Mueller based scatterometry and optical characterization of semiconductor materials

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MUELLER BASED SCATTEROMETRY AND
OPTICAL CHARACTERIZATION OF
SEMICONDUCTOR MATERIALS

by

Gangadhara Raja Muthinti

A Dissertation
Submitted to the University at Albany, State University of New York in
Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy

College of Nanoscale Science and Engineering
2013
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Dedicated to my late grandfather who taught me how to appreciate nature and all the knowledge it can offer.
ACKNOWLEDGEMENTS

I would like to take this opportunity to sincerely offer my thanks to many, who were responsible for this to happen. First and foremost, I am extremely grateful to my advisor, Dr. Alain. C. Diebold, for his thought provoking guidance and constant efforts in the pursuit of knowledge. I whole-heartedly thank him for all the opportunities he had provided me throughout my research and directed me in a positive path to success. I thank all my past and current research members of the optical metrology group for thoughtful discussions and helpful suggestions. I am sincerely grateful to Dr. Brennan Peterson and his team at Nanometrics Inc., for his support, resources and all the critical suggestions throughout the research.

I thank my committee members, Dr. John Hartley (CNSE), Dr. Bakhru Hassaram (CNSE) & Jody Fronheiser (GLOBALFOUNDRIES) for their co-operation and the constructive feed back on the research. I am extremely thankful to the past and present CNSE graduate students, especially Ravi Bonam, Vijay Jain and Vimal Kamineni for their immense help in sample preparation, characterization and lithography. I am gratefully appreciative to all the application engineers at J. A. Woollam Inc., for their constant support on ellipsometry. I am thankful to Dr. Thomas Adams and Dr. Alexander Reznicek for their high quality samples and discussions. I am grateful to engineers at CNSE and SEMATECH for their samples. Thank you to Dr. Todd Bailey and Dr. Bala Haran for their co-operation and suggestions. I am grateful to Dr. Bill Taylor and his team at GLOBALFOUNDRIES for providing samples and advice. I would like to acknowledge Nanometrics Inc., for their funding and support.
Finally, I would like to whole-heartedly thank my family, parents, sister and my dearest wife for their constant support and understanding. Much thanks to my dearest friends Kiran & Malli for their constructive criticism and feedback on my work.
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ABSTRACT

Scatterometry is one of the most useful metrology methods for the characterization and control of critical dimensions (CD) and the detailed topography of periodic structures found in microelectronics fabrication processes. Spectroscopic ellipsometry (SE) and normal incidence reflectometry (NI) based scatterometry are the most widely used optical methodologies for metrology of these structures. Evolution of better optical hardware and faster computing capabilities led to the development of Mueller Matrix (MM) based Scatterometry (MMS). Dimensional metrology using full Mueller Matrix (16 element) scatterometry in the wavelength range of 245nm-1000nm was discussed in this work. Unlike SE and NI, MM data provides complete information about the optical reflection and transmission of polarized light reflected from a sample. MM is a 4x4 transformation matrix (16 elements) describing the change in the intensities of incident polarized light expressed by means of a Stokes Vector. The symmetry properties associated with MM provide an excellent means of measuring and understanding the topography of the periodic nanostructures. Topography here refers to uniformity of the periodic order of arrayed structure. The advantage of MMS over traditional SE Scatterometry is the ability of MMS to measure samples that have anisotropic optical properties and depolarize light.

The present study focuses on understanding the Mueller based Scatterometry with respect to other methodologies by a systematic approach. Several laterally complex nanoscale structures with dimensions in the order of nanometers were designed and fabricated using e-beam lithography. Also Mueller based analysis was used to extract profile information and anisotropy coefficients of complex 3D FinFET, SOI fin grating
structures. Later, Spectroscopic Mueller matrix (all 16 elements) and SE data were collected in planar diffraction mode for the samples using a J.A. Woollam RC2™ Spectroscopic Ellipsometer. NanoDiffract™ (Scatterometry software provided by Nanometrics Inc.) was used to model the nanostructures to precisely calculate the critical dimensions. Complementary techniques like SEM were compared with the results obtained from scatterometry. Mueller and SE based scatterometry techniques were compared commenting on reliability of MM based scatterometry.
CHAPTER 1

Introduction to Scatterometry Technology

Optical scatterometry is a widely used metrology technique in semiconductor/microelectronics manufacturing and advanced process control of various unit operations like lithography and etching. It is an optical method used to measure the critical dimensions of periodic grating structures present on a wafer or mask. Scatterometry tools illuminate light on to the sample of interest and the diffracted (generally specular reflection) light is analyzed to obtain the feature dimensions. The shape information is extracted typically by fitting the data to an optical model or matching to a calibrated reference.

This chapter is divided into four main sections. The first section discusses the timeline, evolution of the scatterometry technology and the recent advancements in both software and hardware components of it. The second section presents an overview of the important complementary optical metrology techniques to scatterometry. It also provides a comparison of the methods focusing on their functionality and measurement routine. Third section focuses on the future challenges of scatterometry technology and provides an outlook on some of the potential solutions. The final section discusses the motivation behind the current research and presents the objectives of this work.

1.1 History of Scatterometry Technology

Scatterometry requires the calculation of diffraction from a periodic grating structure. Though the hardware used to collect the diffraction information was available since the 18th century, lack of analytical software delayed the evolution of scatterometry
technology. In 1981, Moharam and Gaylord from Georgia Institute of Technology (Atlanta, Georgia) were able to rigorously calculate the diffraction from a periodic structure by solving Maxwell’s equation of electromagnetic radiation [1-4]. This method was named as rigorous coupled wave approximation (RCWA) and still remains the foundation of the modern scatterometry optimization software. Later, the first scatterometer was developed in 1987 at University of New Mexico funded by SEMATCH and SRC [5].

Focus and dose control frequently required in lithography was the first application investigated by a scatterometer. Successful results motivated researchers to explore the application horizon of this technology. Later, patterned CD measurements were investigated [5]. The first commercial scatterometer was launched in the year, 1995. Until then, only monochromatic wavelength was used to measure the diffraction data from the sample. University of California, Berkley (1998-2000) modified the source optics capable of illuminating broadband light onto the sample [6,7]. This enabled the improvement of the precision and accuracy of the optimization process of scatterometry analysis software. By early 2000’s, several commercial tools were available in the market, capable of extracting the shape profile from a periodic grating structure (Therma-Wave, Nanometrics, KLA-Tencor, Nova, ASML). In modern semiconductor manufacturing, scatterometry based integrated systems capable of advanced process control plays a crucial role in the critical process steps like lithography, CMP, deposition, SiGe epi-control and etching [8].
1.2 Overview: CD-Metrology techniques

Table 1.1 describes an overview of various critical dimension metrology methods used as a complementary method to scatterometry in semiconductor manufacturing [9]. Scatterometry is not a direct measurement method (or non-linear) as it requires a fit to experimental data. Typically, optical models are validated by other metrology techniques to improve the statistical precision and accuracy of the optimization strategy.

Table 1.1: An overview of CD-metrology techniques used in semiconductor manufacturing.

<table>
<thead>
<tr>
<th></th>
<th>Scatterometry</th>
<th>AFM</th>
<th>CD-SEM</th>
<th>TEM/ X-SEM</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Measuring</strong></td>
<td>CD Profile, Material properties, other etc.,</td>
<td>CD, Roughness</td>
<td>Outer, CD profile</td>
<td>CD Profile, Other</td>
</tr>
<tr>
<td><strong>Sample Specs</strong></td>
<td>Periodic grating</td>
<td>Any</td>
<td>Any</td>
<td>Any</td>
</tr>
<tr>
<td><strong>Measurement time</strong></td>
<td>Seconds</td>
<td>Minutes</td>
<td>Seconds</td>
<td>Days</td>
</tr>
<tr>
<td><strong>Analysis/Time</strong></td>
<td>Days to weeks</td>
<td>Hours</td>
<td>Minutes</td>
<td>Hours to days</td>
</tr>
<tr>
<td><strong>Destructive</strong></td>
<td>Negligible</td>
<td>No</td>
<td>Minor (Resist)</td>
<td>Yes</td>
</tr>
<tr>
<td><strong>Strengths</strong></td>
<td>Fast, Most profile info</td>
<td>Accuracy, Profile info</td>
<td>Quick setup, Fast, Measure everywhere</td>
<td>Full profile info, high accuracy</td>
</tr>
<tr>
<td><strong>Limitations</strong></td>
<td>Model Based, Grating, trade off b/w accuracy &amp; precision</td>
<td>Tip Wear, Large space, low throughput</td>
<td>No profile info</td>
<td>Limited sampling, Sample prep, Resolution is process dependent</td>
</tr>
</tbody>
</table>
The unique advantage of scatterometry is the capability to be implemented as an “in-line” metrology method in manufacturing environment. “In-line”, here refers to the ability to monitor process variation directly without transferring the wafer to another tool. This provides an excellent opportunity to perform process control and improve efficiency of the manufacturing operation. This also minimizes contamination from extraneous factors. Modern CD-SEM tools are also capable of extracting line width as fast as scatterometry. But accurate extraction of the shape profile is extremely difficult and also poses serious effects like charging especially with resist or oxide samples. The down side of using scatterometry is the complex process of creating the optical model and optimizing it to achieve the results. Also, this technique only can be implemented on periodic grating structures. Spot size of the light beam, wavelength of light and pitch of the feature determines the degree of periodicity required for scatterometry measurement. Current, state of the art scatterometry tools are capable of producing a spot size of the order 30-50 microns.

1.3 Metrology challenges in the future

The continuous shrink of the transistors on a chip (Moore’s law) poses several critical challenges that have to be addressed for efficient manufacturability. The performance specifications also shrink together with the feature size and it is extremely important to meet the stringent limits and develop a precise and accurate metrology method. The evolution of 3D transistors (FinFET, Trigate, Buried-gate, Vertical NAND etc.,) for technology nodes beyond 20nm requires even more strict specifications, which made
optical metrology challenging. Further, discovery of novel device architectures based on graphene, CNT, III-V, nanowires creates a new set of challenges for optical metrology.

Optical scatterometry is considered to be a potential candidate for future metrology needs. The following list illustrates some of the unique features of this technology,

- Scaling trend of transistors does not affect the optimization strategy of scatterometry. In order to extract the feature dimensions, the minimum requirement of the technology is that the change in feature dimensions should be optically sensitive (or detectable by the tool). For example, modern tools are capable of detecting a 1nm change in critical dimension in lithography applications (photo-resist grating structures).
- Since, the measurement is fast and non-destructive, statistical variation across the wafer, wafer-to-wafer and lot-to-lot can be measured with ease. Modern manufacturing operations require extensive statistical information to perform routine checks on process quality and variation.
- Scatterometry makes it possible to extract the optical properties of novel materials like graphene, CNT, nanowires, III-V materials, which is needed for precise and accurate optical metrology of novel device architectures.
- Scatterometry enables precise and accurate measurement of the modern device architectures like 3D FinFET, FDSOI in both front-end and back-end of line in manufacturing.
1.4 Motivation and Statement of Thesis

Over the past several years, the evolution of novel 3D device architectures has increased the complexity of the sample geometries. This dramatically increased the number of floating parameters in scatterometry optimization process. Ideal scatterometry models should be such that there exists no correlation between the floating parameters. However, a little correlation (typically less than 40 to 60%) is tolerable based on sample and process specifications. Increase in correlation affects the statistical robustness or accuracy of the model. Significant research has been done to address some of these challenges. “Hybrid” based methodology is considered to be one of the potential solutions to this problem. It involves careful interaction of relevant data between multiple tools and then reduce (sometimes eliminate) the correlation between the most troublesome floating parameters in the optimization process. For example, data from CD-SEM can be fed to the scatterometry tool and reduce the number of parameters. The major problem with this approach is the tool matching compatibility. Fundamentally, each tool has its own share of errors involved in data collection and hence, it is not obvious to transfer data between tools. It can also seriously impact the optimization process between the tools.

Recent advancements in both software and hardware components of scatterometry technology enabled opportunities to analyze complex samples. Previously a part of the diffraction data was only collected due to limitations of scatterometry measurement hardware. Modern ellipsometers or polarimeters are capable of collecting full Mueller data accurately over a wide wavelength range, typically (around 150nm to 1700nm) in a few seconds. Unlike the conventional ellipsometry or reflectometry data, Mueller data provides complete reflection (or transmission) information from a sample.
For complex sample geometries, this additional data may prove useful in improving the statistical robustness of the optical model and also reduce the correlation between the floating parameters. Also, Mueller elements comprise the symmetry information of the sample structure, which provides a way to analyze asymmetric and anisotropic structures. Currently, Mueller based scatterometry is still evolving and limited research has been done understanding the advantages and disadvantages of this new methodology using the state of the art Mueller based ellipsometers. This motivated us to perform a systematic investigation of Mueller properties on complex sample geometries and understand the Mueller based optimization process. Here are the objectives of current research,

- Systematic investigation of Mueller properties of commonly observed sample geometries in semiconductor manufacturing.
- Implement Mueller based Scatterometry optimization process on state of the art samples to extract the feature dimensions and profile information of the structure.
- The effect of optical properties (or dielectric function) on scatterometry models.
- Investigate anisotropy information from complex samples and determine ways interpret the degree of anisotropy in a structure.
- Comparison study between the conventional ellipsometry and Mueller based scatterometry optimization processes.
- Detailed sensitivity analysis of various critical dimensions over Mueller matrix elements.

In summary, This thesis will explore the Mueller properties of complex grating structures, principles of Mueller based scatterometry along with the hardware and software configuration for data collection and analysis, also the effect of stress,
depolarization & anisotropy on the Mueller analysis of strained SiGe FinFET grating structures and finally a comparison of Mueller based scatterometry with ellipsometric based methodology.

