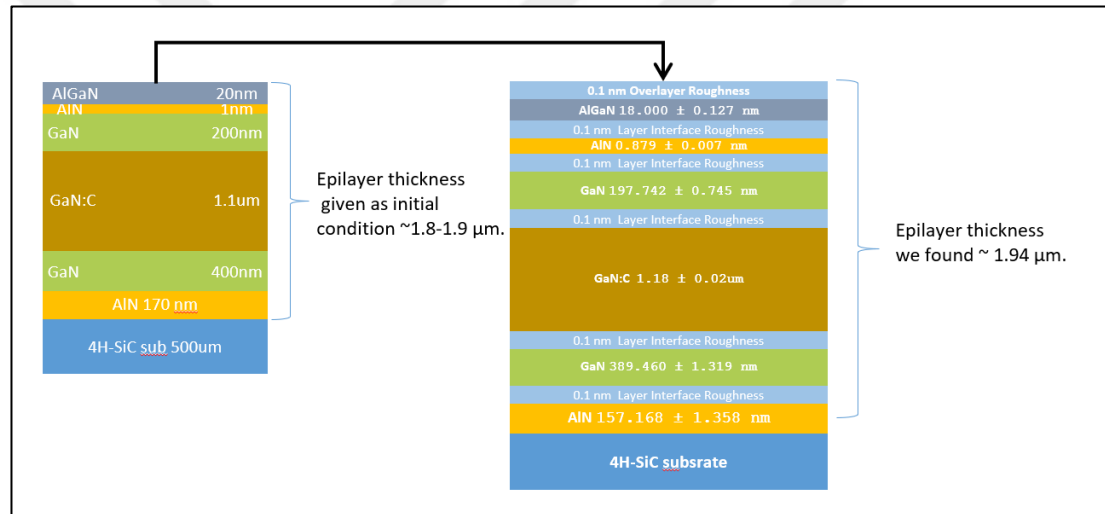


Figure 4.2 : Schematic of GaN on SiC layers

12	☐	0.10	☐	%	☐	AlGaIn_AdnF.dsp	50.00 %	☒	Void.ref	50.00 %	☒	☒
11	☒	18.00				AlGaIn_AdnF.dsp					☒	☒
10	☐	0.10	☒	%	☐	AlN_na.dsp	50.00 %	☒	Void.ref	50.00 %	☒	☒
9	☒	0.90				AlN_na.dsp					☒	☒
8	☐	0.10	☐	%	☐	GaN_HJY.ref	50.00 %	☒	Void.ref	50.00 %	☒	☒
7	☒	197.08				GaN_HJY.ref					☒	☒
6	☐	0.10	☐	%	☐	GaN_HJY.ref	45.00 %	☒	GaN_AdnF.dsp	5.00 %	☒	☒
5	☒	1183.36	☐	%	☐	GaN_HJY.ref	83.79 %	☒	GaN_AdnF.dsp	16.21 %	☒	☒
4	☐	0.10	☐	%	☐	GaN_HJY.ref	50.00 %	☒	Void.ref	50.00 %	☒	☒
3	☒	388.95				GaN_HJY.ref					☒	☒
2	☐	0.10	☐	%	☐	AlN.ref.ref	0.90 %	☒	AlN_osc.dsp	49.55 %	☒	☒
1	☒	157.14	☐	%	☐	AlN.ref.ref	0.90 %	☒	AlN_osc.dsp	99.10 %	☒	☒
5						pwe_c6_3.pwe_c6_3.16h 14mn 34s_II.spe					☒	☒

Figure 4.3 : Simulation of reference layer and material compositions in GaN on SiC

In Figure 4.2, it is stated that the epilayer thickness should be near of 1.8-1.9 μm , according to the initial information provided by the manufacturer. In the analysis

performed, a defect analysis was generally performed based on the possibility of interface and overlayer roughness. During this analysis, the evaluation was made considering that the layer thicknesses were quite close to each other.

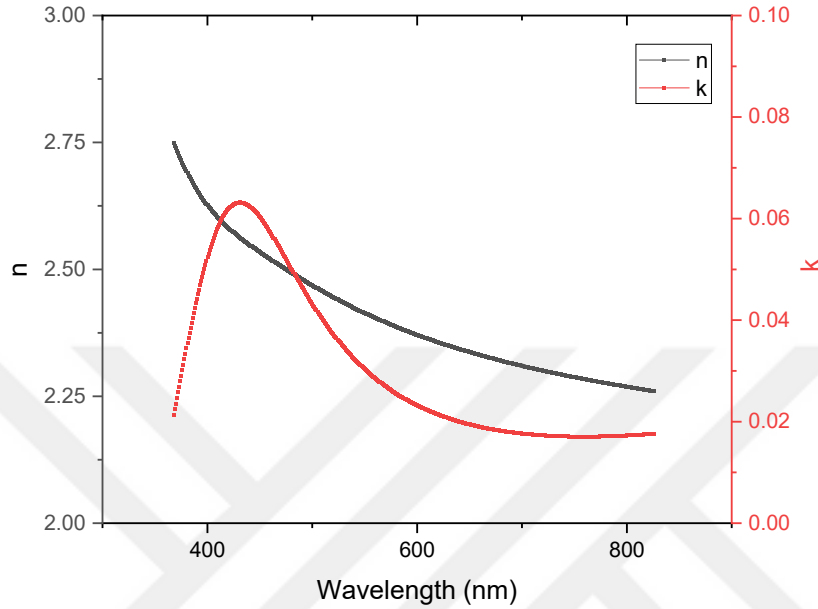


Figure 4.4 : Optical constants of GaN determined from the fit

In Figure 4.4, the analysis results made in the wavelength range of 300-800 nm are presented and the n-k (refractive index and extinction coefficient) parameters were determined for all GaN top-layers. In addition, in Figure 4.5, Psi-Delta values were determined in the measurements made in the wavelength range of 200-1800 nm on the sample. These data permitted a more extensive understanding of the optical and structural properties of GaN layers.

Figure 4.6 shows the chi-square values obtained using different effective medium models such as Bruggeman, EMAMG, SSC, MG, and Best Fit corresponding to five different structural configurations labeled as G8, C4, D5, E6, and F7, all on GaN-on-SiC substrates. Out of the models evaluated, Bruggeman model has the best chi-square values in all cases, and in particular for the F7 configuration, with the highest accuracy in comparison to experimental ellipsometric measurements. This finding supports the accuracy of the Bruggeman Effective Medium Approximation in describing optically inhomogeneous films or rough interfaces, as in the case of GaN-based structures. In

contrast, the SSC model has significantly higher chi-square values for the D5 and G8 geometries, reflecting its inability to accurately capture the complex optical responses for these samples. The Bruggeman model illustrates systematic and clear performance across structures, highlighting its strength and suitability and thereby qualifying it as the most reliable of the efficient medium approximations studied for the characterization of GaN-on-SiC.

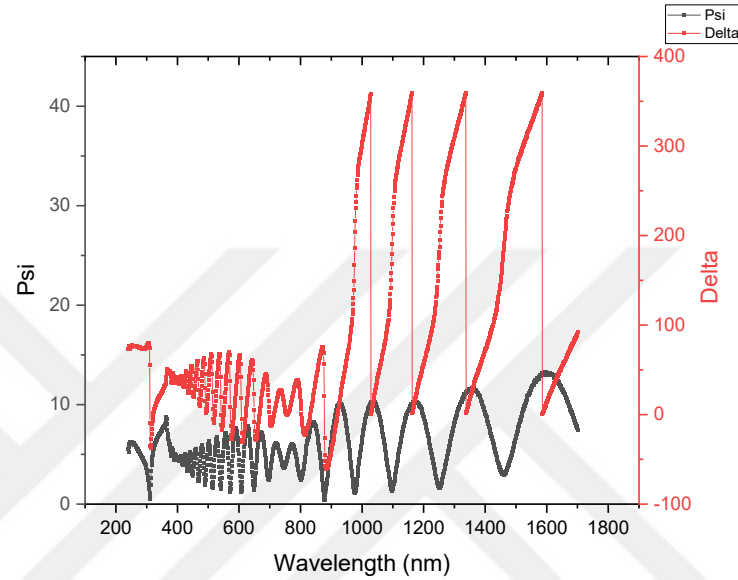


Figure 4.5 : Raw psi and delta of GaN

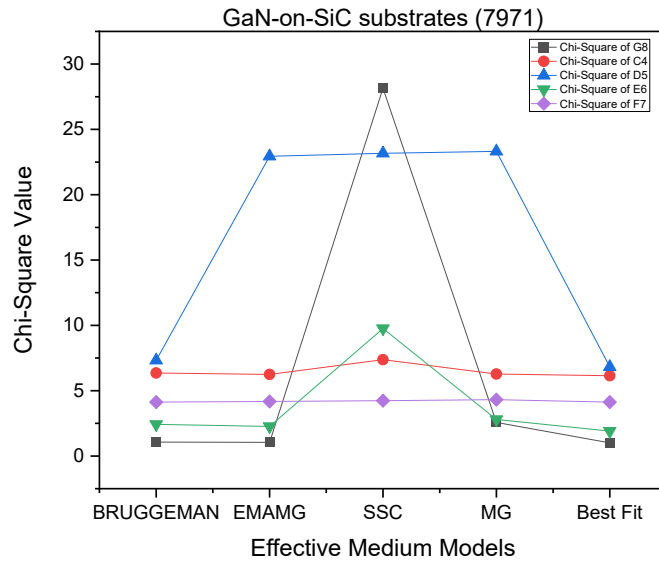


Figure 4.6 : Model fit quality (Chi-Square) for G8, C4, D5, E6 and F14 structures

4.4 Optical Characterization of GaN on Si Material

Sample 7972 is the GaN on Si material provided by CSC and AXITRON within the scope of the EMPIR project named PowerElec [44]. In this thesis, many pieces of these thin films were separated, and sample pieces named D16, F14, H12, and J10 were examined. Preliminary information on these pieces also was obtained by these suppliers.

Sample number 7972 investigated in this thesis consists of a heteroepitaxial structure with a GaN-on-Si structure of 150 mm diameter. The sample has special epitaxial layers optimized for 650 V HEMT devices. The top layer of the structure contains 4 μm thick and $2 \times 10^{16} \text{ cm}^{-3}$ Si-doped GaN, while just below it is a 500 nm thick and $3 \times 10^{18} \text{ cm}^{-3}$ highly doped GaN:Si layer. Under these layers, there is a 1.1 μm thick buffer layer, a 200 nm AlN interlayer, and a 1150 μm thick Si substrate. The sample was grown using the AIX G5+ C MOCVD reactor module with a cassette-cassette chip transport system.

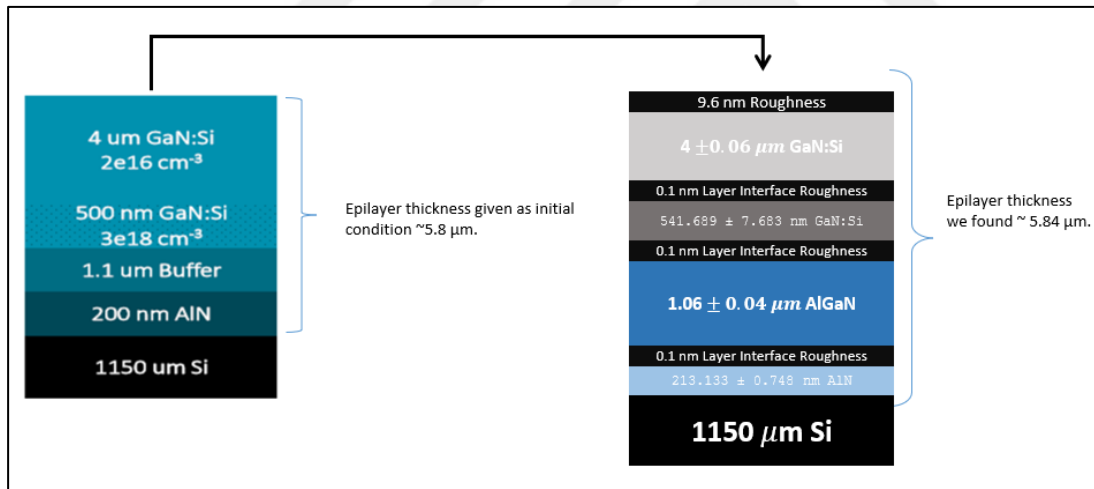


Figure 4.7 : Schematic of GaN on Si layers

In Figure 4.7, it is stated that the epilayer thickness should be near of 5.8 μm , according to the initial condition of top-layers provided by the manufacturer. In the analysis performed, a defect analysis was generally performed based on the possibility of interface and overlayer roughness. During this analysis, the evaluation was made considering that the layer thicknesses were quite close to each other.

8		9.61	%	GaN_HJY.ref	47.84 %	Void.ref	52.16 %	x	x
7	F	4027.25	%	GaN_AdnF2.dsp	17.92 %	GaN_HJY.ref	82.08 %	x	x
6		0.10	%	GaN_HJY.ref	46.00 %	GaN_AdnF.dsp	4.00 %	x	x
5	F	541.67	%	GaN_HJY.ref	92.69 %	GaN_AdnF.dsp	7.31 %	x	x
4		0.10	%	AlGaN_T.dsp	50.00 %	Void.ref	50.00 %	x	x
3	F	1067.00	%	AlGaN_T.dsp				x	x
2		0.10	%	AlN.ref.ref	50.00 %	Void.ref	50.00 %	x	x
1	F	213.31	%	AlN.ref.ref				x	x
				C-si_lsa.ref				x	

Figure 4.8 : Simulation of reference layer and material compositions in GaN on Si

In Figure 4.10, the analysis results made in the wavelength range of 300-800 nm are presented and the n-k (refractive index and extinction coefficient) parameters were determined for all GaN:Si layers. In addition, in Figure 4.9, Psi-Delta values were determined in the measurements made in the wavelength range of 200-1800 nm on the sample. This data allowed a deep understanding of both optical and structural properties of the GaN:Si layers.

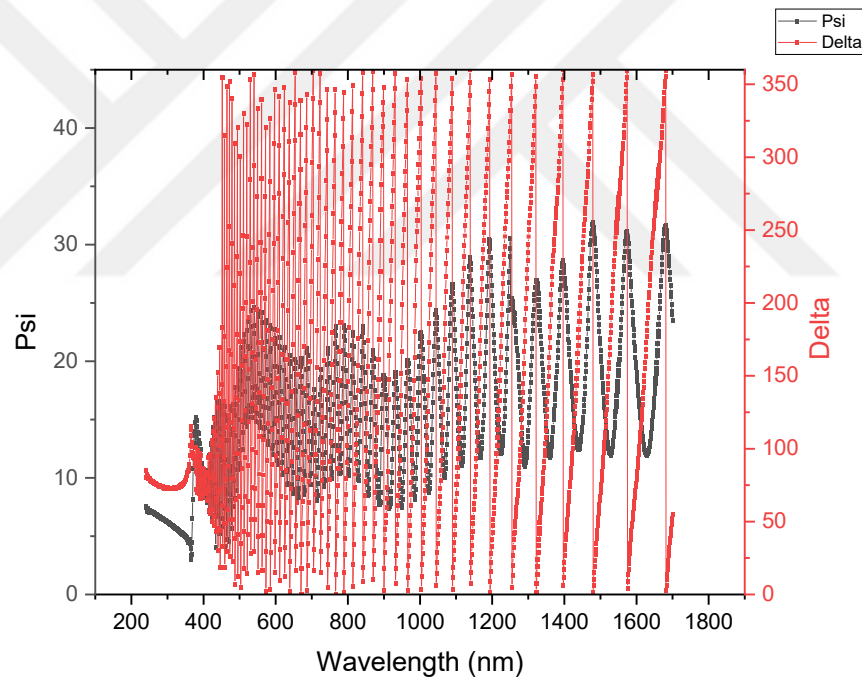


Figure 4.9 : Raw psi and delta of GaN on Si

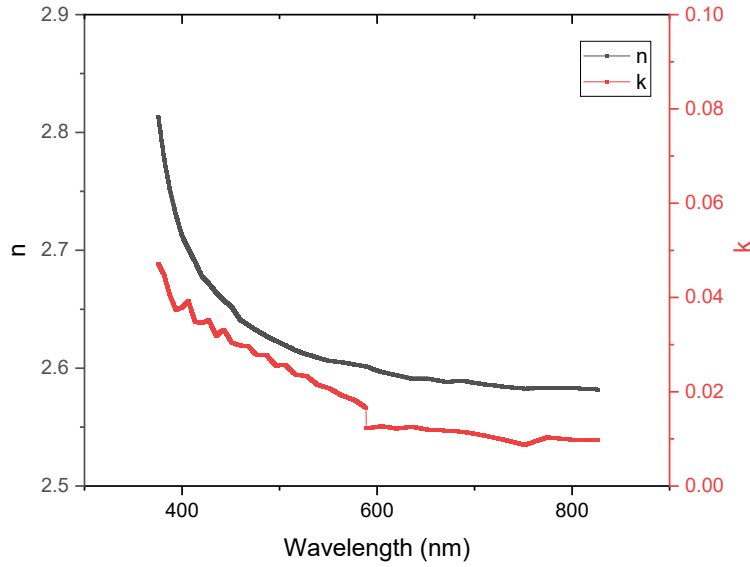


Figure 4.10 : Optical constants of GaN:Si determined from the fit

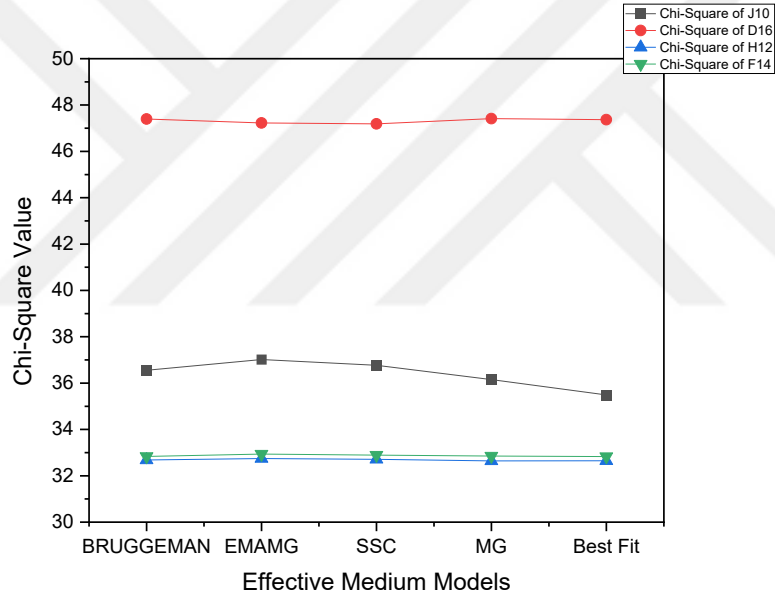


Figure 4.11 : Model fit quality (Chi-Square) for J10, D16, H12, and F14 structures

Figure 4.11 demonstrates the fit goodness of different optical models, i.e., J10, D16, H12, and F14. Of these, the classifications H12 and F14 have lower chi-square values for the entire range of analysis, implying better correspondence between the predicted model and the real-world data. Interestingly enough, the H12 model, which is found to align with Bruggeman Effective Medium Approximation (EMA), records the lowest chi-square values for all through the entire dataset. This phenomenon can imply that using the Bruggeman approach yields the most precise model of the optical response due to its ability to capture inhomogeneous or composite sample

attributes. On the other hand, models like D16, which are presumably built on classical homogeneous layer assumptions, yield considerably higher values for chi-square, implying a poorer correspondence between the model and the observed facts.

4.5 Optical Characterization of SiO₂ on SiC Material

The SiC wafer, WF0053-40-6, tested under this heading is the main sample that will be tested with Imaging-Ellipsometry under the following headings. First of all, this piece has been divided into pieces with and without defects, as stated in other headings, in order to make a defect analysis in an efficient way. The names of these pieces are as follows: E9, C6, B10, E10. According to the preliminary information that the manufacturer has already revealed, no defect has been detected in part E9 of these pieces. Triangle and carrot named defects were encountered in part C6. There is also a triangle defect type in part B10. Finally, there is a carrot defect type in part E10. These defect types are named with these names in the literature[45]. Part C6 was chosen as the piece to be measured under this heading, since this type of defect is larger in size compared to other types of defects and can be seen with an optical microscope.