This thesis has been outlined into seven main chapters. The first chapter starts with discussing the history and timeline of scatterometry technology. It also describes some of the key challenges in optical metrology and the reasons for scatterometry to be a potential candidate. The chapter ends with the motivation behind the current research with clear explanation of the objectives of the work. Chapter two presents a detailed overview of theory, hardware and software aspects of scatterometry technology. Third chapter discusses the effect of stress on the dielectric function of silicon germanium alloy material and presents a detailed understanding of the impact of stress on the critical points of band structure. Fourth chapter presents an elaborate discussion on the investigation of Mueller properties of several sample geometries fabricated using e-beam lithography. Fifth chapter provides a mathematical overview and foundation of the nomenclature used to calculate the effective anisotropic coefficients from a Mueller matrix of a 3D FinFET grating structure and discusses an algorithm used to filter depolarization from experimental Mueller data. Sixth chapter presents a comparison case study of ellipsometry and Mueller based scatterometry optimization processes using silicon fins fabricated on silicon on insulator (SOI) substrate. It also provides the sensitivity analysis of various critical dimensions of SOI fins. Finally, the thesis ends with summary of the work and comments for future work.
1.5 References


CHAPTER 2

Theory and Methodology

This chapter is divided into four main sections providing a detailed discussion on the Mueller theory, nomenclature and mathematical foundation required for experimental data collection, analysis, hardware and software engines used in optical scatterometry. Section 1 will describe the propagation of light or electromagnetic radiation (EM wave) using Maxwell’s equations. Section 2 discusses the theoretical foundation of the Jones and Mueller formalism used to represent the reflection or transmission properties of a sample. Section 3 will provide a detailed description of the optical hardware used to collect both Mueller and ellipsometric data of a sample along with the working principle of optical scatterometry. Section 4 discusses the optimization processes used in scatterometry and the simulation methods implemented in the current work.

2.1 Light fundamentals, Maxwell’s equations

Maxwell’s equations describe many of the classical electromagnetic phenomena and the interaction of light with a medium. Maxwell showed that light has electromagnetic properties with wave like form consisting of mutually perpendicular oscillating electric (E) and magnetic fields (H) propagating with a characteristic frequency (ν). Mathematically, these equations in differential form are given by (MKS units) [1]:

\[\begin{align*}
\nabla \times \mathbf{H} &= \mu_0 \mathbf{E} \\
\nabla \times \mathbf{E} &= -\mu_0 \mathbf{J} - \nabla \phi \\
\nabla \cdot \mathbf{E} &= \frac{
abla \cdot \mathbf{B}}{\mu_0} \\
\nabla \cdot \mathbf{B} &= 0
\end{align*}\]
∇ \times E(r,t) = -\frac{\partial B(r,t)}{\partial t}, \quad (2.1)

∇ \times H(r,t) = J(r,t) + \frac{\partial D(r,t)}{\partial t}, \quad (2.2)

∇ \cdot E(r,t) = \rho(r,t), \quad (2.3)

∇ \cdot B(r,t) = 0. \quad (2.4)

Where \( E, H, D, B, J \) and \( \rho \) represent the electric field, magnetic field, electric displacement, magnetic flux density, current density and the free charge density respectively. Above equations can be solved using the following constitutive relations in a medium [1]:

\[ D = \varepsilon_0 E + P, \quad (2.5) \]

\[ B = \mu_0 (H + M), \quad (2.6) \]

where \( \varepsilon_0 \) and \( \mu_0 \) represent the electric permittivity and magnetic permeability in vacuum respectively. \( P \) and \( M \) respectively, are the electric and magnetic polarizations in the medium. They can be understood as the average electric and magnetic dipole moment per unit volume. In free space, \( P \) and \( M \) are equal to zero as there is no net moment from the dipoles [1]. In a linear optically isotropic dielectric medium, the electric polarization vector is parallel and proportional to the electric field vector.

\[ P = \varepsilon_0 \chi_e E, \quad (2.7) \]

where \( \chi_e \) is the proportionality constant defined as electric susceptibility and is always positive.

Substituting equation (2.7) into (2.5) yields,

\[ D = \varepsilon_0 (1 + \chi_e) E = \varepsilon E, \quad (2.8) \]
giving rise to the relationship between electric permittivity and susceptibility. Likewise, a similar expression relating the magnetic permeability and magnetic susceptibility ($\mu$) is expressed as [1],

$$B = \mu_0 (1 + \chi_m) H = \mu H,$$

where $\chi_m$ is the magnetic susceptibility of a medium.

Further, the electric permittivity defined in equation (2.8) is used to introduce the dielectric function or relative permittivity ($\varepsilon_r$) of a material given by the following equation,

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_0} = 1 + \chi_e.$$

In CGS units, the absolute permittivity ($\varepsilon_0$) of vacuum or air at room temperature is equal to one.

For the case of an anisotropic material, electric (or magnetic) polarization and electric (or magnetic) field vectors need not be in same direction. Electric (or magnetic) susceptibility of these materials exhibits complex behavior and is represented using a second order tensor. The resulting electric permittivity is also a tensor and are described the following equations [1-3].

$$\mathbf{D} = \varepsilon \mathbf{E},$$

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix},$$

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where \( x, y \) and \( z \) represent the principle (also called ‘characteristic’) axes of the anisotropic material. Similar analogous expressions can be used to describe magnetic permeability and susceptibility. Dielectric function of a material is generally extracted or measured using the ‘laboratory’ reference frame or co-ordinate axes and hence, differs from the ‘principle’ reference frame of the anisotropic material. A simple rotary transformation matrix (\( A \)) and Euler angles (\( \phi, \theta, \psi \)) are used to convert the measured dielectric function to the principle axes representation [1-3]. Mathematically, this transformation is expressed as,

\[
e = A \begin{bmatrix} \varepsilon_{x'} & 0 & 0 \\ 0 & \varepsilon_{y'} & 0 \\ 0 & 0 & \varepsilon_{z'} \end{bmatrix} A^{-1}, \tag{2.13}
\]

where \( x', y' \) and \( z' \) represent the axes of the laboratory co-ordinate system. A pictorial representation of both the reference frames along with the Euler angles is shown in figure 2.1 [1,4].

**Figure 2.1:** Representation of laboratory and principle co-ordinate system of an anisotropic material along with the corresponding Euler angles of transformation.
From Maxwell’s equation and the corresponding constitutive relations (equations (2.1) to (2.4) and equation (2.11)), we obtain the following wave equation for the electric field vector \( \mathbf{E} \) [1],

\[
\nabla^2 \mathbf{E} = \frac{\varepsilon \mu}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{4\pi \sigma \mu}{c^2} \frac{\partial \mathbf{E}}{\partial t},
\]

(2.14)

where \( c \), \( \sigma \) are respectively, the speed of light and conductivity in the medium. The solution to the above equation is a sinusoidal function and the resulting \( \mathbf{E} \) field vector is of the form [3],

\[
\mathbf{E} = E_0 e^{i(Kr - \omega t)},
\]

(2.15)

where \( \omega \) is the frequency of light and \( K \) is the complex propagation constant. The real part and imaginary parts of \( K \) are the wave vector and attenuation of light in the material respectively. Substituting equation (2.15) into the wave equation (2.14) yields,

\[
-K^2 = -\frac{\varepsilon \omega^2}{c^2} - \frac{i(4\pi \sigma \omega)}{c^2}.
\]

(2.16)

Assuming the attenuation (imaginary part of \( K \)) of light in the material to be negligible, we arrive at,

\[
\text{Re}(K) = K_0 = \frac{\omega}{c} \sqrt{\varepsilon \mu},
\]

(2.17)

and for the case where the attenuation losses are not small, we get,

\[
K = \frac{\omega}{c} \sqrt{\varepsilon_{\text{complex}}} \mu,
\]

(2.18)

where \( \varepsilon_{\text{complex}} \) is defined as,

\[
\varepsilon_{\text{complex}} = \varepsilon + \frac{i(4\pi \sigma)}{\omega} = \varepsilon_1 + i\varepsilon_2.
\]

(2.19)
Here, $\varepsilon_{\text{complex}}$ is a function of frequency of light and is customary to express the complex dielectric function in terms of $\varepsilon_1$ and $\varepsilon_2$.

Using equation (2.19), complex conductivity is related to the dielectric function by the following equation,

$$
\varepsilon_{\text{complex}} = \frac{4\pi i}{\omega} \left[ \sigma + \frac{\varepsilon \omega}{4\pi i} \right] = \frac{4\pi i}{\omega} \sigma_{\text{complex}}, 
$$

(2.20)

and complex conductivity ($\sigma_{\text{complex}}$) is defined as,

$$
\sigma_{\text{complex}} = \sigma + \frac{\varepsilon \omega}{4\pi i}. 
$$

(2.21)

Further, substituting the solution for $K$, equation (2.16) into the sinusoidal function of electric field vector, equation (2.15) yields the following equation for plane wave propagating in Z-direction [3],

$$
E(z,t) = E_0 e^{-i\omega t} \exp \left( -\frac{i\omega z}{c} \sqrt{\varepsilon \mu} \sqrt{1 + \frac{i(4\pi \sigma)}{\varepsilon \omega}} \right). 
$$

(2.22)

For the light wave propagating in vacuum ($\varepsilon=1$, $\mu=1$ and $\sigma=0$), above equation reduces to a simple wave equation,

$$
E(z,t) = E_0 \exp \left[ -\frac{i\omega z}{c} \right]. 
$$

(2.23)

For a wave propagating in a material of finite electrical conductivity, the amplitude of the wave decays exponentially over a characteristic distance ($\delta$, also called optical skin depth) given by [1],

$$
\delta = \frac{c}{\omega N_2(\omega)} = \frac{c}{\omega k(\omega)}, 
$$

(2.24)
where $N_2 (=k)$ is the imaginary part of the complex refractive index (also called the extinction coefficient). Complex refractive index is related to the dielectric function of a material described by the following equation [1,3],

$$N(\omega) = \sqrt{\mu \varepsilon_{\text{complex}}} = \sqrt{\varepsilon \mu \left(1 + \frac{i(4\pi\sigma)}{\varepsilon\omega}\right)} = n(\omega) + ik(\omega). \quad (2.25)$$

For non-magnetic materials, above equation can be simplified further and is expressed as,

$$N(\omega) = \sqrt{\varepsilon_{\text{complex}}} = n(\omega) + ik(\omega), \quad (2.26)$$

and comparing the real and imaginary parts of above equation, we arrive at,

$$\varepsilon_1 = n^2 - k^2, \quad (2.27)$$

$$\varepsilon_2 = 2nk. \quad (2.28)$$

Also, absorption coefficient ($\alpha$) is defined as the distance from the surface of the material where the intensity of electric field vector ($|E|^2$) falls off to 1/e and is expressed as,

$$\alpha = \frac{2\omega k}{c} = \frac{4\pi k}{\lambda}. \quad (2.29)$$

### 2.2 Plane waves and polarization of light

A plane wave is a constant frequency wave with wavefronts (infinite parallel planes) of constant amplitude and normal to the phase velocity vector. These plane waves are a particular solution of Maxwell’s equation describing the electromagnetic phenomena in a homogeneous region of the space. For a plane wave propagating in z-direction, Maxwell’s equation enforce that both electric and magnetic field should be mutually perpendicular to each other and to the direction of propagation. Typically, the magnetic
moments induced in a material are negligible when compared to optical moments induced by the electric field. Conventionally, the polarization of light is described using the electric field vector (E). Polarization of light refers to the orientation of electric field oscillations in a specific plane, which is perpendicular to the direction of propagation. The electric field components for a fully polarized light propagating along z-axis can be decomposed into x and y directions represented by the following equations [2,3],

\[
E_x(z, t) = \text{Re} \left[ E_{x0} \exp \left( i\omega t - \frac{2\pi z}{\lambda} + \delta_x \right) \right],
\]

\[
E_y(z, t) = \text{Re} \left[ E_{y0} \exp \left( i\omega t - \frac{2\pi z}{\lambda} + \delta_y \right) \right],
\]

where \(E_{x0}\) and \(E_{y0}\) are amplitudes and \(\delta_x\) and \(\delta_y\) are the phases for the electric field’s x and y polarization components, respectively. The polarization of light is defined based on the relative difference in magnitude and phase between the two components of the electric field. Polarization is schematically expressed using polarization ellipse as shown in figure 2.2. The polarization ellipse is obtained by tracing the end point of electric field intensity vector in space over one time period (\(T = \frac{2\pi}{\omega}\)). Ellipticity (\(\varepsilon\)) and azimuth (\(\theta\)) angles are used to characterize polarization ellipse and its orientation and are calculated using the following equations [3],

\[
\sin(2\varepsilon) = \frac{2E_{x0}E_{y0}}{E_{x0}^2 + E_{y0}^2} \sin(\delta),
\]

\[
\tan(2\theta) = \frac{2E_{x0}E_{y0}}{E_{x0}^2 + E_{y0}^2} \cos(\delta),
\]

\[
\delta = \delta_y - \delta_x.
\]
Here, ellipticity is defined as the tangent between the half axes of the polarization ellipse and azimuth is the rotation of its major axis. For a linearly polarized light, the two components of the electric field are in phase ($\delta = 0$, $\varepsilon = 0$) and for circularly polarized light, the ellipticity becomes $\pm \pi/4$. For all other conditions of $\varepsilon$, light wave is elliptically polarized. The handedness of the polarization ellipse defines the rotation sense of the polarized light. Light is “right handed” when the electric field vector rotates clock-wise for the beam traveling into the reference plane. Likewise, polarized light is “left handed” when the electric field vector rotates in counter-clock sense.