SiC wafers used in this study have an n⁺ (nitrogen-doped) 4H polycrystalline structure and were cut at a 4-degree angle. The amount of wafers used was determined as $12.5 \pm 0.2 \mu\text{m}$ as seen in Figure 4.12. The doping density is approximately $1.0 \times 10^{16} \text{ cm}^{-3}$. In addition, the wafers have a thermally grown SiO₂ layer. The pre-characterization of these samples was changed with the PerkinElmer Frontier MappIR system and the mapping was done using the Polytec Cvmapp 92A. The growth of these structures was carried out using the AIX-G5-WW-C MOCVD system.

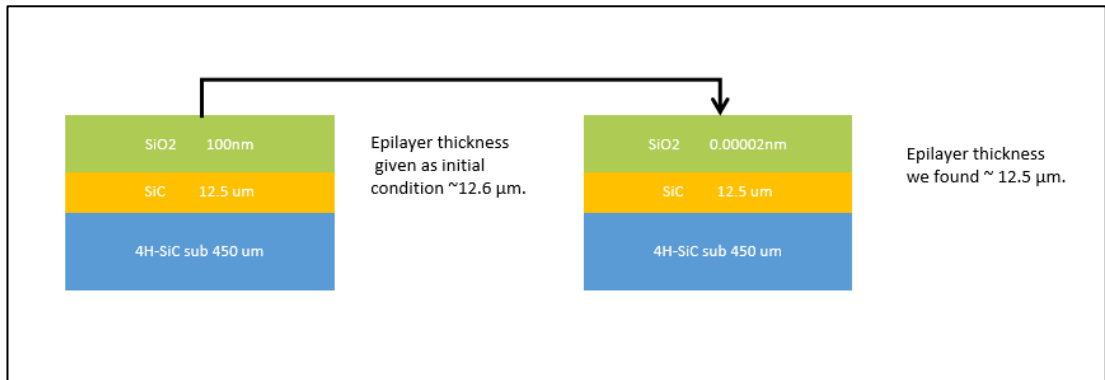


Figure 4.12 : Schematic of SiO₂ on SiC

In Figure 4.12, according to the first data given by the manufacturer, the thickness of the epilayer is about 12.6 μm . Generally, in this analysis, all defect analyses were done considering the possibility of an interface and upper layer roughness. In such a case, considering the fact that the layer thicknesses are very close to each other during this analysis, the assessment is done. The reason it does not exactly equal this initial thickness in this analysis part is that the SiO_2 layer could not be traced in the analysis result.

In Figure 4.13, the SiC-based backscatter baffle has been fully integrated into the device. This was also discussed with other partners and agreement was reached on the same issue. In the study conducted by Kildemo (2004), backscattering and similar optical phenomena observed in 4H-SiC samples were investigated in detail. Similar phenomena were also observed in the samples used in my study. In this context, the effect of backscattering and similar phenomena on the optical properties of 4H-SiC was evaluated in line with the findings of the relevant study [45].

3	[F]	0.00002	SiO2_1sa.ref	x	x
2	[F]	12.50000	SiC_New_amorphous.udf	x	x
1	[F]	449.87495	SiC 4H E.ref	x	x
5			Void.ref		x

Figure 4.13 : Simulation of reference layer and material compositions in SiO_2 on SiC

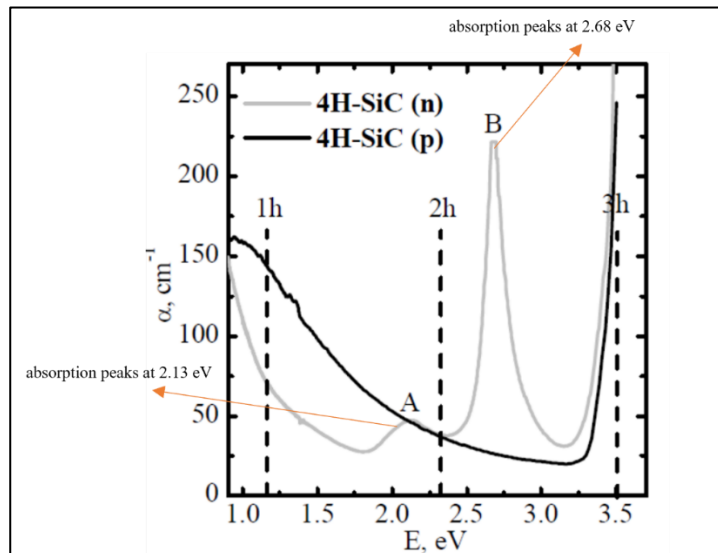


Figure 4.14 : Absorption spectra of n- and p- type 4H-SiC substrates [46]

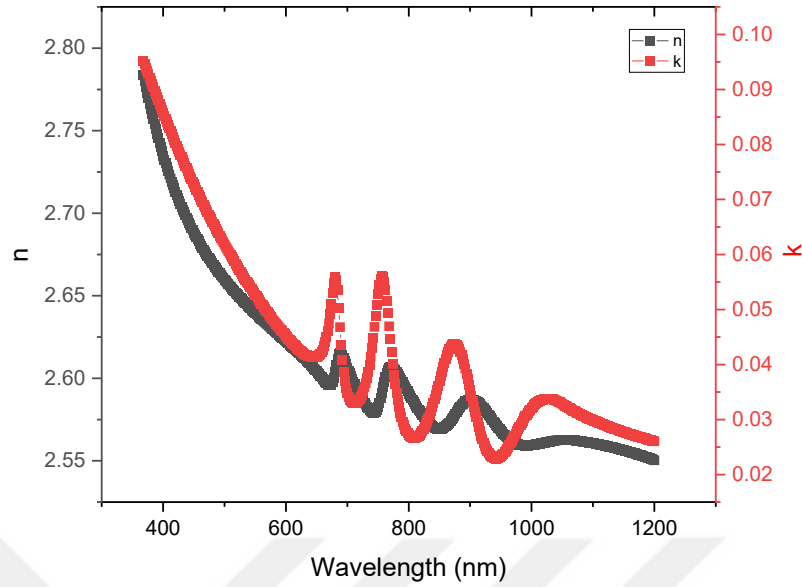


Figure 4.15 : Optical constants of SiC determined from the fit

In this view, the absorption bands referred to in Figure 4.14 were also measured in the present work and as such served as supporting measurements for Kildemo. In the latter study, it was reported that the oscillations observed in 4H-SiC samples were due to interference effects between ordinary and extraordinary modes [47]. This was said to occur as a result of backside reflection in double-sided polished samples, whose thickness reaching to hundreds of micrometers allowed the interference effect [48]. However, as deduced for the investigated samples, the main cause for the oscillations was the interference effect between ordinary and extraordinary wave components reflected from a thick anisotropic layer or plate [49]. This reiterated again the significance of sample structure in the present observations.

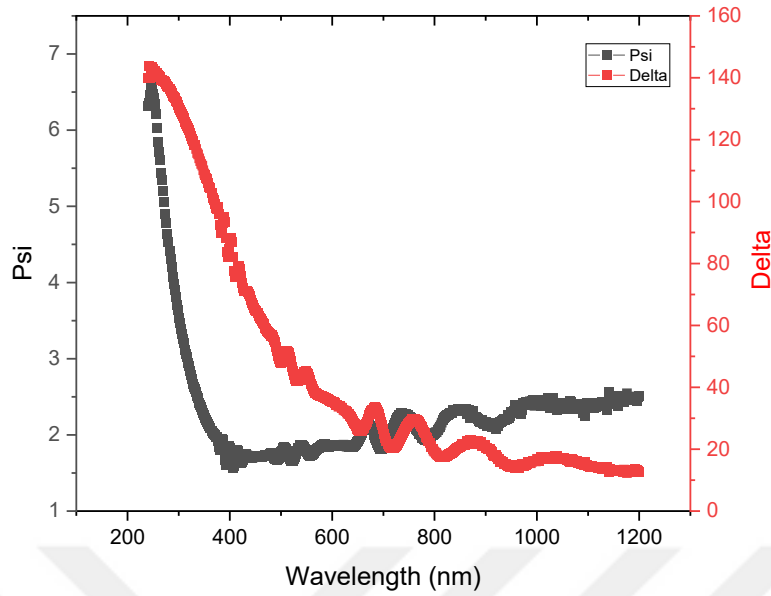


Figure 4.16 : Raw psi and delta of SiO₂ on SiC

4.6 Optical Characterization of Metallic Thin Films for Optical Metrology

In this part of study, the optical characterization of metal thin films was conducted using three types of spectroscopic ellipsometry systems each with a differing modulation mechanism. These systems are found at diverse national research institutes in Türkiye. The ellipsometric structure with rotating analyzer utilized in the present research is the SENresearch 4.0 Spectroscopic Ellipsometer located at the TÜBİTAK UME Quantum Metrology Laboratory. The rotating compensator ellipsometry system utilized was the RC2 Ellipsometer from J.A. Woollam Co., which is an extremely precise instrument currently located at the Sabancı University SUNUM Research Center. Finally, all the measurements related to the photo-elastic modulator (PEM) ellipsometry were performed using instruments at TÜBİTAK MAM (Marmara Research Center).

The refractive index (n) and extinction coefficient (k) of thin films made of sputtered Pt, Nb, and Ru were found using three ellipsometers under identical deposition conditions. Results obtained from the comparison of measurements are relevant to the development of correlations among the instruments and to the ongoing process in the standardization of metrological methods in the case of nanostructured surfaces and metal coatings.

Thin films made from platinum, niobium, and ruthenium were prepared in this current study using direct current magnetron sputtering, which is a commonly followed physical vapor deposition technique for conductive thin films. Deposition was done under ambient temperature under low base pressure conditions less than 10^{-5} Pa for a nominal thickness of 30 nm for all the samples. A pre-cleaning treatment using Argon plasma was done beforehand for removing native oxides from the surface. This fabrication technique ensures minimum surface impurity and compliance under industrial standards for making metrological thin films.

The suitability of such deposition conditions for traceable optical metrology was previously validated in Hansen et al. (2025), where thin films prepared under comparable vacuum levels and sputtering parameters were shown to achieve expanded uncertainties in refractive index determination as low as 0.002 ($k=2$) across the 400–1000 nm spectral range [50].

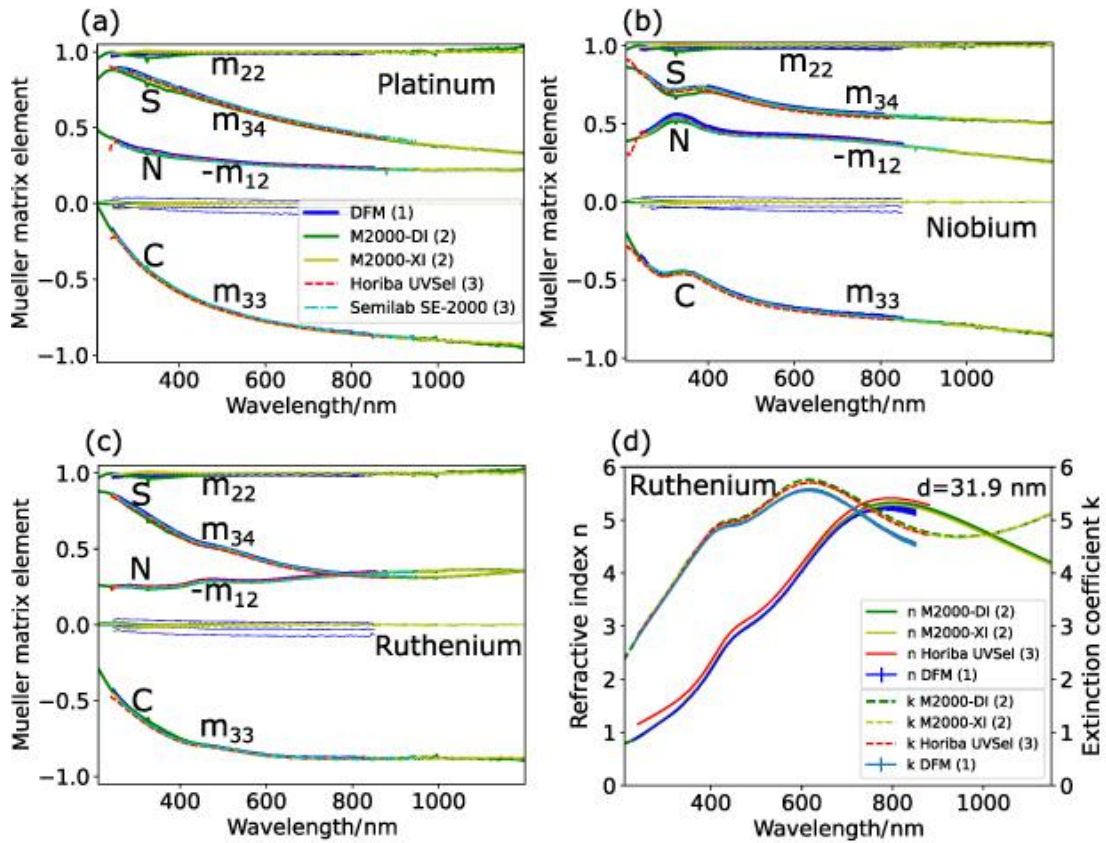


Figure 4.17 (a)–(d) : Data reproduced from Hansen et al. [50] for validation

The accuracy of results acquired was assessed through comparison between n and k spectra for platinum (Pt), niobium (Nb), and ruthenium (Ru) films and well-established reference databases from published work in learned journals. For example, Hansen et al. (2025) carried out comprehensive multi-instrumental research using five different commercial ellipsometers for analyzing metallic thin films, all of nominal 30 nm thickness, under different modulation modes.

Figure 4.17 (a)–(d), given by Hansen et al., shows that ruthenium's refractive index and extinction coefficient values have similar dispersion behavior using different instruments such as DFM, M2000-DI/XI, Horiba UVISEL, and Semilab SE-2000. The deviation is normally limited to ± 0.05 for n and ± 0.1 for k for a wavelength range from 400 to 1000 nm [50].

Current research has produced similar results using the RC2, PEM, and rotating compensator ellipsometers located at TÜBİTAK and SUNUM. The spectral results characterizing the extinction coefficient (k) and its relation to the refractive index (n) for ruthenium (Ru), niobium (Nb), and platinum (Pt) (see Figures 4.18–4.20) present a high degree of correlation for different systems, with discrepancies identified being well within those defined by Hansen for such a study. This result provides a solid demonstration of reproducibility between instruments and justifies metrological calibration between these devices and their counterpart commercial instruments.

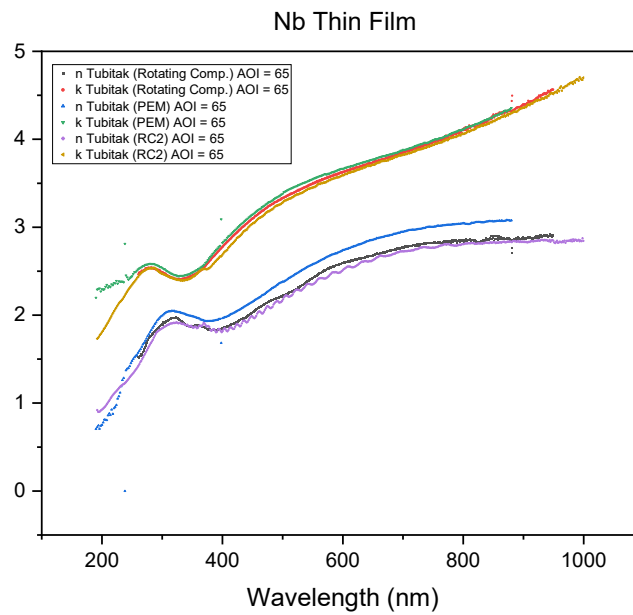


Figure 4.18 : Niobium thin film refractive index (n) and extinction coefficient (k) measurements using multiple ellipsometers

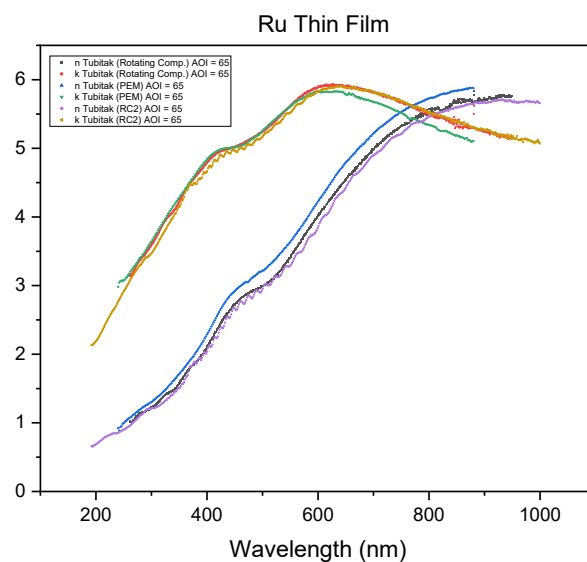


Figure 4.19 : Ruthenium thin film refractive index (n) and extinction coefficient (k) measurements using multiple ellipsometers

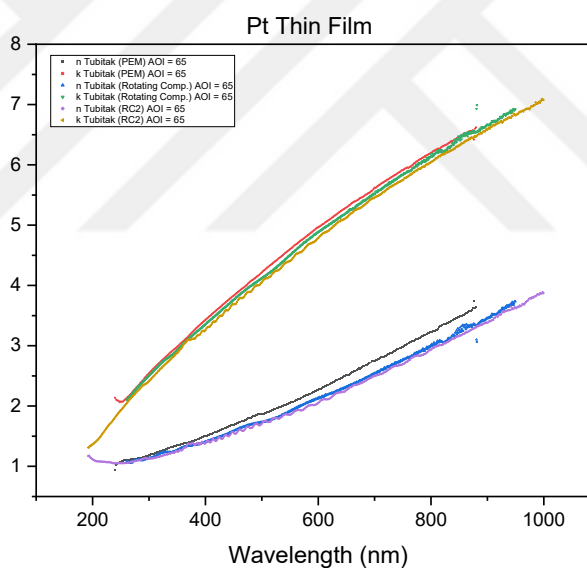


Figure 4.20 : Platinum thin film refractive index (n) and extinction coefficient (k) measurements using multiple ellipsometers

5. HOME-MADE IMAGING ELLIPSOMETRY SETUP

It was understood from the findings and evaluations made in the previous sections that spectroscopic ellipsometry has some limitations when analyzing defects in materials. To get rid of such limitations, an analysis technique of defects which is more sensitive and comprehensive has been developed. In this respect, this section of the thesis will introduce the Imaging-Ellipsometry system that was designed and realized in the lab for these purposes.

The basic principles, technical details, and the way this system works will be introduced and discussed in detail. Applications and findings received by using this novel setup to get more precise and accurate analyses for defects in materials examined within this thesis are also given.

These analyses will probably contribute significantly to further investigations of the influence of defects on the optical and physical properties of materials and a better understanding of these parameters critical for material performance. Finally, this contribution tries to present Imaging Ellipsometry as the new, effective technique for defect analysis in material sciences.

5.1 Imaging Ellipsometry Setup

In classical spectroscopic ellipsometry, the area under investigation is illuminated by a focused beam from a broadband spectral light source, such as a Xenon arc lamp, and detected by spectrally resolved detectors such as CCD or diode arrays. The illuminated spot is typically on the order of a few square millimeters, but it can be further reduced using focusing optics. However, the resulting data represent a spatial average over the illuminated region and therefore do not provide direct information about the shape, size, or spatial distribution of individual surface features or defects on the micrometer scale.

Imaging ellipsometry offers an alternative approach in which a single-wavelength laser source is used in combination with a two-dimensional CCD detector. In this configuration, each pixel of the CCD array captures the reflected light independently, allowing for spatially resolved analysis of the sample. By analyzing the polarization state at each pixel, local variations in the sample's optical response can be mapped. These pixel-wise results can then be reconstructed into a spatially resolved dataset, enabling the characterization of defect shape, size, and distribution across the sample surface [51].