**Figure 2.2: Schematic representation of polarization ellipse used to describe polarized light.**

The other commonly used characteristic angles to describe polarized light are $\psi$ and $\Delta$. There are preferred quantities in majority of the ellipsometric and scatterometry measurements and widely used to investigate material and optical properties. These angles are related to the polarization ellipse given by the relations [3],
\[ \tan \psi = \frac{E_x}{E_y} \], \hspace{1cm} (2.35)

\[ \Delta = \delta_x - \delta_y. \] \hspace{1cm} (2.36)

### 2.3 Jones representation of polarized light (The Jones formalism)

The Jones vector describes polarized light using the electric field components and is a direct representation of a single uniform monochromatic transverse electric plane wave. The Jones vector of a fully polarized light is expressed as a 2x1 column vector using the equations (2.30) and (2.31), given by [3,5,6],

\[
E(z,t) = \begin{bmatrix} E_x \exp\left[i(\omega t - kz + \delta_x)\right] \\ E_y \exp\left[i(\omega t - kz + \delta_y)\right] \end{bmatrix} = \exp\left[i(\omega t - kz)\right] \begin{bmatrix} E_x \exp(i\delta_x) \\ E_y \exp(i\delta_y) \end{bmatrix}, \tag{2.37}
\]

where \( k = \frac{2\pi}{\lambda} \), the propagation number. The exponential multiplication factor outside the column vector in equation (2.37) is generally ignored, thus simplifying the representation as,

\[
E(z,t) = \begin{bmatrix} E_x \\ E_y \end{bmatrix}, \tag{2.38}
\]

\[
E_x = E_{x0} \exp(i\delta_x), \tag{2.39}
\]

\[
E_y = E_{y0} \exp(i\delta_y), \tag{2.40}
\]

where \( E_x \) and \( E_y \) are the complex amplitudes of the polarized plane wave. Jones vector provide complete information regarding the state of polarization of the light beam and are capable of describing fully or completely polarized light. Jones formalism fails describing depolarized or partially polarized light. Most of the optical interactions with a medium or optical elements cause some depolarization in the incoming light beam, the Jones
formalism of representation is not an efficient way of characterizing the optical path. However, this representation works well for quasi-monochromatic and negligible depolarizing optical interactions. Intensity of light (for example, a monochromatic laser light source) is calculated by pre-multiplying the Jones vector by its Hermitian adjoint vector matrix. The Hermitian adjoint matrix is defined as the complex conjugate of the corresponding transposed matrix. Mathematically, light intensity (I) is expressed as [6],

$$ I = E^\dagger E = E_x^* E_x + E_y^* E_y. $$

(2.41)

The transformation of light after interacting with a medium or optical element is characterized using a 2x2 matrix referred as the Jones matrix (J) given by [6],

$$ \begin{bmatrix} E'_x \\ E'_y \end{bmatrix} = J \begin{bmatrix} E_x \\ E_y \end{bmatrix}, $$

(2.42)

$$ J = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix}, $$

(2.43)

where $E'_x, E'_y$ are the electric field components of the light beam after interaction. There are 4 elements in the Jones matrix and a total of 8 independent components as each element is a complex number. Therefore, 8 independent real parameters are required to characterize the Jones matrix [7]. The emergent intensity of light after interacting with a series of optical elements is calculated by a cascade of matrix multiplications of the corresponding Jones matrices and described by the following equation [5].

$$ E_f = J_n J_{n-1} J_{n-2} \ldots J_2 J_1 E_i = J_{\text{net}} E_i, $$

(2.44)

where $J_{\text{net}}$ is the combined Jones matrix calculated by the multiplication of individual Jones matrices of all the optical elements ($J_1, J_2, \ldots J_n$). The co-ordinate system used to
calculate individual Jones matrices can vary from one another and a rotary transformation matrix, \( R(\alpha) \) is used to include this effect of rotation. For example, the effect of rotating the co-ordinate system associated with an optical element by angle \((\alpha)\) is expressed as \[2.45\],

\[ J' = R(\alpha)JR(-\alpha), \]

where \( J' \), is the Jones matrix calculated after including the effect of rotation. Jones vectors of various kinds of polarized light and Jones matrices for commonly used optical elements are shown in tables 2.1 and 2.2 \[2,3\].

2.4 **Mueller description of polarized light (Stokes-Mueller formalism)**

Polarized light can also be described using the scalar intensity quantities rather than electric field vectors. The polarization state of light is expressed in terms of a 4x1 column matrix referred to as Stokes vector (S) and defined as \[3,5,6\],

\[
S = \begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4
\end{bmatrix} = \begin{bmatrix}
\langle E_x^*E_x + E_y^*E_y \rangle \\
\langle E_x^*E_x - E_y^*E_y \rangle \\
\langle E_y^*E_x + E_x^*E_y \rangle \\
\langle i(E_y^*E_x - E_x^*E_y) \rangle
\end{bmatrix},
\]

where \( E_r^* \), is the complex conjugate of \( r^{th} \) component of electric field component, \( E_r \). The brackets \(<...>\) used in equation \(2.47\) signifies that the variables are time-averaged and introduced to account for variations in amplitude and phase of quasi-monochromatic light beam. \( S_1 \) is the total intensity of the light, \( S_2 \) is the net intensity of linearly polarized light, \( S_3 \) is the net intensity of linearly polarized light oriented at \( 45^0 \) and \( S_4 \) is the net intensity...
of right circularly polarized light. The necessary and sufficient condition for the Stokes vector to be physical is given by [8,9],

$$S_1^2 \geq S_2^2 + S_3^2 + S_4^2.$$  \hfill (2.48)

Equality in the equation (2.48) holds for the case when light is completely or fully polarized while inequality is satisfied for partially polarized light. This enables the calculation of the percent degree of polarization associated with a light beam. Degree of polarization (p) is calculated using the mathematical expression [8,10],

$$p = \frac{\sqrt{S_2^2 + S_3^2 + S_4^2}}{S_1},$$  \hfill (2.49)

where the degree of polarization (p) varies from 0 (unpolarized light) to 1 (fully polarized light). The transformation of light beam expressed in Stokes representation after interacting with a medium or optical element is described using a 16 element, 4x4 square matrix referred to as Mueller matrix (M) given by [3,5],

$$S_f = MS_i,$$  \hfill (2.50)

$$M = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} \\
M_{21} & M_{22} & M_{23} & M_{24} \\
M_{31} & M_{32} & M_{33} & M_{34} \\
M_{41} & M_{42} & M_{43} & M_{44}
\end{bmatrix},$$  \hfill (2.51)

where $S_i$ and $S_f$ are the incoming and emergent Stokes vector of light after interaction. Physically, a Mueller matrix element ($M_{nm}$) refers to the degree of transformation of incident light in a state $S_n$ (incident light) to a state $S_m$ (transmitted/reflected) after interaction, where variables ‘m’ ($1 \leq m \leq 4$) and ‘n’ ($1 \leq n \leq 4$), are the components of Stokes vector. Specifically the matrix element $M_{11}$ represents the total reflectivity (or
transmittivity) of the optical medium or material. Experimentally measured Mueller matrices are typically normalized with $M_{11}$ to simplify data analysis. The normalized Mueller matrix ($M^*$), is expressed as [11],

$$M^* = \begin{bmatrix}
1 & M_{12}/M_{11} & M_{13}/M_{11} & M_{14}/M_{11} \\
M_{21}/M_{11} & M_{22}/M_{11} & M_{23}/M_{11} & M_{24}/M_{11} \\
M_{31}/M_{11} & M_{32}/M_{11} & M_{33}/M_{11} & M_{34}/M_{11} \\
M_{41}/M_{11} & M_{42}/M_{11} & M_{43}/M_{11} & M_{44}/M_{11}
\end{bmatrix}. \quad \text{(2.52)}$$

The elements in the normalized matrix have the values between -1 and 1. Normalized Mueller matrices of various commonly used optical elements are shown in table 2.2 [3]. Analogous to Jones formalism, the effect of rotation of the co-ordinate system by a positive angle ($\alpha$) on a Mueller matrix is adjusted by a multiplication factor, $R(\alpha)$ and the resultant Mueller matrix ($M_\alpha$) is calculated using the relation [2,3],

$$M_\alpha = R(\alpha)M R(-\alpha), \quad \text{(2.53)}$$

where,

$$R(\alpha) = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos 2\alpha & \sin 2\alpha & 0 \\
0 & -\sin 2\alpha & \cos 2\alpha & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}. \quad \text{(2.54)}$$

For non-depolarizing optical interactions with a material, a corresponding Mueller matrix can be calculated from Jones matrix described in equation (2.43). The necessary and sufficient condition for a Mueller matrix to be non-depolarizing is given by the following expression [10].

$$\text{trace}(MM^T) = 4M_{11}^2. \quad \text{(2.55)}$$

A Mueller matrix calculated from the Jones matrix is referred to as the Mueller-Jones matrix (MJ), computed using the relation [12],
\[ MJ = A(J \otimes J^*)A^{-1}, \]  

(2.56)

where \( \otimes \) denotes the Kronecker product and A is,

\[
A = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & i & -i & 0 \end{bmatrix}. \]  

(2.57)

Using equations (2.42), (2.43) and substituting in equation (2.56) yields the expression relating the Jones matrix elements to the corresponding Mueller-Jones matrix elements [13],

\[
MJ = \begin{bmatrix} \frac{1}{2}(|J_{11}|^2 + |J_{21}|^2) & \frac{1}{2}(|J_{11}|^2 - |J_{21}|^2) & \text{Re}(J_{11}^*J_{21} + J_{12}^*J_{22}) & -\text{Im}(J_{11}^*J_{12} + J_{12}^*J_{22}) \\ \frac{1}{2}(|J_{12}|^2 + |J_{22}|^2) & \frac{1}{2}(|J_{12}|^2 - |J_{22}|^2) & \text{Re}(J_{11}^*J_{12} + J_{12}^*J_{22}) & \text{Im}(J_{11}^*J_{12} + J_{12}^*J_{22}) \\ \text{Re}(J_{11}^*J_{12} + J_{12}^*J_{22}) & \text{Re}(J_{11}^*J_{22} + J_{12}^*J_{21}) & \text{Re}(J_{11}^*J_{12} + J_{12}^*J_{22}) & \text{Im}(J_{11}^*J_{12} + J_{12}^*J_{22}) \\ -\text{Im}(J_{11}^*J_{12} + J_{12}^*J_{22}) & \text{Im}(J_{11}^*J_{22} + J_{12}^*J_{21}) & \text{Im}(J_{11}^*J_{12} + J_{12}^*J_{22}) & \text{Re}(J_{11}^*J_{12} + J_{12}^*J_{22}) \end{bmatrix} \]  

(2.58)

Not all 4x4 matrices are Mueller matrices and the physical constraints that must be satisfied by a 4x4 matrix to be a physically realizable Mueller matrix are the polarization and gain constraints. Polarization constraint refers that M cannot produce an outgoing or emergent Stokes vector with a degree of polarization greater than one. Gain constraint represents that M cannot produce emergent Stokes vector of intensities greater than that of the incoming or incident Stokes vector. Figure 2.3 shows the various mathematical domains of 4x4 square matrices [6].
An equivalent relation to the equation (2.49), used to calculate the degree of polarization (p) can be computed using the Mueller matrix elements given by [8,14],

\[
p = \left( \sum_{i,j=1}^{4} M_{ij}^2 - M_{11}^2 \right)^{1/2} \sqrt{3} M_{11},
\]

where the physical values of p vary from 0 (ideal depolarizing system) to 1 (ideal polarizing system).

The critical advantage of using Mueller formalism over the Jones representation is its ability to account for the optical interactions exhibiting scattering or depolarizing electromagnetic phenomena. Also, the quantities used to measure Mueller elements are
directly related to intensity transformations making the interpretation of the optical spectra and the corresponding effect of optical properties relatively easier.

Table 2.1: Jones and Stokes vectors of different kinds of polarized light.

<table>
<thead>
<tr>
<th>Polarization</th>
<th>Polarization state</th>
<th>Jones vector</th>
<th>Stokes vector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unpolarized light</td>
<td>Does not exist</td>
<td>[1]</td>
<td>[1]</td>
</tr>
<tr>
<td>Linear polarization parallel to x-axis</td>
<td></td>
<td>[1]</td>
<td>[1]</td>
</tr>
<tr>
<td>Linear polarization parallel to y-axis</td>
<td></td>
<td>[0]</td>
<td>[1]</td>
</tr>
<tr>
<td>Linear polarization orientated at 45°</td>
<td></td>
<td>[1/√2]</td>
<td>[1]</td>
</tr>
<tr>
<td>Right circular polarization</td>
<td></td>
<td>[1/√2]</td>
<td>[1]</td>
</tr>
<tr>
<td>Left circular polarization</td>
<td></td>
<td>[1/√2]</td>
<td>[1]</td>
</tr>
<tr>
<td>Elliptically polarized light</td>
<td></td>
<td>sinψ exp(iΔ)</td>
<td>[1]</td>
</tr>
</tbody>
</table>

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Table 2.2: Jones and Mueller matrices of commonly used optical elements.