5.1.1 Optical Configuration and principle

Figure 5.1 shows the optical configuration of our Imaging Ellipsometry system. As a light source multiple wavelength laser source (Research Electro-optic Tunable Helium-Neon Laser, 633nm, 612nm, 604nm, 594nm and 543nm) used with diffusers or spectral lamps with wavelength filters can be used. It is collimated by a spatial filter system (Thorlabs, KT311). Polarization state is controlled by a motorized compensator (X-RSW-E series motorized rotary stage, and B-Halle zero-order quarter wave plate), C, and motorized-analyzer (X-RSW-E series motorized rotary stage and B-Halle Glan-Thompson Polarizing Prisms). A high NA objective (40X Nikon Plan Fluorite Imaging Objective, 0.75 NA) provides a wide range of incident angles and focuses beam to a small spot size. Beam splitter, BS (BS-013, 50:50 non-polarizing beamsplitter cube), provides align the laser source to the optical path. Finally, through a tube lens (TTL200-S8, 200mm tube lens), the amplitude distribution in the BFP (Back Focal Plane) of the objective is transmitted to the image plane of a CDD camera (Retiga-R6) which periodically captures the BFP image at compensator angles.

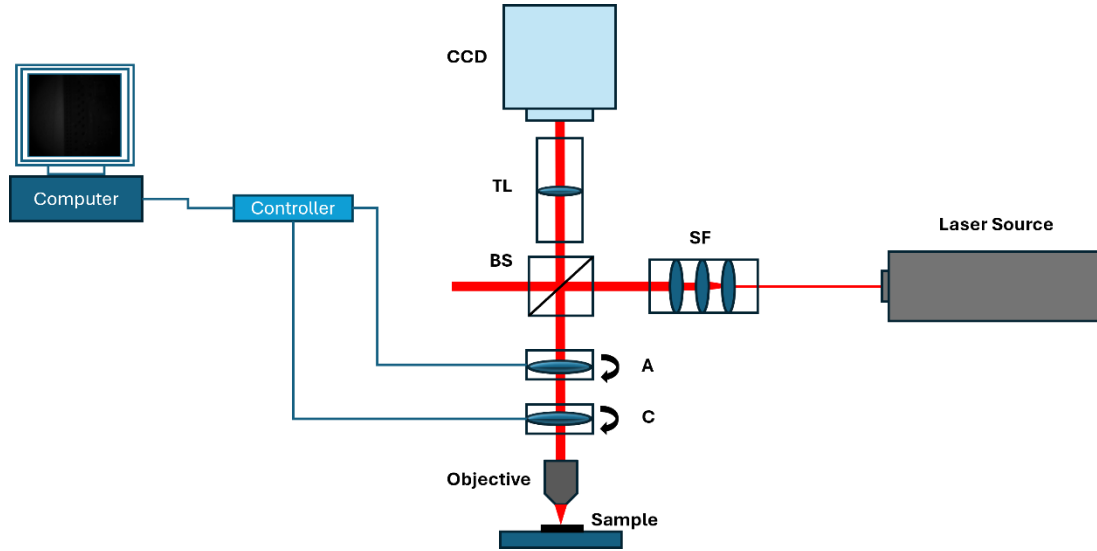


Figure 5.1 : Schematic of a Imaging-ellipsometry optical configuration with rotary compensator and analyzer : TL - tube lens, A - polarizer and analyzer, C - rotary compensator, BS - beam splitter, SF – Spatial filter

CCD takes pictures at various compensator angles. Generally, for an isotropic case, the Jones matrix can model the electric field of the optical system, defined as in Eq. (5.1).

Here, J_A , J_C , J_P , and J_S represent the Jones matrices of the analyzer, compensator, polarizer and sample, respectively. These matrices incorporate the corresponding rotation matrices and δ represents the retardance of a quarter-wave plate.

$$\begin{aligned}
 L_{OUT} = & J_A \times R(A') \times R(-C') \times J_C(\delta) \times R(C') \\
 & \times J_S \times R(-C') \times J_C(\delta) \times R(C') \times R(-P') \times J_P \times L_{IN}
 \end{aligned} \tag{5.1}$$

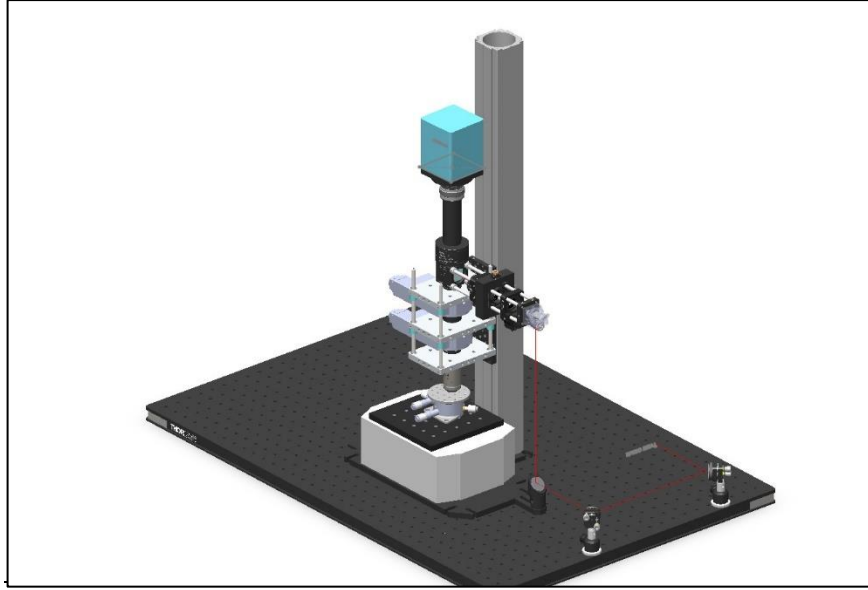


Figure 5.2 : SolidWorks view of Imaging-Ellipsometry setup

Figure 5.2 also presents the SolidWorks schematic of Imaging Ellipsometry setup. For this setup, a motorized Z-stage holds a CCD camera which illuminates a test specimen placed in a horizontal position. The polarizer is placed in front of the sample, with an analyzer placed behind, which ensures examination of the polarization state of light coming from the sample.

Figure 5.3 shows a 3D cone illustrating how light rays at various angles of incidence form a conical volume. Each ray corresponds to a specific in-plane wave vector component. Equation 5.2 expresses how the angular distribution of these rays can be computed using the numerical aperture (NA) and the normalized radial position:

$$\theta = \sin^{-1} \left(\frac{\rho(\theta)}{\rho(\theta_{max})} \times NA \right) \quad (5.2)$$

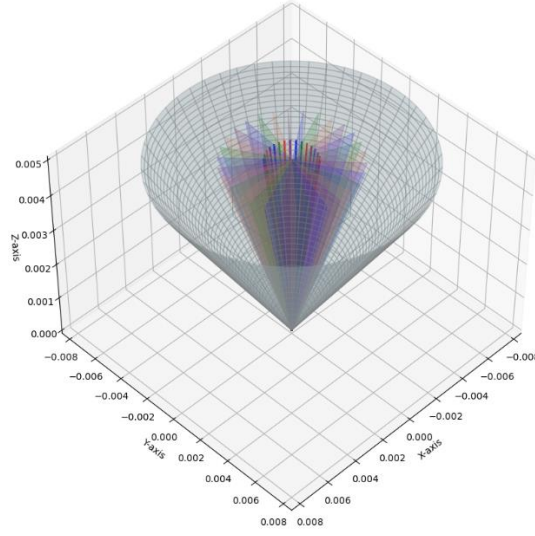


Figure 5.3 : 3D Cone view with rays and planes of incidence

Figure 5.4 shows the circular light pattern captured on the CCD along with sampled grid points. These points, evenly distributed within the circular area, enable angle-resolved ellipsometric measurements. Each pixel corresponds to a distinct angular component, making it possible to resolve local deviations or defects on the sample surface with high angular precision.

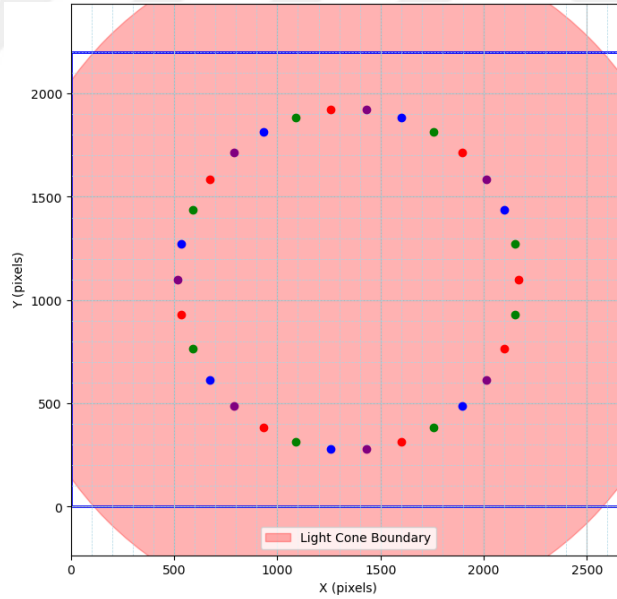


Figure 5.4 : CCD with circular light area and gridlines

The optical design outlined in this paper allows for research into surface defects in materials such as silicon carbide (SiC), similar to research by Grundmann et al. (2024) [52]. The goal of this project is to replicate and improve upon the methods described in the reference publication in order to achieve high-resolution angle measurements that allow for in-depth defect analysis.

6. RESULTS AND DISCUSSION

Classical spectroscopic ellipsometry, which is used throughout this study as a probing tool for defect detection, shows us that this tool has some drawbacks for the assessment of defects. The ellipsometer has a beam spot of about 1.2 mm and, from this beam on a macroscopic average, does the inverse calculation for microscopic properties such as defects in materials. However, comparing the defect sizes/shapes in this study to such beam spot size and also considering that the method relies on fitting measurement data to a proper model, only defect sizes of certain defect concentrations that can be modelled as voids in layers can be analyzed. Classically, spectroscopic ellipsometry is not suited to evaluating shapes at micrometer scales.

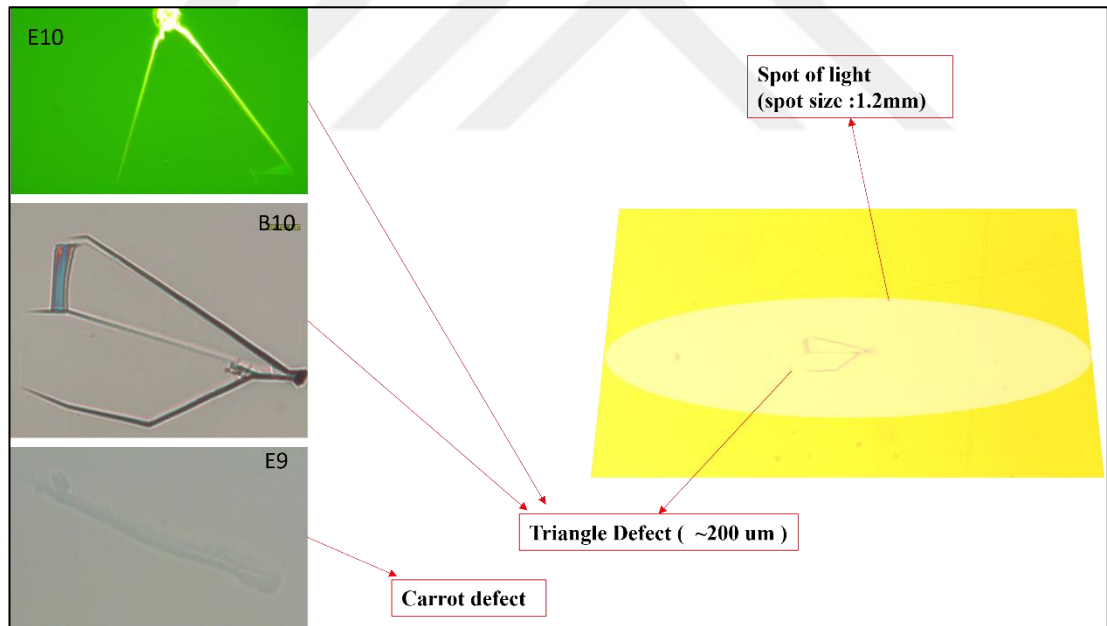


Figure 6.1 : Illustrate of the defect size and shapes

Throughout the project, with several discussions during the project meetings and online discussions, it is concluded that the imaging ellipsometry, which uses 2D camera pixels as a detector array to decrease the area under test to a significantly smaller spot, would be a better-suited approach to investigate defect sizes and shapes.

This technique can be supported by other techniques, such as AFM, which, in turn, is not possible in the case of spectroscopic ellipsometry.

The spectroscopic ellipsometry could further support in sample property characterization-a priori information for other methods like imaging ellipsometry in multiple layers.



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APPENDICES

APPENDIX A: C++ libraries for rotary analyzer configuration

```
// furkans.forellipsometry.cpp
#include <vector>
#include <random>
#include <tuple>
#include <furkans.fresnelcalculations.h>
#include <furkans.forellipsometry.h>
#include <cmath>
#include <complex>
#include <iomanip>
#include <iostream>
using namespace std::complex_literals;
namespace furkans
{
    namespace forellipsometry
    {
        std::complex<double> r_f_m(std::complex<double> ref_index,
double theta_i, bool deg)
        {
            auto rp = furkans::fresnelcalculations::r_u_amp(ref_index,
theta_i, deg);
            auto rs = furkans::fresnelcalculations::r_a_amp(ref_index,
theta_i, deg);

            return rp / rs;
        }

        double degrees_to_radians(double degrees)
        {
            return degrees * M_PI / 180.0;
        }

        std::complex<double> r_f_tpsi_Delta(double tanpsi, double
Delta, bool deg)
        {
            double d = deg ?
furkans::forellipsometry::degrees_to_radians(Delta) : Delta;
```

Figure A.6.1 : C++ code for ellipsometry system outputs

```

std::pair<double, double> tpsi_Delta_f_r(const std::complex<double>
&rho, bool deg)
{
    double Delta = std::atan2(-1.0 * rho.imag(), rho.real());

    if (rho.real() < 0)
    {
        if (rho.imag() > 0)
        {
            Delta += M_PI;
        }
        else
        {
            Delta -= M_PI;
        }
    }

    double tanpsi = std::abs(rho);

    if (deg)
    {
        Delta = Delta * 180.0 / M_PI;
        Delta =
furkans::forellipsometry::normalizeDelta(Delta);
    }

    return std::make_pair(tanpsi, Delta);
}

double normalizeDelta(double Delta)
{
    if (Delta < 0.0)
    {
        Delta += 180.0;
    }
    if (Delta >= 180.0)
    {
        Delta -= 180.0;
    }
    return Delta;
}

```

Figure A.1 (continue) : C++ code for ellipsometry system outputs

```

std::complex<double> m_f_r(std::complex<double> rho, double theta_i,
bool deg)
{
    double theta;
    if (deg = true)
    {
        theta = theta_i * M_PI / 180.0;
    }
    else
    {
        theta = theta_i;
    }
    std::complex<double> e_index = std::sqrt(1.0 - 4.0 * rho *
std::pow(sin(theta), 2) / (std::pow((1.0 + rho), 2)));

    return std::tan(theta) * e_index;
}
std::complex<double> m_f_tpsi_Delta(double tanpsi, double
Delta, double theta_i, bool deg)
{
    std::complex<double> rho = r_f_tpsi_Delta(tanpsi, Delta,
deg = true);

    return m_f_r(rho, theta_i, true);
}
std::vector<double> generate_signal(const std::vector<double> &phi,
double IDC, double IS, double IC, double noise, bool deg)
{
    std::vector<double> result;
    result.reserve(phi.size());

    std::random_device rd;
    std::mt19937 gen(rd());
    std::normal_distribution<double> distribution(0, noise);
    for (const auto &angle : phi)
    {
        double phi_radians;
        if (deg = true)
        {
            phi_radians = angle * M_PI / 180.0;
        }
    }
}

```

Figure A.1 (continue): C++ code for ellipsometry system outputs

```

else
    {
        phi_radians = angle;
    }
    double base = (IDC + (IS * std::sin(2.0 * phi_radians))
+ (IC * std::cos(2.0 * phi_radians)));
    double noise_value = distribution(gen);
    result.push_back(base + noise_value);
}

return result;
}

std::vector<double> generate_signal_f_m(const
std::vector<double> &phi, std::complex<double> ref_index, double
theta_i, double Polarizer_angle, double average, double noise, bool
deg)
{
    std::vector<double> result;
    result.reserve(phi.size());

    double P_r;

    if (deg = true)
    {
        P_r = Polarizer_angle * M_PI / 180.0;
    }
    else
    {
        P_r = Polarizer_angle;
    }

    for (const auto &angle : phi)
    {
        double phi_r;
        if (deg = true)
        {
            phi_r = angle * M_PI / 180.0;
        }
        else
        {
            phi_r = angle;
        }
    }
}

```

Figure A.1 (continue) : C++ code for ellipsometry system outputs

```

std::complex<double> par =
furkans::fresnelcalculations::r_u_amp(ref_index, theta_i, true) *
std::cos(P_r) * std::cos(phi_r);
    std::complex<double> per =
furkans::fresnelcalculations::r_a_amp(ref_index, theta_i, true) *
std::sin(P_r) * std::sin(phi_r);
        double base = std::pow(std::cos(P_r), 2) *
std::pow(std::abs(par + per), 2);

        std::random_device rd;
        std::mt19937 gen(rd());
        double noise_value =
std::normal_distribution<double>(0, noise)(gen);

        result.push_back((average * base) + noise_value); //
    }

    return result;
}

std::pair<std::complex<double>, std::vector<double>> r_f_data(
    const std::vector<double> &phi, const std::vector<double>
&signal, double Polarizer_angle, bool Quarter_wave_plate = false, bool
deg = false)
{

    double P_radians;
    std::vector<double> phi_radians;

    if (deg)
    {
        P_radians = M_PI * Polarizer_angle / 180.0;
        for (const auto &angle : phi)
        {
            phi_radians.push_back(M_PI * angle / 180.0);
        }
    }
    else
    {
        P_radians = Polarizer_angle;
        phi_radians = phi;
    }
    double I_ave, alpha, beta;

```

Figure A.1 (continue): C++ code for ellipsometry system outputs

```

std::tie(I_ave, alpha, beta) = ff_coeffie(phi, signal, deg);

    std::complex<double> factor;

    double tanPC;
    if (Quarter_wave_plate)
    {
        tanPC = std::tan(P_radians + M_PI / 4.0);
        factor = (1.0 + 1i * tanPC) / (1.0 - 1i * tanPC);
    }
    else
    {
        factor = std::tan(P_radians);
    }

    std::complex<double> delta(1.0 - alpha * alpha - beta *
beta, 0.0);
    std::complex<double> rho = (1.0 + alpha) / (beta - 1i *
std::sqrt(delta)) * factor;

    std::vector<double> fit;
    for (const auto &angle : phi_radians)
    {
        fit.push_back(I_ave * (1.0 + alpha * std::cos(2.0 *
angle) + beta * std::sin(2.0 * angle)));
    }

    if (0.0 <= Polarizer_angle && Polarizer_angle <= M_PI /
2.0)
    {
        return std::make_pair(rho, fit);
    }

    return std::make_pair(std::conj(rho), fit);
}

std::pair<std::complex<double>, std::vector<double>>
r_f_POA(const std::vector<double> &phi, const std::vector<double>
&signal, double Polarizer_angle, bool deg = false)
{
    size_t n = phi.size();
    std::vector<double> phi_radians(n);
    double P_radians;