<table>
<thead>
<tr>
<th>Optical Element</th>
<th>Jones matrix</th>
<th>Mueller matrix</th>
</tr>
</thead>
</table>
| Polarizer (Analyzer), P(A) | \[
\begin{bmatrix}
1 & 0 \\
0 & 0
\end{bmatrix}
\] | \[
\begin{bmatrix}
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\] |
| Compensator (Retarder), C | \[
\begin{bmatrix}
1 & 0 \\
0 & \exp(-i\delta)
\end{bmatrix}
\] | \[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos\delta & \sin\delta \\
0 & 0 & -\sin\delta & \cos\delta
\end{bmatrix}
\] |
| Photoelastic modulator, M | \[
\begin{bmatrix}
1 & 0 \\
0 & \exp(i\delta)
\end{bmatrix}
\] | \[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos\delta & -\sin\delta \\
0 & 0 & \sin\delta & \cos\delta
\end{bmatrix}
\] |
| Coordinate rotation, R(\alpha) | \[
\begin{bmatrix}
\cos\alpha & \sin\alpha \\
-\sin\alpha & \cos\alpha
\end{bmatrix}
\] | \[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos 2\alpha & \sin 2\alpha & 0 \\
0 & -\sin 2\alpha & \cos 2\alpha & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\] |
| Isotropic sample, S | \[
\begin{bmatrix}
\sin\psi \exp(i\Delta) & 0 \\
0 & \cos\psi
\end{bmatrix}
\] | \[
\begin{bmatrix}
1 & -\cos 2\psi & 0 & 0 \\
-\cos 2\psi & 1 & 0 & 0 \\
0 & 0 & \sin 2\psi \cos \Delta & \sin 2\psi \sin \Delta \\
0 & 0 & -\sin 2\psi \sin \Delta & \sin 2\psi \cos \Delta
\end{bmatrix}
\] |
| Depolarizer, D | Does not exist | \[
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\] |
2.5 Spectroscopic ellipsometry (SE): Working principle

SE is a fast, non-destructive and accurate optical metrology method used extensively in the characterization of wide variety of materials (metals, dielectrics, semiconductors, polymers, graphene, carbon nanotubes etc.). SE uses a regression based modeling approach to match the experimental data using an optical model. The interaction of polarized light with a sample is calculated using Maxwell’s equations and Fresnel reflection (transmission) coefficients. The typical experimental parameters collected using an ellipsometer are $\psi$ and $\Delta$ described in equations (2.35), (2.36). Based on the hardware capabilities, some ellipsometers enable the collection of full Mueller matrix data (16 elements) of a sample. A dual rotating compensator ellipsometer was used in the current work. Presence of dual compensators enables the collection of both the full Mueller and SE data. The optical path along with the measurement method is described in the subsequent section. This section focuses on the theoretical framework required for optical modeling of measured data.

The origin of SE is based on the principle that a material’s optical response (reflection or transmission coefficient) varies with the state of polarization of the incident light beam. The reflection coefficient of a sample is a function of the complex refractive index (or dielectric function) and thin film thickness of all the layers in the stack. The reflection coefficients of ‘p’ (parallel) and ‘s’ (perpendicular) components of a linearly polarized light exhibit different properties after reflection (or transmission). A schematic diagram showing the interaction of polarized light with an arbitrary material is shown in figure 2.4 [3]. The Fresnel reflection coefficients of ‘p’ and ‘s’ components of the polarized light are given by [2,3],

28
\[ r_p = \frac{N_i \cos \theta - N_i \cos \theta_i}{N_i \cos \theta + N_i \cos \theta_i}, \]  
(2.60)

\[ r_s = \frac{N_i \cos \theta - N_i \cos \theta_i}{N_i \cos \theta + N_i \cos \theta_i}, \]  
(2.61)

where the subscripts ‘i’ and ‘t’ represent the incident and transmitting mediums respectively. \( N \) is the complex refractive index consisting of a real (refractive index, \( n \)) and imaginary (extinction coefficient, \( k \)) parts described in equation (2.26). The relationship between the dielectric function (\( \varepsilon \)) and complex refractive index (\( N \)) of a material was discussed in section 2.1, equations (2.27) and (2.28). \( \theta_i \) and \( \theta_t \) are the angles of incidence and refraction.

Figure 2.4: Fresnel reflection and transmission of linearly polarized light with an arbitrary material.

Figure 2.5 shows the optical model of a sample (ambient/thin film/substrate). Here, optical model represents the knowledge of complex refractive index and thickness information of all the layers in the stack. Optical interference of light occurs due to
multiple reflections of light at the ambient/thin film and thin film/substrate interfaces. The secondary reflections from the backside of the substrate are assumed not to interfere due to its relatively large thickness (typically in the order of millimeters). The total reflection coefficients can be calculated for ‘p’ and ‘s’ components of polarized light using the summation of Fresnel reflection coefficients at the interfaces in the stack and expressed as [3],

\[
R_{012,p} = \frac{r_{01,p} + r_{12,p} \exp(-i2\beta)}{1 + r_{01,p}r_{12,p} \exp(-i2\beta)},
\]

\[
R_{012,s} = \frac{r_{01,s} + r_{12,s} \exp(-i2\beta)}{1 + r_{01,s}r_{12,s} \exp(-i2\beta)},
\]

where \( r_{01,p}, r_{12,p}, \) and \( r_{012,p} \) represent the reflection coefficients for p-polarized light calculated using equation (2.60) for ambient/thin film, thin film/substrate and ambient/thin film/substrate interfaces. Similarly, \( r_{01,s}, r_{12,s}, \) and \( r_{012,s} \) refer to the reflection coefficients for s-polarized light calculated using equation (2.61). Here, exponential term, phase variation \( \beta \) is defined as [3],

\[
\beta = \frac{2\pi d}{\lambda} N_1 \cos \theta_1 = \frac{2\pi d}{\lambda} \left(N_1^2 - N_0^2 \sin^2 \theta_0 \right)^{1/2},
\]

where \( d \) is the thickness of the thin film and \( \lambda \) is the wavelength of light.
Figure 2.5: Optical interference of light after reflection from ambient/thin film/substrate sample system.

SE measures the characteristic angles $\psi$ and $\Delta$ of polarization ellipse after reflection (or transmission) for multiple wavelengths of light at various incident angles. In other words, SE measures the change in ellipticity of polarized light, hence the name ‘ellipsometry’. The measured $\psi$ and $\Delta$ are related to the total reflection coefficients described in equations (2.62) and (2.63) [3],

$$\frac{R_p}{R_s} = \tan \psi \exp(i\Delta), \quad (2.65) \text{ (a)}$$

$$\psi = \tan^{-1}\left(\frac{R_p}{R_s}\right) = \tan^{-1}\left(\frac{\sqrt{R_p}}{R_s}\right), \quad (2.65) \text{ (b)}$$

$$\Delta = \delta_p - \delta_s. \quad (2.65) \text{ (c)}$$

Unlike the definition explained in equation (2.36), $\Delta$ used in the above equation is defined as the relative phase change between ‘p’ and ‘s’ waves before and after reflection (or transmission). And $\psi$ is defined as the inverse tangent of the ratio of the magnitudes of the change in amplitudes of ‘p’ and ‘s’ waves before and after reflection (or
transmission). From equations (2.62), (2.63) and (2.65), it can be understood that $\psi$ and $\Delta$ are a function of the complex refractive index of all the materials in the stack and thin film thickness ($d$). Since, the equation needed is in non-linear form, a regression based optical modeling is generally employed to extract optical properties and thin film thickness.

2.6 Hardware: Optical elements, different optical configurations

Tools used to collect SE or Mueller data can be broadly classified into two categories: Tools with rotating optical elements and tools with photoelastic modulators. Ellipsometers with rotating element configuration can be further classified into rotating analyzer (RAE) and rotating compensator (RCE) ellipsometers [2]. All instruments have a light source (laser or broadband) and polarizer on incident side of the sample and an analyzer with a detector (typically solid state) on the reflection (or transmission) side of the sample. The polarizer (or analyzer) is generally made of anisotropic crystal capable of producing linearly polarized light from the unpolarized light source. Analyzer and polarizer are essentially the same optical elements but named based on the role they play in the measurement method. Generally, a polarizer consists of prisms made of a uniaxial anisotropic material (CaCO$_3$ or calcite). Uniaxial crystals have one characteristic optic axis (defined based on the symmetry) with two unique refractive indices ($n_e$, $n_o$ and generally $n_o > n_e$). Light propagating along the optic axis obeys Snell’s law and travels with a velocity, c/$n_o$ and referred to as ordinary ray. Here, c is the speed of light in vacuum. Light propagating oblique or perpendicular to optic axis (sometimes called fast
axis) travels with a velocity \( c/n_e \) and is defined as extraordinary ray. Since \( n_o > n_e \), extraordinary ray travels faster than the ordinary ray.

Glan-Taylor prism is the most widely used polarizer due to its high transmission efficiency over a wide wavelength range (typically, 210 -2000 nm) [3,15]. Glan-Taylor prism consists of two prisms (made of anisotropic crystal) aligned with their optic axis parallel to each other with air as the medium between them. The first prism blocks the ordinary ray by means of total internal reflection (occurs when incident angle is greater than critical angle, \( \theta_c = \sin^{-1} \frac{1}{n_o} \)) and allows only the extraordinary ray to pass through the second prism. Second prism is installed so that the emergent extraordinary ray is parallel to the incident light. Thus, unpolarized light is transformed to linearly polarized light. Several variations of Glan-Taylor prism polarizer were also developed with different materials and dielectric coatings to improve transmission efficiency and correct for wavelength spread. The performance of a polarizer is represented by extinction ratio \( (\kappa) \) defined as [2,3],

\[
\kappa = \frac{E_{x0}^2}{E_{y0}^2} = \frac{I_x}{I_y},
\]

where \( I_x \) and \( I_y \) represent the intensity of light along \( x \) and \( y \) directions of the polarizer. Extinction ratios \( (\kappa) \) of high performance polarizers are typically in the order of \( 10^5 \) [2].

Compensators (or retarders) are used to convert linearly polarized light to circularly polarized light (or vice-versa) by creating a phase difference between the electric field vector components. A compensator operates on optical anisotropy (similar to that of a polarizer) and is made of a birefringent material. Birefringence (having two
characteristic refractive indices) is a phenomenon exhibited by a uniaxial anisotropic crystal. As discussed earlier that light propagating in a birefringent crystal is split into ordinary and extraordinary rays traveling at two different characteristic velocities. This creates a phase difference ($\delta$) between both the rays exiting the crystal and is calculated by the equation [2,3],

$$\delta = \frac{2\pi}{\lambda} |n_e - n_o|d,$$

(2.67)

where $d$ denotes the thickness of the compensator. It is evident from equation (2.67) that phase difference ($\delta$) is a function of wavelength. Since, calcite exhibits a strong birefringence, the thickness ($d$) of material needed to induce a required phase difference is small. Thus, making it extremely useful for ellipsometric applications. When the phase difference ($\delta$) equals $\pi/2$ (or path difference $= \lambda/4$), the compensator is defined as quarter-wave plate. In ellipsometric or scatterometry applications, quarter-wave compensators are frequently used to generate (or detect) circularly polarized light.

Optical anisotropy can be induced in an isotropic material by applying stress in certain symmetric directions of the crystal. This phenomenon is called photo-elasticity and is employed by photo-elastic modulators. Generally, the birefringence induced in an isotropic material is proportional to the stress applied and the direction of stress coincides with the optic axis. Since the degree of anisotropy induced can be controlled by stress, a precise control on the induced phase difference is possible. But, these can be sensitive to temperature (and pressure) fluctuations and a careful calibration procedure is generally developed to account for these effects. For semiconductor metrology applications, these modulators are rarely used due to their complicated functioning and calibration.
Nevertheless, they are capable of generating high quality data when compared to rotating compensator ellipsometers.

A summary of commonly used ellipsometric hardware configurations is shown in table 2.3 [2,3,16,17]. Each configuration has its own pros and cons of measurement and the choice of ellipsometer is based on the properties of the samples to be characterized. Full Mueller matrix data is required to characterize complex samples exhibiting anisotropy and depolarization.
Table 2.3: Hardware configurations of commonly used ellipsometers.

<table>
<thead>
<tr>
<th>Ellipsometer</th>
<th>Optical configurations</th>
<th>Data collected (Stokes parameters)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PSA&lt;sub&gt;R&lt;/sub&gt;</td>
<td><img src="image" alt="PSAR Diagram" /></td>
<td>$S_1, S_2$ and $S_3$ (12 Mueller elements)</td>
</tr>
<tr>
<td>PSCA&lt;sub&gt;R&lt;/sub&gt;</td>
<td><img src="image" alt="PSCAR Diagram" /></td>
<td>$S_1, S_2$ and $S_3$ (12 Mueller elements). $S_4$ can be collected by changing the compensator angle: Needs 2 measurements.</td>
</tr>
<tr>
<td>PSC&lt;sub&gt;R&lt;/sub&gt;A</td>
<td><img src="image" alt="PSCRA Diagram" /></td>
<td>$S_1, S_2, S_3$ and $S_4$ (16 Mueller elements)</td>
</tr>
<tr>
<td>PSMA</td>
<td><img src="image" alt="PSMA Diagram" /></td>
<td>$S_1, S_2$ and $S_4$ or $S_1, S_3$ and $S_4$ (12 Mueller elements)</td>
</tr>
</tbody>
</table>
2.7 Dual rotating compensator ellipsometer

Full Mueller and ellipsometric data was collected using a state of the art dual rotating compensator ellipsometer (J. A. Woollam Inc., RC2™). The optical path of light beam traveling from the source to the detector is shown in figure 2.6. Light source consists of two lamps: a 150 Watt Xe arc lamp and a 6 Watt QTH (quartz-tungsten-halogen) lamp. The high pressure Xe lamp produces light in the ultra violet to visible wavelength spectrum (245 nm -1000 nm) and the QTH lamp generates light in the near IR region (1000 nm -1700 nm). A thin Si wafer is used to produce a single collimated beam by combining the UV-VIS and NIR light. The resultant beam passes through a fixed polarizer and later through a continuously rotating achromatic prism compensator and finally focused on the sample. The rotational frequency of the compensator is fixed after calibration and can be controlled using a hollow shaft servo-motor. Light after reflection (or transmission) passes through another continuously rotating compensator, later through another fixed polarizer (analyzer) and finally detected using two spectrometers: Si CCD detector (for UV-VIS region, 245 nm-1000 nm) and InGaAs photo diode array detector (for NIR region, 1000 nm -1700 nm). The resolution of detected light is approximately 1nm. A computer-controlled software (Complete EASE™) provided by J. A. Woollam Inc., was used to align, calibrate and collect data from the ellipsometer. Typical data acquisitions times are in the order of 5 to 15 seconds.

Intensity detected in an ellipsometric experiment can be expressed using the Jones and Mueller matrix formalism discussed in sections 2.3 and 2.4. Applying the Stokes vector description and Jones matrices for each optical element (shown in table 2.1 & 2.2), the intensity of light detected can be calculated by the following equation [2,3],
\[
\mathbf{L}_{\text{out}} = \left[ \mathbf{AR}(A) \right] \left[ \mathbf{R}(-C)\mathbf{CR}(C) \right] \left[ \mathbf{S} \right] \left[ \mathbf{R}(-C)\mathbf{CR}(C) \right] \left[ \mathbf{R}(-P)\mathbf{P} \right] \mathbf{L}_{\text{in}},
\]

(2.68)

where \( \mathbf{L}_{\text{in}} \), \( \mathbf{L}_{\text{out}} \) represent the Jones (or Stokes) vectors of the incoming and outgoing light respectively. Here, \( \mathbf{P}, \mathbf{C} \) and \( \mathbf{A} \) are the rotation angles of polarizer, compensator and analyzer with respect to the sample co-ordinate system. Substituting the Mueller matrices for each optical element (from table 2.2) in equation (2.68), we get,

\[
\mathbf{L}_{\text{out}} = \frac{1}{2} \begin{bmatrix}
1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix} \times \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos 2A & \sin 2A & 0 \\
0 & -\sin 2A & \cos 2A & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \times
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos 2C & -\sin 2C & 0 \\
0 & \sin 2C & \cos 2C & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \times
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \delta & -\sin \delta & \cos \delta \\
0 & \sin \delta & \cos \delta & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \times
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos 2P & -\sin 2P & 0 \\
0 & \sin 2P & \cos 2P & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} \times \mathbf{L}_{\text{in}}.
\]

(2.69)

The number of unknowns to be extracted from equation (2.69) is 16, which are the full Mueller matrix elements of the sample. Simplifying the above equation by substituting the characteristic frequencies (\( \omega t \)) for both compensators rotating with frequencies in the ratio 1:5, we get the following time-dependent waveform for the intensity of the light detected [16-18],

38
\[
I(t) = I_0 \left\{ 1 + \sum_{n=1}^{16} \left[ \alpha_{2n} \cos(2n\omega t - \phi_{2n}) + \beta_{2n} \sin(2n\omega t - \phi_{2n}) \right] \right\},
\]

(2.70)

where \( I_0 \) is the normalized Fourier dc coefficient, \( \alpha_{2n} \) and \( \beta_{2n} \) (\( n = 1, 2, 3, \ldots, 16 \)) are the normalized ac Fourier coefficients with phase corrections \( \Phi_{2n} \). A detector reading \( N \) times per fundamental optical cycle \( (\pi/\omega) \) leads to \( N \) equal exposure times \( (t_e = \pi/N\omega) \) generating \( N \) spectra and can be described as [2,16],

\[
S_j = I_0' \int_{\frac{j\pi}{N\omega}}^{\frac{(j+1)\pi}{N\omega}} \left\{ 1 + \sum_{n=1}^{16} \left[ \alpha_{2n} \cos(2n\omega t) + \beta_{2n} \sin(2n\omega t) \right] \right\} dt,
\]

(2.71)

For each pixel on the solid-state detector, equation (2.71) represents a system of \( N \) equations with 25 unknowns (Fourier coefficients). Inversion matrix calculations are carried to extract all the Fourier coefficients. These Fourier coefficients are directly related to the 16 Mueller elements of the sample and are extracted by balancing equations (2.69) and (2.70).

Further, both ellipsometric and Mueller matrix elements can be related each other using Mueller formalism. For an isotropic sample, the off-diagonal block elements (M13, M14, M23, M24, M31, M32, M41 and M42) are zero as there are no cross-polarization effects. The on-diagonal elements (M11, M12, M21, M22, M33, M34, M43, M44) are directly related to the ellipsometric parameters and can be described by the following equations [11,19,20].
\[
M = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} \\
M_{21} & M_{22} & M_{23} & M_{24} \\
M_{31} & M_{32} & M_{33} & M_{34} \\
M_{41} & M_{42} & M_{43} & M_{44}
\end{bmatrix} = \begin{bmatrix}
1 & -N & 0 & 0 \\
-N & 1 & 0 & 0 \\
0 & 0 & C & S \\
0 & 0 & -S & C
\end{bmatrix},
\]

(2.72)

where,

\[N = \cos(2\psi),\]
\[S = \sin(2\psi)\sin(\Delta),\text{ and}\]
\[C = \sin(2\psi)\cos(\Delta).\]

For optically anisotropic samples, due to cross-polarization effects, the off-diagonal block-elements (or off-diagonal Jones matrix elements) are non-zero. The resulting non-depolarizing MM is related to the ellipsometric parameters by the following set of equations [20-24].

\[
M = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} \\
M_{21} & M_{22} & M_{23} & M_{24} \\
M_{31} & M_{32} & M_{33} & M_{34} \\
M_{41} & M_{42} & M_{43} & M_{44}
\end{bmatrix} = \begin{bmatrix}
1 & -N - \alpha_{ps} & C_{sp} + \zeta_1 & S_{sp} + \zeta_2 \\
-N - \alpha_{sp} & 1 - \alpha_{sp} - \alpha_{ps} & -C_{sp} + \zeta_1 & -S_{sp} + \zeta_2 \\
C_{ps} + \xi_1 & -C_{ps} + \xi_1 & C_{pp} + \beta_1 & S_{pp} + \beta_2 \\
-S_{ps} + \xi_2 & S_{ps} + \xi_2 & -S_{pp} + \beta_2 & C_{pp} - \beta_1
\end{bmatrix},
\]

(2.74)

where,
\[ N = \frac{1 - \tan^2(\psi_{pp}) - \tan^2(\psi_{ps}) - \tan^2(\psi_{sp})}{D}, \]
\[ D = \frac{1 + \tan^2(\psi_{pp}) + \tan^2(\psi_{ps}) + \tan^2(\psi_{sp})}{1}, \]
\[ C = 2 \tan(\psi_{pp}) \cos(\Delta_{pp}) / D, \]
\[ S = 2 \tan(\psi_{pp}) \sin(\Delta_{pp}) / D, \]
\[ S_{ij} = 2 \tan(\psi_{ij}) \sin(\Delta_{ij}) / D, \]
\[ C_{ij} = 2 \tan(\psi_{ij}) \cos(\Delta_{ij}) / D, \]
\[ \alpha_{ij} = 2 \tan^2(\psi_{ij}) / D, \]
\[ \zeta_1 = \left( \frac{D}{2} \right) (CC_{ps} + SS_{ps}), \]
\[ \zeta_2 = \left( \frac{D}{2} \right) (CC_{ps} - SS_{ps}), \]
\[ \xi_1 = \left( \frac{D}{2} \right) (CC_{sp} + SS_{sp}), \]
\[ \xi_2 = \left( \frac{D}{2} \right) (CC_{sp} - SS_{sp}), \]
\[ \beta_1 = \left( \frac{D}{2} \right) (C_{sp} C_{ps} + S_{sp} S_{ps}), \]
\[ \text{and} \]
\[ \beta_2 = \left( \frac{D}{2} \right) (C_{sp} C_{ps} - S_{sp} S_{ps}). \]

Here, \( i, j \) represent \( p, s \) (parallel & perpendicular) components of polarized light respectively.

**Figure 2.6:** Optical configuration of dual rotating compensator ellipsometer used to collect full 16 element Mueller and ellipsometric data in a single measurement.
2.8 Software: RCWA, Scatterometry optimization methods

Optical scatterometry requires modeling of the diffraction of light from a periodic grating structure. Rigorous coupled wave approximation (RCWA) is a powerful and efficient numerical simulation analysis technique used widely in the development of scatterometry software engines. Moharam and Gaylord first developed RCWA to solve the diffraction of light from a 2D dielectric and sinusoidal planar grating structure. RCWA method solves the Maxwell’s equations to calculate the diffraction from a periodic grating structure. A schematic diagram of RCWA method used to calculate diffraction from 2D grating structure is shown in figure 2.7 [25,26]. RCWA is based on the assumption that the dielectric function of the grating can be expanded in the direction of periodicity. This is done using a Fourier series expansion of the dielectric region and is expressed as [27,28],

\[ \varepsilon(r) = \sum_h \varepsilon_h \exp \left( i \frac{2\pi h}{\Lambda} r \right), \]  

(2.76)

where \( \varepsilon(r) \) is the effective dielectric function of the periodic grating and \( h \) is the spatial expansion parameter. The periodic grating is sliced into a series of rectangular slabs and the effective dielectric function, shown in equation (2.76) is applied on each slab. The electromagnetic scattering problem (reflection or transmission) can be calculated for each slab using Maxwell’s equations by matching the boundary conditions at each slice. If the spatial expansion parameter, \( h \) is expanded over \( \pm \infty \), the exact solution of diffraction of light from the grating structure can be achieved i.e., slicing the grating into a series of infinitesimally thin slices results in an exact solution. However, this is computationally difficult and time consuming. An approximate solution is obtained by assuming finite
number of slices (s) and spatial orders (N), which works very well for a majority of the scatterometry problems. Typically, N can vary from 10 to 100 based on the dielectric function of the materials present in the grating structure [28]. Number of slices (s) to be used typically vary from 1 to 50 and depends on the line shape of the grating. Care should be taken in optimizing the analysis method to obtain an adequate solution and convergence to the diffraction problem.

Optical response simulators (RCWA) used in scatterometry only solves the “forward” problem i.e., simulates optical response for a given grating structure. They cannot extract dimensional information from an experimentally measured optical signature, which is a “reverse” problem. This requires an optimization method to match the measured data with the simulated data. Optimization processes employed to extract the critical dimensions and other structural info can be broadly classified into two categories: Library based approach and direct regression based approach. An overview of both the optimization procedures are shown in the figures 2.8 and 2.9 [27, 29]. Library method is generally used as an in-line optical metrology solution for characterization of grating structures due to faster convergence time. A large library of optical response data for varying feature dimensions of the grating structure is developed off-line using the optical response simulator and transferred onto the scatterometry measurement tool. Later, measured response of an unknown grating is matched to closest spectra in the library to extract the critical dimensional information. This method works well when the number of parameters to be measured is small (typically 3 to 6) and having little to no correlation between them. For complex samples, off-line generation of library and
sensitivity analysis of critical parameters takes considerable amount of time due to limited computational capacity.

Direct regression optimization employs a regression algorithm (typically, least squares or Marquardt-Levenberg method [30]) to extract the feature dimensions directly from the measured data. Since, it is a multi-parameter, non-linear optimization problem, the strategy to develop to a robust scatterometry model changes with sample complexity. Also, the number of local minima rapidly increases with the number of unknown parameters resulting a larger computational effort. However, due to advancements in processing speed and complex algorithms, these bottlenecks for a large extent have been addressed. Typical regression times vary from 10 seconds or longer and for samples with simple geometries, direct regression method works well and can be directly implemented on the measurement tool.

Figure 2.7: Schematic representation of RCWA method used for calculating diffraction from a periodic grating structure.
Figure 2.8: Overview of regression based optimization process used in optical scatterometry.

Polarized light (Broadband) → Optical Response Simulator → Optimizer

Sample/Structure → Simulated Response

Optical Response (Scatterometry Signature) → Match

Optical model (Initial CD parameters), Prior knowledge of shape required

Regression results (OCD profile)
Figure 2.9: Overview of library based optimization process used in optical scatterometry.

1. **Polarized light (Broadband)**
2. **Sample/Structure**
3. **Optical Response (Scatterometry Signature)**
4. **Optical Response Simulator**
5. **Simulated Spectral library**
6. **Best Match**
7. **OCD Profile**

- **Define Structure, Parameter space, Resolution**
- **Pilot samples calibrated with CD-SEM, CD-AFM etc.**
- **Off-line process**
2.9 References


CHAPTER 3

Effect of stress on the optical properties of strained materials

The precision, accuracy and robustness of both scatterometry and ellipsometric optical models strongly depend on the correctness of the optical properties of all the materials in the stack. Here, optical properties refer to the dielectric function (or complex refractive index) of the material. Dielectric function (DF) of a material is a function of wavelength (or frequency) of light. Temperature, stress and spatial confinement affect the critical point behavior of the DF of a material and it is extremely important to use the appropriate optical properties during scatterometry or ellipsometric analysis for obtaining accurate results. This chapter focuses on the effects of stress on the dielectric function of biaxially strained, pseudomorphic Si$_{1-x}$ Ge$_x$ (0$<$X$<$0.75) alloy layers grown on a Si (001) substrate. Strained materials are currently being employed to improve the electron or hole mobility of both non-planar FinFET and MOSFET devices for 22nm technology node and beyond. Understanding the effects of strain would be essential for accurate process control and metrology in IC manufacturing.