```

Figure A.1 (continue) : C++ code for ellipsometry system outputs

```

if (deg)
{
    P_radians = Polarizer_angle * M_PI / 180.0;
    std::transform(phi.begin(), phi.end(),
        phi_radians.begin(), [](double deg)
        { return deg * M_PI / 180.0; });
    else
    {
        P_radians = Polarizer_angle; phi_radians = phi; }
    auto [I_ave, alpha, beta] = ff_coeffie(phi, signal, deg);
    double tanpsi = std::sqrt((1.0 + alpha) / (1.0 - alpha)) *
std::fabs(std::tan(P_radians));
    double Delta = std::acos(beta / std::sqrt(1.0 -
std::pow(alpha, 2)));
    std::complex<double> rho = tanpsi * std::exp(1i * Delta);
    std::vector<double> fit(n);
    for (size_t i = 0; i < n; ++i)
    { fit[i] = I_ave * (1 + alpha * std::cos(2.0 *
phi_radians[i]) + beta * std::sin(2.0 * phi_radians[i]));
    }
    return std::make_pair(rho, fit);
}
std::tuple<double, double, double> ff_coeffie(const std::vector<double>
&phi, const std::vector<double> &signal, bool deg)
{
    size_t n = phi.size();
    std::vector<double> phi_radians;
    if (deg)
    { phi_radians.reserve(n);
if (deg)
    {
        P_radians = Polarizer_angle * M_PI / 180.0;
        std::transform(phi.begin(), phi.end(),
            phi_radians.begin(), [](double deg)
            { return deg * M_PI / 180.0; });
        else
        {
            P_radians = Polarizer_angle;
            phi_radians = phi; }
        auto [I_ave, alpha, beta] = ff_coeffie(phi, signal, deg);
        double tanpsi = std::sqrt((1.0 + alpha) / (1.0 - alpha)) *
std::fabs(std::tan(P_radians));
        double Delta = std::acos(beta / std::sqrt(1.0 -
std::pow(alpha, 2)));
        std::complex<double> rho = tanpsi * std::exp(1i * Delta);
        std::vector<double> fit(n);
        for (size_t i = 0; i < n; ++i)
        { fit[i] = I_ave * (1 + alpha * std::cos(2.0 *
phi_radians[i]) + beta * std::sin(2.0 * phi_radians[i]));
        }
    }
}

```

Figure A.1 (continue): C++ code for ellipsometry system outputs

```

for (size_t i = 0; i < n; ++i)
{
    phi_radians.push_back(phi[i] * M_PI / 180.0);
}
else
{
    phi_radians = phi;
}

double I_ave = 0.0;
double I_S = 0.0;
double I_C = 0.0;

for (size_t i = 0; i < n; ++i)
{
    I_ave += signal[i];
    I_S += 2.0 * signal[i] * std::sin(2.0 *
phi_radians[i]);
    I_C += 2.0 * signal[i] * std::cos(2.0 *
phi_radians[i]);
}

I_ave /= n;
I_S /= n;
I_C /= n;

double alpha = I_C / I_ave;
double beta = I_S / I_ave;

return std::make_tuple(I_ave, alpha, beta);
}

std::vector<double> generate_signal_f_r(const std::vector<double> &phi,
const std::complex<double> &rho, double Polarizer_angle, bool
Quarter_wave_plate, int average, double noise, bool deg)
{
    {
        double P_radians;
        if (deg = true)
        {
            P_radians = Polarizer_angle * M_PI / 180.0;
        }
    }
}

```

Figure A.1 (continue) : C++ code for ellipsometry system outputs

```

else
{
    P_radians = Polarizer_angle;
}
std::vector<double> phi_radians;
phi_radians.reserve(phi.size());
for (double angle : phi)
{
    phi_radians.push_back(deg ? M_PI * angle / 180.0 :
angle);
}
double tanpsi = std::abs(rho);
double Delta = std::arg(rho);

double alpha, beta;
if (Quarter_wave_plate)
{
    double psi = std::atan(tanpsi);
    alpha = -std::cos(2.0 * psi);
    beta = std::sin(2.0 * psi) * std::cos(Delta + 2.0 *
P_radians);
}
else
{
    double tanP = std::tan(P_radians);
    double denom = tanpsi * tanpsi + tanP * tanP;
    alpha = (tanpsi * tanpsi - tanP * tanP) / denom;
    beta = (2.0 * tanpsi * std::cos(Delta) * tanP) /
denom;
}
std::vector<double> signal(phi.size());
for (int i = 0; i < phi.size(); ++i)
{
    signal[i] = average * (1.0 + alpha * std::cos(2.0 *
phi_radians[i]) + beta * std::sin(2.0 * phi_radians[i]));
    if (noise > 0)
    {
        signal[i] +=
std::normal_distribution<double>(0,
noise)(std::mt19937(std::random_device())));
    }
} return signal;
} } }

```

Figure A.1 (continue) : C++ code for ellipsometry system outputs

```

// furkans_fresnel.cpp
#ifndef FURKANS_FRESNEL_CPP
#define FURKANS_FRESNEL_CPP
#include <cmath>
#include <furkans.fresnelcalculations.h>
namespace furkans
{
    namespace fresnelcalculations
    {
        std::pair<double, std::complex<double>>
_underlee(std::complex<double> ref_index, double theta_i, double n_i,
bool deg)
        {
            double theta;
            if (deg == true)
            {
                theta = theta_i * M_PI / 180.0;
            }
            else
            {
                theta = theta_i;
            }

            std::complex<double> m2 = std::pow(ref_index / n_i, 2);
            double c = std::cos(theta);
            double s = std::sin(theta);
            double a = std::pow(s, 2);
            std::complex<double> d = std::sqrt(m2 - a);

            if (ref_index.imag() == 0)
            {
                d = std::conj(d);
            }

            return std::make_pair(c, d);
        }

        double R_u(double ref_index, double theta_i, double n_i, bool
deg)
        {
            return std::abs(std::pow(r_u_amp(ref_index, theta_i, n_i,
deg), 2));
        }
    }
}

```

Figure A.6.4 : C++ code for Fresnel equations

```

double R_a(double ref_index, double theta_i, double n_i, bool deg)
{
    return std::abs(pow(r_a_amp(ref_index, theta_i, n_i, deg),
2));
}

std::complex<double> real_if_close(const std::complex<double>
&value, double tol)
{
    if (std::abs(value.imag()) < tol)
    {
        return std::complex<double>(value.real(), 0.0);
    }
    return value;
}

std::complex<double> r_a_amp(std::complex<double> ref_index,
double theta_i, double n_i, bool deg)
{
    auto cosines = _underlee(ref_index, theta_i, n_i, deg);
    std::complex<double> rs = (cosines.first - cosines.second)
/ (cosines.first + cosines.second);

    return real_if_close(rs);
}

std::complex<double> r_u_amp(std::complex<double> ref_index,
double theta_i, double n_i, bool deg)
{
    auto cos_values = _underlee(ref_index, theta_i, n_i, deg);

    std::complex<double> m2 = (ref_index / n_i) * (ref_index /
n_i);

    std::complex<double> rp = (m2 * cos_values.first -
cos_values.second) / (m2 * cos_values.first + cos_values.second);

    return real_if_close(rp);
}

double R_a(double ref_index, double theta_i, double n_i, bool deg)
{

```

Figure A.2 (continue) : C++ code for Fresnel equations

```

    double r_un_light(double ref_index, double theta_i, double n_i,
bool deg)
    {
        return (R_u(ref_index, theta_i, n_i, deg) + R_a(ref_index,
theta_i, n_i, deg)) / 2;
    }

    double t_un_light(double ref_index, double theta_i, double n_i,
bool deg)
    {
        return (T_u(ref_index, theta_i, n_i, deg) + T_a(ref_index,
theta_i, n_i, deg)) / 2;
    }

    double t_u_amp(double ref_index, double theta_i, double n_i,
bool deg)
    {
        auto cosines = _underlee(ref_index, theta_i, n_i, deg);
        double m2 = pow(ref_index / n_i, 2);
        double tp = 2 * std::real(cosines.first) * (ref_index /
n_i) / (m2 * std::real(cosines.first) + std::real(cosines.second));
        return std::abs(tp);
    }

    double t_a_amp(double ref_index, double theta_i, double n_i,
bool deg)
    {
        auto cosines = _underlee(ref_index, theta_i, n_i, deg);
        double ts = 2 * std::real(cosines.second) / (ref_index /
n_i) / (std::real(cosines.first) + std::real(cosines.second));
        return std::abs(ts);
    }

    double T_u(double ref_index, double theta_i, double n_i, bool
deg)
    {
        auto cosines = _underlee(ref_index, theta_i, n_i, deg);
        double m2 = pow(ref_index / n_i, 2);
        double tp = 2 * std::real(cosines.first) * (ref_index /
n_i) / (m2 * std::real(cosines.first) + std::real(cosines.second));
        return std::abs(std::real(cosines.second) /
std::real(cosines.first) * std::pow(std::abs(tp), 2));
    }

```

Figure A.2 (continue) : C++ code for Fresnel equations

```

double critical_angle(double ref_index, double n_i, bool deg)
{
    std::complex<double> argument = ref_index / n_i;
    double asin_result = std::asin(std::abs(argument));

    if (deg)
    {
        return asin_result * 180.0 / M_PI;
    }

    return asin_result;
}

double T_a(double ref_index, double theta_i, double n_i, bool
deg)
{
    auto cosines = _underlee(ref_index, theta_i, n_i, deg);
    double ts = 2 * std::real(cosines.first) /
(std::real(cosines.first) + std::real(cosines.second));
    return std::abs(std::real(cosines.second) /
std::real(cosines.first) * std::pow(std::abs(ts), 2));
}

double brewster_calculation(double ref_index, double n_i, bool
deg)
{
    if (deg)
    {
        return std::atan2(ref_index, n_i) * 180 / M_PI;
    }
    return std::atan2(ref_index, n_i);
}
}
#endif // FURKANS_FRESNEL_CPP

```

Figure A.6.6 : Programme code named light intensity

```

double critical_angle(double
ref_index, double n_i, bool deg)
{

```

Figure A.2 (continue) : C++ code for Fresnel equations

```

//.\isikyogunlugu.exe
#include <iostream>
#include <cmath>
#include <vector>
#include <complex>
#include "furkans.forellipsometry.h"
#include "furkans.fresnelcalculations.h"
#include <algorithm>
#include <random>
#include <numeric>

int main()
{

    double a = 4.0;
    double b = 1.0;
    double c = 1.0;
    double error = 0.0001;

    const int num_points = 90;
    std::vector<double> degrees(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        degrees[i] = i * 360.0 / num_points;
    }

    std::vector<double> phi_X(degrees.size());
    std::transform(degrees.begin(), degrees.end(), phi_X.begin(),
[] (double deg)
        { return deg * M_PI / 180.0; });

    std::vector<double> signal =
furkans::forellipsometry::generate_signal(degrees, a, b, c, error,
false);

    double I_ave, alpha, beta;

    std::tie(I_ave, alpha, beta) =
furkans::forellipsometry::ff_coeffie(phi_X, signal, false);
    alpha = alpha * 4;
    beta = beta * 4;
    double c = 1.0;
    {
        degrees[i] = i * 360.0 / num_points;
    }
}