The optical properties of un-doped, bi-axially strained, fully pseudomorphic Si$_{1-x}$ Ge$_x$ alloy layers (0$<$X$<$0.75) grown on silicon (100) were measured using spectroscopic ellipsometry over a spectral range of 245nm to 1000nm. The composition of Ge, thickness of the alloy layer along with strain was measured using high resolution X-ray diffraction (HRXRD). HRXRD showed that all the samples were fully strained with no relaxation. Also, AFM (Atomic Force Microscopy) showed that the samples exhibit low values of surface roughness, which facilitates the extraction of the dielectric function.
Stress in the Si$_{1-x}$Ge$_x$ films affects the optical properties and induces shift in the $E_1$ and $E_1+\Delta_1$ critical point energies. This relative shift in energies can be explained using elastic theory (based on the principles of $k*p$ theory) [1].

This chapter is divided into six main sections. The first section gives a brief introduction of the origin of critical points using the band structure of silicon. The second section provides the mathematical foundation for calculating the shift in critical point energies using elastic theory. The third and fourth sections discuss the deposition technique used for sample preparation and HRXRD characterization used to determine the strain, concentration and film thickness. The fifth section provides the experimental details regarding the measurement of dielectric function using spectroscopic ellipsometry. Later, direct space analysis (both second and third derivative methods) calculations that are used to extract critical point energies are discussed. Also, the measurement results were compared with elastic theory calculations [1, 14]. Tabulated values of the extracted dielectric functions for various concentration of germanium can be found in appendix I.

3.1 Introduction: Critical Points

Strain in a crystalline semiconductor material affects its band structure and several novel strained alloy materials (like SiGe, GeSn) are used to increase carrier mobility and tune the band gap of devices. Both hydrostatic and shear compressive stress components occur in biaxial strained Si$_{1-x}$Ge$_x$ causing a shift in the critical point energies. The typical stress observed in a strained pseudomorphic Si$_{1-x}$Ge$_x$ film is in the order of 1 GPa for films with germanium concentration less than 20% Ge and increases with a rise in concentration to more than 3Gpa. Though epitaxial growth of Si$_{1-x}$Ge$_x$ is well understood [2-4], growth of
high quality, strained, high concentration Si$_{1-x}$Ge$_x$ films still remains a challenge. Recent advancements in deposition methods enabled epitaxial growth of fully strained high concentrations of germanium alloy layers (>50%) [5]. Few publications describe the study of the dielectric function for fully strained, high quality Si$_{1-x}$Ge$_x$ films, especially for concentrations greater than 50% [1, 6-9]. Humlíček et al. studied the dielectric function of fully relaxed or strain-free Si$_{1-x}$Ge$_x$ alloys and a comparison of results obtained from the current work validated the effect of strain on optical behavior [10]. Elastic theory calculations and comparisons were possible due to the availability of wide range of samples with varying Ge concentrations (0% to 75% Ge). Appropriate and accurate determination of optical properties for strained alloy materials is necessary for successful implementation of optical metrology in scatterometry and ellipsometry applications. Also, data from this study work shows that the relative error resulted in using strain-free properties for fully strained material was found to be significant (typically around 15% for 20%Ge sample) in ellipsometric thickness measurements and would increase with rise in concentration of Ge.

Direct band optical transitions observed as sharp peaks in the dielectric function are called critical points (CP). They arise when there exists approximately a constant energy gap between conduction band (CB) and valence band (VB) with high joint density of states [11]. The transition from $\Lambda_3$ (VB) to $\Lambda_1$ (CB) along $k = (2\pi/a_0) <1/4,1/4,1/4>$ to the edge of the Brillouin zone (BZ) gives rise to the E$_1$ CP [12]. For Si (room temperature), it occurs at 3.4eV [12]. The E$_1$ CP of Si also has a nearly degenerate, E$_1$+$\Delta_1$ CP where $\Delta_1$ (= ~ 0.03 eV) is the spin orbit splitting and is difficult to measure at room temperature. Ge has a large spin orbit splitting of ~ 0.19 eV which is easily detectable by an
ellipsometer at room temperature. Room temperature CP energies of Ge are lower than Si and occur at 2.11 eV ($E_1$) and 2.3 eV ($E_1+\Delta_1$) [13]. Rohlfing et al determined that strong electron-hole interactions were responsible for large oscillator strength and energy of $E_1$ CP of Si [13]. For concentrations of Ge less than 20%, $E_0'$ CP is nearly degenerate with the $E_1$. $E_0'$ CP was found to occur due to optical transitions from the $\Gamma_{25'}$ (VB) to $\Gamma_{15}$ (CB) at the center of the BZ [14]. Low temperature measurements of Si can be used for accurate determination of $E_0'$ and $E_1$. The $E_0'$ CPs of Si and Ge occur at 3.20 eV and 3.123 eV respectively [1]. A linear interpolation method is generally employed for extracting $E_0'$ CP from the nearly overlapping $E_1$ and $E_1+\Delta_1$ of a strained alloy and an overview can be found in reference 1. There is some ambiguity in the reported values of $E_1'$ CP for Ge. For Si, $E_1'$ was found to occur at 5.45 eV whereas for Ge, the values reported in literature varied between 4.35 to 4.5 eV [15,16]. $E_1'$ results due to the optical transitions occurring from the $\Lambda_3$ (VB) to the second CB along the $<111>$ direction [15,16]. Finally, the $E_2$ CP for Si and Ge show higher intensity than the $E_1$ CP and occur at 4.27 eV and 4.36 eV respectively [11]. The optical transition responsible for $E_2$ CP is not well defined but considered to occur as an optical transition close to the edge of the BZ along the $\Sigma$ and $\Delta$ directions [11].

3.2 Theory: Elastic theory calculations

An overview of elastic theory calculations that describe the effect of strain on optical properties can be found in reference 17. Equations describing the effect of concentration of Ge on $E_1$, $E_1+\Delta_1$ and $E_2$ CP of relaxed or strain free alloy films are stated in reference 1 and 10, represented as:
Equation Chapter 3 Section 1

\[ E_1(x) = 3.395 - 1.287x - 0.153x(1-x), \text{eV}, \quad (3.1) \]

\[ [E_1 + \Delta_1](x) = 3.428 - 1.132x - 0.062x(1-x), \text{eV}, \quad (3.2) \]

\[ E_2(x) = 4.372 - 0.00069(1-x), \text{eV}. \quad (3.3) \]

Equations (3.1) to (3.3) are also a function of strain. Here, Zollner’s [17] nomenclature has been used to define the strain parameters. The ‘in-plane’ of the sample is defined as the direction perpendicular to growth direction and the corresponding lattice constant of the pseudomorphic Si\(_{1-x}\)Ge\(_x\) alloy was assumed to be that of silicon. HRXRD measurements were used to confirm the pseudomorphic nature of Si\(_{1-x}\)Ge\(_x\) alloys. The experimental details can be found in the subsequent sections. The equation describing the lattice constant of strain-free and bulk Si\(_{1-x}\)Ge\(_x\) at room temperature can be represented as [18, 19]:

\[ a_{\text{Si}(1-x)Ge(x)}(x) = a_0(\text{Si}) + 0.200326x(1-x) + [a_0(\text{Ge}) - a_0(\text{Si})]x^2 \text{ Å}. \quad (3.4) \]

And, the equation describing the lattice constant along the growth direction of pseudomorphic Si\(_{1-x}\)Ge\(_x\) alloys grown on Si(001) is given by [20],

\[ a_{\text{Si}(1-x)Ge(x)}(x)[||] = a_0(\text{Si}) + 0.4005x - 0.0063x^2 \text{ Å}. \quad (3.5) \]

Equation (3.5) holds true at room temperature and shows small deviations from elastic theory. Further, the in-plane strain component, \(e_{\perp}\), and the strain component along the growth direction, \(e_{||}\), are defined by the following equations [1, 16, 17, 21]:

\[ e_{\perp} = \frac{a_{\text{Si}}}{a_{\text{Si}(1-x)Ge(x)}} - 1, \quad (3.6) \]

\[ e_{||} = 2\frac{S_{12}}{S_{11} + S_{12}} e_{\perp}. \]
The linear interpolation method (Vegard’s law) was used to calculate the elastic compliance constants $S_{11}$ and $S_{12}$ for $Si_{1-x}Ge_x$ alloys. Table 3.1 shows the elastic compliance and stiffness constants used in the calculations. The elastic stiffness constants $C_{11}, C_{12}$ are related to the elastic compliance constants by $C_{11}-C_{12}=(S_{11}-S_{12})^{-1}$. As a result, the hydrostatic and shear strain components can be calculated using the following equations [1, 17, 21, 22, 23]:

\[ e_H = \frac{e_\parallel + 2e_\perp}{3} \quad \text{and} \quad e_S = \frac{e_\parallel - e_\perp}{2}. \quad (3.7) \]

In summary, equations (3.1) through (3.7) can be used to calculate both the hydrostatic and shear strain components of a pseudomorphic strained alloy film. Now, shear and hydrostatic shifts in the critical point energies for a biaxially strained $Si_{1-x}Ge_x$ film can be related to the corresponding strain components and are calculated using the following expressions [1, 16, 17].

\[ \Delta E_H = \sqrt{3}D_1^1 e_H \quad \text{and} \quad \Delta E_S = \sqrt{6}D_3^1 e_S. \quad (3.8) \]

Where $D_1^1$ and $D_3^1$ represent the volume and shear deformation potentials.

Etchegoin, et al, calculated the deformation potentials for pure Si (0 to ~ 2 GPa) and Ge (~ 1 GPa) [24, 25]. Pseudomorphic $Si_{1-x}Ge_x$ alloys can experience stresses greater than 3 GPa, and the stress versus the shift in CP energy is non-linear for Ge [25]. Here, Vegard’s law was used to approximately estimate the values of the deformation potentials of $Si_{1-x}Ge_x$ alloys using bulk values as the basis. Table 3.1 lists the values of lattice constant, elastic properties and phonon deformation potentials of Si and Ge.
Table 3.1. Elastic constants, phonon deformation potentials and lattice constant values for Silicon and Germanium at room temperature. Values are taken from Ref. 1 and 19.

<table>
<thead>
<tr>
<th></th>
<th>$C_{11}$ $(10^{12}$ dyn cm$^{-2}$)</th>
<th>$C_{12}$ $(10^{12}$ dyn cm$^{-2}$)</th>
<th>$D_1^1$ (eV)</th>
<th>$D_3^3$ (eV)</th>
<th>$a$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>1.66</td>
<td>0.64</td>
<td>-9.72</td>
<td>4.36</td>
<td>5.432</td>
</tr>
<tr>
<td>Ge</td>
<td>1.29</td>
<td>0.48</td>
<td>-8.6</td>
<td>5.9</td>
<td>5.657</td>
</tr>
</tbody>
</table>

Further, the energies of the $E_1$ and $E_1+\Delta_1$ CP for bi-axially strained tetrahedral semiconductors can be calculated using the following equations [1, 16, 17, 21, 26]:

$$E_1 = E_1^0 + \frac{\Delta_1}{2} + \Delta E_H - \sqrt{\left(\frac{\Delta_1}{2}\right)^2 + (\Delta E_S)^2}, \quad (3.9)$$

$$E_1 + \Delta_1 = (E_1^0 + \Delta_1) - \frac{\Delta_1}{2} + \Delta E_H + \sqrt{\left(\frac{\Delta_1}{2}\right)^2 + (\Delta E_S)^2}. \quad (3.10)$$

The energy shift of a critical point can be calculated from strain. The calculations are classified into two cases: small shear ($\Delta E_S < \Delta_1$) and large shear ($\Delta E_S > \Delta_1$) approximations. These approximations would be useful to estimate the relative intensities of both $E_1$ and $E_1+\Delta_1$ critical points. For the case of small shear approximation, the critical point energies are related by the following equations:

$$E_1 = E_1^0 + \Delta E_H - (\Delta E_S)^2 / \Delta_1, \quad (3.11)$$

$$E_1 + \Delta_1 = (E_1^0 + \Delta_1) + \Delta E_H + (\Delta E_S)^2 / \Delta_1. \quad (3.12)$$

And the relative intensities of $E_1$ and $E_1+\Delta_1$ critical point energies are calculated by

(Small shear approximation),
\[ I_{E_1}(e_S) = I_{E_1}(e_S = 0) \left( 1 - \frac{\sqrt{6}D_3^3e_S}{\Delta_1} \right) \], \quad (3.13) \\
\[ I_{E_1+\Delta_1}(e_S) = I_{E_1+\Delta_1}(e_S = 0) \left( 1 + \frac{\sqrt{6}D_3^3e_S}{\Delta_1} \right) \]. \quad (3.14) 

For the case of large shear approximation, the critical point energies are in general named as \( E_a \) and \( E_b \). Assuming negligible spin orbit interactions, \( E_a \) and \( E_b \) can be related to the hydrostatic and shear strain energy values and expressed as [1, 17, 21, 23]:

\[ E_a = E_1 + \Delta E_H + \Delta E_S, \quad (3.15) \]
\[ E_b = E_1 + \Delta E_H - \Delta E_S. \quad (3.16) \]

The relative intensities of both the critical points change with the concentration of germanium. For the case of small shear, the intensity calculated for \( E_1+\Delta_1 \) CP is higher than the intensity of \( E_1 \). Also, the relative difference of this intensity increases with rise in concentration of Ge. Similarly, for the case of large shear, the intensity calculated for lower energy \( E_b \) is estimated to be almost three times that of the intensity of the \( E_a \) critical point. This relative difference in intensities has a prominent effect on the line shape of the dielectric function of the alloy film. In conclusion, calculations from elastic theory estimate a significant change in the line shape of the dielectric function with an increase in concentration of Ge. The regime change from small shear to large shear was observed to occur for alloy films with concentrations ranging from 40% to 50% Ge. The critical point energies calculated using elastic theory for alloy films as a function Ge concentration are shown in figure 3.1.

It is extremely important to verify the pseudomorphic nature of the alloy film grown on the substrate for accurate determination of dielectric function. It is also useful
for relevant comparison with elastic theory calculations. Photo-luminescence and X-ray diffraction are commonly employed to experimentally determine concentration of germanium and pseudomorphic nature of the epi layer [27]. Also, variations in growth and process conditions strongly influence the percentage of relaxation in the film. Hence, it is necessary to confirm the pseudomorphic nature of the epi layer. HRXRD was used in the present work for validation of strain and concentration of germanium.

**Figure 3.1**: Comparison between the values of the $E_1$ and $E_1 + \Delta_1$ critical point energies for Si$_{1-x}$Ge$_x$ alloys for unstrained alloys and those calculated using the elastic theory described in section II for pseudomorphic, bi-axially strained Si$_{1-x}$Ge$_x$ alloys on Si(001). The experimental values were taken from reference 10.

![Comparison between the values of the $E_1$ and $E_1 + \Delta_1$ critical point energies for Si$_{1-x}$Ge$_x$ alloys for unstrained alloys and those calculated using the elastic theory described in section II for pseudomorphic, bi-axially strained Si$_{1-x}$Ge$_x$ alloys on Si(001). The experimental values were taken from reference 10.](image)

Similar to the behavior of the critical points discussed earlier, both $E_0'$ and $E_2$ critical points are affected by strain [1, 28]. $E_0'$ CP of pseudomorphic Si$_{1-x}$Ge$_x$ epi layer was observed to follow a linear trend with concentration of Ge (for X<20%) [28, 29]. While
the oscillator strength of E2 CP was predicted to decrease with rise in Ge concentration (for X<30%) [15,16]. Also, E2 was observed to collapse from single CP to multiple peaks at low temperatures [15].

3.3 Experimental Details

The Si1-xGex alloy films described in this section were provided by IBM. Chemical vapor deposition at low temperature and reduced pressure was used to grow high quality, pseudomorphic, fully strained intrinsic Si1-xGex alloy films on blanket double-sided polished 300mm p-type Boron-doped (1-10 Ωcm) (100) silicon wafers. A mixture of disilane and germane was used to deposit these alloy layers (up to a concentration of Ge = 75%). Careful control of temperature below the critical point for 3D growth mode (375C to 575C) was responsible for good quality of deposition. Later, an aqueous HF solution was used to remove the native oxide and terminate the surface with hydrogen. Following a water rinse and isopropyl drying process, the wafers were loaded into the UHV batch load lock of the CVD reactor within one hour. Prior to deposition, the wafers were heated for 2 - 3 minutes at 700 – 750C to desorb the remaining sub-stoichiometric surface oxide that re-formed during the exposure to air. Untreated wafers were cleaned employing an in-situ high-temperature (1050C) hydrogen pre-bake that removed organic contamination and native oxide. The BEDE Metrix L (Jordan Valley Semiconductors) X-ray diffraction tool was used to characterize layer thickness, germanium concentration and strain of all wafers. AFM data indicated that all films had less than 0.1 nm RMS (route mean square roughness) over a 10 micron x 10 micron area except for x=0.75
where the RMS value was \( \sim 0.14 \) nm. This enabled successful optical characterization using spectroscopic ellipsometry.

In order to characterize the strained induced effects on the complex dielectric function, spectroscopic ellipsometry (SE) measurements were performed on the series of high pseudomorphic Si\(_{1-x}\)Ge\(_x\) (0<\(x<0.75\)) alloy layers characterized by high resolution X-ray diffraction, The ellipsometric angles \( \Psi \) & \( \Delta \) were collected in the spectral range of 0.73 – 5.06eV (1700 nm – 245 nm) with a resolution of 0.01eV using a computer controlled, high accurate dual rotating compensator ellipsometer, J.A. Woollam RC2™.

Along with the standard ellipsometric parameters, depolarization data was also collected to account for non-ideal effects due to backside reflections in the IR region (\( \approx \)1000-1700nm). The dielectric functions were extracted from the experimental data by determining the optimum model using minimization of least squares method known as Marquardt-Levenberg algorithm [30]. Surface oxide effects were also incorporated in the developed model to extract the ‘true’ dielectric function of the alloy layer.

### 3.4 Characterization of strain: High resolution X-ray diffraction

High resolution X-ray diffraction was used to validate the pseudomorphic nature of all the epi layers grown on the silicon substrate [8,9]. Also, it was used to measure the thickness, strain and concentration of germanium in the layer. A combination of symmetric and asymmetric scans was used to verify the pseudomorphic nature of the alloy films. The lattice constant perpendicular to growth direction was measured using symmetric (004), \( \omega-2\theta \) rocking curves. The lattice spacing between the planes was measured using glancing exit asymmetric 224 relaxation scans [31, 32]. Figure 3.2 shows
the overlay plot of triple axis, (004) ω-2θ rocking curves plots for all the Si_{1-x}Ge_x alloy films with concentration of germanium varying from x= 0.05 to x= 0.75. Also, Table 3.2 shows a consolidated report of the concentration and thickness for all the films.

The periodicity of the interference fringes observed near the epi layer’s diffraction peak are used to determine the thickness of alloy layer. The concentration of germanium is determined by calculating the angular difference between substrate and layer peak. Based on diffraction theory, the intensity of the peak is proportional to the square of the number of diffracting planes while the width and periodicity of interference fringes is inversely proportional to the number of planes.

Layer thickness and composition were extracted using a curve–fitting methodology [32]. For a Bragg angle θ, if the peak angular separation between layer and substrate is δθ, the change in the plane spacing δd with reference to substrate lattice plane spacing d, is given by [31]

$$\frac{\delta d}{d} = -\delta \theta \cot \theta.$$  \hspace{1cm} (3.17)

For 004 symmetric reflections, experimental mismatch of lattice parameter of the layer with the lattice parameter ‘a’ of the substrate is given by [31]

$$m^* = \frac{\delta a}{a} = \frac{\delta d}{d}.$$  \hspace{1cm} (3.18)

But mismatch when layers are fully relaxed is [31]

$$m = \left[\frac{a(\text{layer}) - a(\text{substrate})}{a(\text{substrate})}\right].$$  \hspace{1cm} (3.19)

By using elastic theory [31],
Further, composition (or concentration) of Ge can be calculated from the corresponding lattice parameter. Here, lattice parameter is related to the mismatch defined in equations (3.18) & (3.19). Linear interpolation (Vegard’s law) is generally assumed during the calculation of the concentration from lattice parameter. The maximum relative error of calculated Ge is 0.5%.

Triple axis HRXRD was used to differentiate tilt and strain of the layer, which is extremely important in accurate characterization of epi-layers. Further, both relaxation scans and reciprocal space maps were measured on all the wafers. Both the layer and substrate can have the same crystal orientation even though a relaxed layer’s lattice parameter does not match with the substrate [31]. Reciprocal space maps collect the diffracted intensity around a lattice point by scanning different offset omega angles along each step of \( \omega-2\theta \) to consider the effect of strain parameter and tilt separately. Symmetric (004) reciprocal maps are used to determine the presence of tilt in the epi-layer with respect to the substrate. Figure 3.3 shows the (004) reciprocal space maps for two samples with concentration of Ge = 30% and 70%. It is evident from the figure that both the layer and substrate peak have the same tilt angle. The 00l axis relates to the d-spacing changes in the alloy layer whereas the hh0 axis relates to the tilt of the diffraction planes. Figure 3.3 also shows (224) grazing exit reciprocal space maps for the same samples with concentration of Ge = 30% and 70%. These (224) maps validate that there is no relaxation. It can be clearly observed from the figure that the layer and substrate peaks
are perfectly aligned indicating the substrate and the epi-layer materials have equal parallel lattice spacing. The same measurement routine was implemented on rest of the samples to validate strain, composition and thickness.

Table 3.2: Measured and Calculated Values of the energies of the $E_1$ and $E_1 + \Delta_1$ Critical Points for Pseudomorphic Si$_{1-x}$Ge$_x$ on Si(001). The k*p theory results are listed along with the values obtained using the small and high shear approximations. The germanium concentration and thickness for the Si$_{1-x}$Ge$_x$ films measured in this study are listed. The concentration and thickness data has a relative total error of 0.5 atomic % or better. Thus, for $x=0.10$, the Ge percentage is 10% ± 0.5% and for $x=0.7$ the Ge percentage is 70% ± 3.5%.

<table>
<thead>
<tr>
<th>Wafer No.</th>
<th>Ge Fraction X</th>
<th>Si$_{1-x}$Ge$_x$ Thickness (nm)</th>
<th>$E_1$ (eV) Strained</th>
<th>$E_1+\Delta_1$ (eV) Strained</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Measured</td>
<td>k*p Theory</td>
<td>Small Shear</td>
</tr>
<tr>
<td>1</td>
<td>0.05</td>
<td>64.0</td>
<td>3.31</td>
<td>3.33</td>
</tr>
<tr>
<td>2</td>
<td>0.10</td>
<td>75.0</td>
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<td>3.27</td>
</tr>
<tr>
<td>3</td>
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<td>3.14</td>
</tr>
<tr>
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<td>3.10</td>
<td>3.09</td>
</tr>
<tr>
<td>6</td>
<td>0.27</td>
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</tr>
<tr>
<td>7</td>
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<td>46.0</td>
<td>2.97</td>
<td>2.96</td>
</tr>
<tr>
<td>8</td>
<td>0.40</td>
<td>24.6</td>
<td>2.88</td>
<td>2.86</td>
</tr>
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<td>9</td>
<td>0.45</td>
<td>18.8</td>
<td>2.85</td>
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</tr>
<tr>
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<td>2.76</td>
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</tr>
<tr>
<td>11</td>
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<td>14</td>
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</tr>
<tr>
<td>15</td>
<td>0.75</td>
<td>9.9</td>
<td>2.48</td>
<td>2.41</td>
</tr>
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</table>
Figure 3.2: Symmetric 004, $\omega$-2$\theta$ rocking curves of Si$_{1-x}$Ge$_x$ alloy films for selected Ge concentrations from $x = 0.05$ to $x = 0.75$. 
Figure 3.3: 004 and 224 Reciprocal Space Maps were plotted in hkl crystallographic dimensions showing the pseudomorphic nature of Si$_{1-x}$Ge$_x$ ($x=0.3$ and $x=0.7$) alloys on Si (001). The 004 RSMs characterize the Si$_{1-x}$Ge$_x$ 004 lattice planes that are parallel to the Si 004 lattice planes while the 224 RSM characterize both the quality of the lattice both parallel and perpendicular to the Si lattice.
3.5 Extraction of dielectric function of strained Si$_{1-x}$Ge$_x$ alloy layers

Determination of the complex dielectric functions of the pseudomorphic Si$_{1-x}$Ge$_x$ ($0 < x < 0.75$) alloy layers requires careful modeling of the surface oxide layer. Previous studies of Si$_{1-x}$Ge$_x$ with $x < 0.3$ modeled the surface oxide as pure silicon dioxide. Since this study included alloys with high concentrations of Ge ($x = 0.75$), the complex dielectric function of the native oxide on a pure Ge sample was measured. GeO$_2$ dielectric function extracted from the crystalline Ge wafer is consistent with that of Hu, et al [32]. Both silicon and germanium dioxide do not absorb in the wavelength region sampled in this study (245nm-1000nm). The real part of the dielectric function of the Si$_1$Ge$_x$ transitions from SiO$_2$ to GeO$_2$ like as Ge concentration increases. The complex dielectric functions for selected Si$_{1-x}$Ge$_x$ alloys are shown in figure 3.4 and the complex refractive index in figure 3.5. A table listing the values of $\varepsilon_1$ and $\varepsilon_2$ for all the different concentrations at different energy values (resolution 0.1eV) is provided in appendix I. Figure 3.6 shows a direct comparison between the imaginary part of the dielectric function of pseudomorphic versus stress free Si$_{1-x}$Ge$_x$ for various concentrations. The use of the un-strained complex refractive index of Si$_{0.5}$Ge$_{0.5}$ instead of the values for a strained film can result in an error of 15% or more when determining the thickness of pseudomorphic films. The percentage error was estimated by generating $\Psi$ and $\Delta$ from 0.74 eV to 5.06 eV for a 10 nm pseudomorphic Si$_{0.5}$Ge$_{0.5}$ layer using the complex refractive index listed in appendix I and then calculating the film thickness using the complex refractive index for an unstrained layer from reference 10.
Figure 3.4: The complex refractive index of $\text{Si}_{1-x}\text{Ge}_x$ alloys for selected concentrations of germanium.