```

Figure A.6.7 : Programme code named light intensity

```

std::vector<double> asil(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        asil[i] = I_ave + alpha * std::sin(2.0 * phi_X[i]) + beta *
std::cos(2.0 * phi_X[i]);
    }

    for (int i = 0; i < num_points; ++i)
    {
        std::cout << "degrees=" << degrees[i] << " " << signal[i] << "
" << asil[i] << std::endl;
    }

    std::cout << "I_DC expected=" << a << " obtained=" << I_ave <<
std::endl;
    std::cout << "I_S expected=" << b << " obtained=" << alpha <<
std::endl;
    std::cout << "I_C expected=" << c << " obtained=" << beta <<
std::endl;

    return 0;
}

std::vector<double> asil(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        asil[i] = I_ave + alpha * std::sin(2.0 * phi_X[i]) + beta *
std::cos(2.0 * phi_X[i]);
    }

    for (int i = 0; i < num_points; ++i)
    {
        std::cout << "degrees=" << degrees[i] << " " << signal[i] << "
" << asil[i] << std::endl;
    }

    std::cout << "I_DC expected=" << a << " obtained=" << I_ave <<
std::endl;
    std::cout << "I_S expected=" << b << " obtained=" << alpha <<
std::endl;
    std::cout << "I_C expected=" << c << " obtained=" << beta <<
std::endl;

    return 0;
}

```

Figure A.3 (continue) : Programme code named light intensity

```

//.\ellipsometriolcumu_RAE.exe
#include <iostream>
#include <cmath>
#include <vector>
#include <complex>
#include "furkans.forellipsometry.h"
#include "furkans.fresnelcalculations.h"

int main()
{

    const int num_points = 90;
    std::vector<double> degrees(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        degrees[i] = i * 360 / num_points;
    }

    std::vector<double> phi(degrees.begin(), degrees.end());
    std::complex<double> ref_index = {2.0, -0.5};
    double theta_i = 70.0;
    double Polarizer_angle = 45.0;
    bool deg = true;
    bool Quarter_wave_plate = false;

    std::vector<double> signal =
furkans::forellipsometry::generate_signal_f_m(phi, ref_index, theta_i,
Polarizer_angle, 1.0, 0.0001, deg);

    auto [rho, fit] = furkans::forellipsometry::r_f_data(phi, signal,
Polarizer_angle, Quarter_wave_plate, deg);

    std::complex<double> m2 = furkans::forellipsometry::m_f_r(rho,
theta_i, true);

    std::cout << "Original ref_index: " << ref_index << std::endl;
    std::cout << "Calculated ref_index: " << m2 << std::endl;

    std::complex<double> rho2 =
furkans::forellipsometry::r_f_m(ref_index, theta_i, true);
    std::cout << "Calculated rho from ref_index: " << rho2.real() << "
+ " << rho2.imag() << "j" << std::endl;
    std::cout << "Expected rho: " << rho.real() << " + " << rho.imag()
<< "j" << std::endl;

```

Figure A.6.8 : Programme code named ellipsometry_RAE

```

std::cout << "signal: ";
for (const auto &value : signal)
{
    std::cout << value << " ";
}

std::cout << "fit: ";
for (const auto &value : fit)
{
    std::cout << value << " ";
}
std::cout << std::endl;

return 0;
}

```

Figure A.6.10 : Programme code named fitting_Delta_Psi_programme

```

std::cout << "signal: ";
for (const auto &value : signal)
{
    std::cout << value << " ";
}

std::cout << "fit: ";
for (const auto &value : fit)
{
    std::cout << value << " ";
}
std::cout << std::endl;

return 0;
}

```

Figure A.4 (continue) : Programme code named ellipsometry_RAE

```

// .\fitting_Delta_Psi_program.exe
#include <iostream>
#include <cmath>
#include <vector>
#include <complex>
#include "furkans.forellipsometry.h"
#include "furkans.fresnelcalculations.h"

int main()
{
    const int num_points = 90;
    std::vector<double> degrees(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        degrees[i] = i * 360.0 / num_points;
    }

    std::vector<double> phi(degrees.begin(), degrees.end());

    std::complex<double> ref_index = {1.5, -0.0};
    double Polarizer_angle = 45.0;
    double theta_i = 70.0;

    double average = 1.0;
    bool deg = true;
    bool Quarter_wave_plate = false;

    double noise = 0.0000001;
    std::vector<double> signal =
furkans::forellipsometry::generate_signal_f_m(degrees, ref_index,
theta_i, Polarizer_angle, average, noise, deg);

    auto [rho, fit] = furkans::forellipsometry::r_f_data(degrees,
signal, Polarizer_angle, Quarter_wave_plate, deg);
    std::complex<double> m_fit = furkans::forellipsometry::m_f_r(rho,
theta_i, deg);

    std::pair<double, double> tanpsi_Delta =
furkans::forellipsometry::tpsi_Delta_f_r(rho, deg);
    double Delta = tanpsi_Delta.second;
    double tanpsi = tanpsi_Delta.first;

// .\fitting_Delta_Psi_program.exe

```

Figure A.6.11 : Programme code named fitting_Delta_Psi_programme

```

std::cout << "Original refractive index = " << ref_index.real() <<
std::showpos << ref_index.imag() << "j" << std::endl;
    std::cout << "Recovered refractive index = " << m_fit.real() <<
std::showpos << m_fit.imag() << "j" << std::endl;
    std::cout << "Fitted Delta = " << Delta << "degree, tanpsi = " <<
tanpsi << std::endl;

    std::cout << "signal: ";
    for (const auto &value : signal)
    {
        std::cout << value << " ";
    }

    std::cout << "fit: ";
    for (const auto &value : fit)
    {
        std::cout << value << " ";
    }
    std::cout << std::endl;
    return 0;
}

```

Figure A.6.13 : Programme code named fitting_Delta_Psi_programme

```

std::cout <<
"Original refractive index = " << ref_index.real() << std::showpos <<
ref_index.imag() << "j" << std::endl;
    std::cout << "Recovered refractive index = " << m_fit.real() <<
std::showpos << m_fit.imag() << "j" << std::endl;
    std::cout << "Fitted Delta = " << Delta << "degree, tanpsi = " <<
tanpsi << std::endl;

    std::cout << "signal: ";
    for (const auto &value : signal)
    {
        std::cout << value << " ";
    }

    std::cout << "fit: ";
    for (const auto &value : fit)
    {
        std::cout << value << " ";
    }
    std::cout << std::endl;
    return 0;

```

Figure A.5 (continue): Programme code named fitting_Delta_Psi_programme

```

//.\acquisition_Delta_Psi_program.exe
#include <iostream>
#include <cmath>
#include <vector>
#include <complex>
#include "furkans.forellipsometry.h"
#include "furkans.fresnelcalculations.h"
#include <algorithm>
#include <random>
#include <numeric>
#include <fstream>

int main()
{

    const int num_points = 90;
    std::vector<double> degrees(num_points);
    for (int i = 0; i < num_points; ++i)
    {
        degrees[i] = i * 360.0 / num_points;
    }

    std::ofstream
outputFile("Phi_and_Delta_Values_from_dummy_signal.csv");

    outputFile <<
"a,b,c,error,rho_real,rho_imag,tanpsi,Delta,Signal1,Signal2,...,Signal9
0\n";

    std::random_device rd;
    std::mt19937 gen(rd());
    std::uniform_real_distribution<double> distribution_a(0.01, 0.4);
    std::uniform_real_distribution<double> distribution_b(-0.1, 0.1);
    std::uniform_real_distribution<double> distribution_c(-0.1, 0.1);
    std::uniform_real_distribution<double> distribution_error(0.0001,
0.001);

    const int num_iterations = 200;

//.\acquisition_Delta_Psi_program.exe
#include <iostream>
#include <cmath>
#include <vector>

```

Figure A.6.14 : Programme code named fitting_Delta_Psi_programme

```

for (int i = 0; i < num_iterations; ++i)
{

    double a = distribution_a(gen);
    double b = distribution_b(gen);
    double c = distribution_c(gen);
    double error = distribution_error(gen);

    bool deg = true;

    std::vector<double> signal =
furkans::forellipsometry::generate_signal(degrees, a, b, c, error,
deg);

    double Polarizer_angle = 45;
    bool Quarter_wave_plate = false;
    auto [rho, fit] = furkans::forellipsometry::r_f_data(degrees,
signal, Polarizer_angle, Quarter_wave_plate, deg);

    auto tanpsi_Delta =
furkans::forellipsometry::tpsi_Delta_f_r(rho, deg);
    double psi = (std::atan(tanpsi_Delta.first)) * 180.0 / M_PI;

    outputFile << a << "," << b << "," << c << "," << error << ","
        << std::real(rho) << "," << std::imag(rho) << ","
        << psi << "," << tanpsi_Delta.second;

    for (const auto &value : signal)
    {
        outputFile << "," << value;
    }
    outputFile << "\n";
}

outputFile.close();

std::cout << "CSV file 'Phi_and_Delta_Values_from_dummy_signal.csv'
has been generated.\n";

return 0;
}

for (int i = 0; i < num iterations; ++i)

```

Figure A.6 (continue): Programme code named fitting_Delta_Psi_programme



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PUBLICATIONS, PRESENTATIONS AND PATENTS ON THE THESIS:

- **Hansen, P.-E., et al.** "Instrumentation and uncertainty evaluation for absolute characterization of thin films and nanostructured surfaces in advanced optical metrology." Metrologia, 62(2), 025010, 2025.
- **Yıldız, Furkan, et al.** "Imaging Ellipsometry for Material Characterization and Defect Analysis." 4th International Graduate Research Symposium (IGRS'25), İstanbul Technical University, May 12–14, 2025, İstanbul, Türkiye.