Figure 3.5: The complex dielectric function of $\text{Si}_{1-x}\text{Ge}_x$ alloys for selected concentrations of germanium.
Figure 3.6. Comparison of the dielectric function of pseudomorphic Si$_{1-x}$Ge$_x$ alloys films with strain free Si$_{1-x}$Ge$_x$ alloys. The effect of strain on the line shape of the E$_1$ critical point is evident as the concentration of Ge increases. ‘Hum’ refers to Humlíček’s data for unstrained Si$_{1-x}$Ge$_x$ alloy layer [10].
3.6  **Direct space analysis: Second and third derivative methods**

A comparison of the observed changes in line shape with the predictions of elastic theory requires careful fitting of dielectric function to analytical CP line shapes for $E_1$ and $E_1+\Delta_1$. The standard analytical CP line shapes described below were found to give excellent fits to the data measured on all the samples [1, 15]. First and higher order derivatives of the complex dielectric function were calculated by first fitting a polynomial expression to the dielectric function in the energy range of interest. Then, second derivatives were calculated by differentiating the resulting polynomial expression. Critical points transitions $E_1$ and $E_1+\Delta_1$ were extracted by fitting the second derivatives of complex dielectric function using direct space analysis. The second derivative of the dielectric function is given below,

$$\frac{d^2\varepsilon}{dE^2} = \sum_{j=1}^{3} n(n-1)A_je^{i\Phi_j}(E - E_j + i\Gamma_j)^{n-2}.$$  \hspace{1cm} (3.21)

Where $\varepsilon$ is the complex dielectric function, $A_j$, $\Gamma_j$ are the amplitudes and broadening parameters, and $\Phi_j$ are the phase angles. The spin orbit splitting energy $\Delta_1$ is less than 0.1 eV for $x < 0.3$, and it is useful to remember that the $E_0'$ CP of Si is 3.20 eV and for Ge is 3.123 eV [1]. For concentrations less than $x \approx 0.32$, the critical points values of $E_0'$ and $E_1$ and $E_1+\Delta_1$ are almost degenerate [1]. For higher Ge concentrations, the spin orbit splitting, $\Delta_1$, and the strain induced separation of $E_1, E_1+\Delta_1$ both increase. The $E_1+\Delta_1$ peak becomes apparent in the double derivative of the dielectric function. Since, $E_0'$ and $E_1$ and $E_1+\Delta_1$ are almost degenerate, previous studies found that it is very difficult to resolve them [1, 6]. Here, a thorough investigation was performed for all three critical points including degenerate peaks using standard CP line shapes. Addition of a CP line shape...
for $E_0'$ with initial values for the transition energy, amplitude, phase, and broadening based on literature values [16, 28] for strain free alloys did not improve the fit or change the values of $E_1$ and $E_1+\Delta_1$. Including $E_0'$ in the analysis increased the correlation between critical energies and amplitude values during fitting, and hence, $E_0'$ values are not reported here. Determining the $E_0'$ energy and broadening requires a low temperature measurement followed by extrapolation to room temperature. Optimal fits for $E_1/E_1+\Delta_1$ were obtained by using $n = -1$ and allowing the phase angles to be different for each critical point structure [1, 15], as expected for an excitonic $E_1$ and a mixed excitonic and two-dimensional (2D) nature for $E_0'$ and $E_1+\Delta_1$ critical point. Although the $E_0'$ and $E_1+\Delta_1$ are degenerate, best fits with the second derivative were obtained by including both CP’s in the fit. This is especially true for lower concentrations of germanium.

The extracted values of $E_1/E_1+\Delta_1$ are listed in table 3.2 and compared to the elastic theory results calculated using equations (3.9), (3.10) and the small shear (equation (3.11), (3.12)) and high shear (equations (3.16), (3.17)) approximations. A comparison between elastic theory and experiment is shown in figure 3.7. These results are well represented by the complete elastic theory predictions for $E_1/E_1+\Delta_1$. The small shear approximation closely predicts the stress induced shifts of $E_1$ for low concentrations of Ge up to approximately 40% while the small shear approximation over predicts the shift of $E_1+\Delta_1$. Experimental shifts are larger than those predicted by the high shear approximation for Ge concentrations above 40%. It is interesting that the experimental results are well represented by elastic theory predictions, considering that the values of the volume and shear deformation potentials $D_1^1$ and $D_3^3$ used to calculate the hydrostatic and shear shifts were calculated using Vegard’s law [25, 34].
Figure 3.7. Comparison between the experimental values of the $E_1$ and $E_1+\Delta_1$ critical point energies for pseudomorphic, bi-axially strained $Si_{1-x}Ge_x$ alloys grown on Si(001) and the elastic theory described in Section II. The elastic theory results were calculated using the exact $k*p$ expression for the energy shifts.

Humlíček and Garriga studied the temperature dependence of the optical spectra of $Si_{1-x}Ge_x$ alloys [35]. In that work, CP energies of strain free alloys were determined by fitting the third derivative of the dielectric function. For the sake of completeness, $E_1/E_1+\Delta_1$ CP energies were also determined using third derivative of the dielectric function. The equation used to fit the third derivative is given below [28],

$$\frac{d^3(\varepsilon E^2)}{dE^3} = \sum_{j=1}^{3} C_j e^{i\Phi_j} (E - E_j + i\Gamma_j)^{-4+n/2}.$$  \hspace{1cm} (3.22)

Where $n, \Phi_j, C_j, \Gamma_j, E_j$ denote dimensionality of the critical point, the phase angle, scaling factor, broadening energy, and the transition energy of the $j^{th}$ CP, respectively. Only small differences were observed between the CP energies determined using the second and third derivatives. Significant difference will be observed when alternate line shapes are used. For example, CP energies will differ when the Lorentzian profile modified by a
normalized Gaussian used to fit the temperature dependent data in reference 35 is used instead of the analytical CP line shape used here. In table 3.3, a comparison between the $E_1/E_1+\Delta_1$ energies of strained Si$_{1-x}$Ge$_x$ alloys measured by other studies and the values obtained for the samples characterized in this study is shown [17, 36, 37]. The CP energies determined using the third derivative of the dielectric function from this study are also listed in table 3.4. Table 3.3 shows the CP energies for alloys having the same Ge concentration as studied here. The data from reference 36 was analyzed using a 2-D CP line shape, while an excitonic line shape was used in this study. It is important to note that the $E_1$ CP of silicon and germanium and their alloys is typically considered to have an excitonic CP line shape [1, 11, 13, 15, 16, 17, 23, 24, 25, 26]. There are two reasons that the CP energies might vary between studies. The first one is the selection of line shape and method used to fit to that line shape. The second is the quality of the pseudomorphic alloys. As mentioned above, the surface of these alloys is extremely smooth as indicated by the AFM data. Another indication of the surface smoothness and of the sample homogeneity is that none of the samples exhibited depolarization ($< 1\%$) for the wavelength range studied here. This amount of depolarization is typical of the data obtained by the spectroscopic ellipsometer for high quality samples such as ultra-smooth SiO$_2$/Si.
Table 3.3: Comparison of Experimental $E_1$ and $E_1+\Delta_1$ Critical Point Energies with literature values. Comparison data has been shown only for the samples that exactly match the Ge concentrations published in the above-mentioned references. The samples characterized in Reference 1 were capped with an epitaxial silicon layer making determination of $E_1$ and $E_1+\Delta_1$ difficult due to the overlap with $E_0'$. In addition, the silicon-capping layer may affect the stress experienced by the $\text{Si}_{1-x}\text{Ge}_x$ alloys making comparison difficult.

<table>
<thead>
<tr>
<th>Ge Fraction (X)</th>
<th>$E_1$ (eV)</th>
<th>$E_1+\Delta_1$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Strained</td>
<td>Strained</td>
</tr>
<tr>
<td>0.05</td>
<td>3.31$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.27$^a$</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>3.28$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.16$^c$</td>
<td></td>
</tr>
<tr>
<td>0.14</td>
<td>3.20$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.20$^b$</td>
<td>3.08$^c$</td>
</tr>
<tr>
<td>0.19</td>
<td>3.13$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.12$^b$</td>
<td>3.01$^c$</td>
</tr>
<tr>
<td>0.23</td>
<td>3.10$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.07$^b$</td>
<td>3.24$^b$</td>
</tr>
<tr>
<td>0.32</td>
<td>2.96$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3.14$^a$</td>
<td></td>
</tr>
<tr>
<td>0.45</td>
<td>2.85$^a$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2.75$^c$</td>
<td>3.04$^a$</td>
</tr>
</tbody>
</table>

$^a$ Present work

$^b$ From Reference 36

$^c$ From Reference 37 (Third derivative line shape analysis was performed to extract the critical points in this reference)
Table 3.4: Comparison of critical point values extracted using second and third derivative analysis techniques.

<table>
<thead>
<tr>
<th>Wafer No.</th>
<th>Ge Fraction (X)</th>
<th>$E_1$(eV) Strained</th>
<th>$E_1$+$\Delta_1$(eV) Strained</th>
<th>$k*p$ Theory</th>
<th>$k*p$ Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Measured 2$^\text{nd}$ Der. Analysis</td>
<td>Measured 3$^\text{rd}$ Der. Analysis</td>
<td>Measured 2$^\text{nd}$ Der. Analysis</td>
<td>Measured 3$^\text{rd}$ Der. Analysis</td>
</tr>
<tr>
<td>1</td>
<td>0.05</td>
<td>3.31</td>
<td>3.30</td>
<td>3.33</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>0.10</td>
<td>3.28</td>
<td>3.26</td>
<td>3.27</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
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<td>3.18</td>
<td>3.21</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
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<td>3.15</td>
<td>3.14</td>
<td>-</td>
</tr>
<tr>
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<td>3.09</td>
<td>3.09</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>0.27</td>
<td>3.01</td>
<td>3.01</td>
<td>3.03</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>0.32</td>
<td>2.97</td>
<td>2.97</td>
<td>2.96</td>
<td>3.14</td>
</tr>
<tr>
<td>8</td>
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<td>2.87</td>
<td>2.86</td>
<td>3.08</td>
</tr>
<tr>
<td>9</td>
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<td>2.85</td>
<td>2.85</td>
<td>2.80</td>
<td>3.04</td>
</tr>
<tr>
<td>10</td>
<td>0.51</td>
<td>2.76</td>
<td>2.76</td>
<td>2.72</td>
<td>2.98</td>
</tr>
<tr>
<td>11</td>
<td>0.54</td>
<td>2.68</td>
<td>2.70</td>
<td>2.68</td>
<td>3.07</td>
</tr>
<tr>
<td>12</td>
<td>0.61</td>
<td>2.62</td>
<td>2.63</td>
<td>2.59</td>
<td>3.01</td>
</tr>
<tr>
<td>13</td>
<td>0.64</td>
<td>2.57</td>
<td>2.58</td>
<td>2.55</td>
<td>2.99</td>
</tr>
<tr>
<td>14</td>
<td>0.70</td>
<td>2.51</td>
<td>2.52</td>
<td>2.48</td>
<td>2.92</td>
</tr>
<tr>
<td>15</td>
<td>0.75</td>
<td>2.48</td>
<td>2.49</td>
<td>2.41</td>
<td>2.98</td>
</tr>
</tbody>
</table>

3.7 Summary

Dielectric function (optical properties) of fully strained, pseudomorphic Si$_{1-x}$Ge$_x$ alloys was extracted using spectroscopic ellipsometry from 0.74 eV to 5.06 eV (245nm to 1000nm). HRXRD was used to validate the pseudomorphic nature of the alloys and measure strain, thickness and composition. Elastic theory calculations were performed to calculate the shift in critical point energies due to stress and compared with experimental results. Direct space analysis was used to extract the critical point energies from the experimental dielectric function. Both second and third derivative methods were used to resolve the critical point energies. There is a clear change in line shape for the $E_1$ and
$E_{1+\Delta_1}$ CPs as the Ge concentration increases. The room temperature shift in the energies of $E_1$ and $E_{1+\Delta_1}$ CPs with stress closely follows elastic theory predictions.
3.8 References


CHAPTER 4

Systematic investigation of Mueller properties

Knowledge of Mueller properties is extremely useful for efficient implementation of both library and regression based scatterometry methodologies. Systematic investigation of Mueller properties of grating structures provides critical information regarding symmetric properties and depolarization caused by a sample. This chapter is divided into four main sections. The first section provides a brief literature review of the work performed on Mueller properties and its implementation in the field of optical metrology. The second section discusses the origin of symmetric properties of Mueller and Jones matrices for grating structures using Stokes-Mueller formalism. The third section provides experimental details regarding sample layout and fabrication using e-beam lithography. It also discusses the configuration of ellipsometer used for data collection and software used for scatterometry analysis. Finally, the last section discusses the key observations regarding Mueller properties of the samples and gives detailed information regarding scatterometry modeling and analysis.

4.1 Mueller based optical metrology: Introduction

Evolution of complex three-dimensional structures along with shrinking feature dimensions provides significant challenges for optical dimensional metrology. According to the 2011 International Technology Road map for Semiconductors (ITRS), the requirements for uncertainty in the critical dimension measurement (CD) for forth-
coming process nodes is less than 2nm[1]. This requires unprecedented levels of precision and matching from metrology equipment. The ITRS Metrology roadmap also indicates that existing critical dimension measurement methods such as SEM and scatterometry are quickly reaching their limits and require improvements for future process nodes. Currently, the optical scatterometry that is used to measure the CD, sidewall angle (SWA) and other topographical parameters is based on spectroscopic ellipsometry (SE) and reflectometry (SR). The spectral data is interpreted through simulations of optical scattering using the rigorous coupled wave approximation[2]. This approach is widely referred to as OCD (optical critical dimension) or scatterometry in the semiconductor industry. Both the techniques are based on an inverse approach where the measured optical spectra are fitted by assuming a multi-parameter optical model and calculating the diffraction from a periodic grating [3]. The precision and accuracy of the results depend on the model, sensitivity of parameters to small changes and incorporation of several non-idealities such as signal noise. Often, complete characterization of a complex structure requires more data than available from traditional SE resulting in unresolved correlation between variables. Data from other complementary techniques like CD-SEM, CD-AFM etc., can reduce the correlation between the modeling parameters, and this hybrid metrology approach has been suggested as a means of establishing manufacturing metrology [4]. Thus, there is a need to improve OCD. Here, Mueller matrix (MM) scatterometry is investigated. The unique aspect of this technology is that MM data provides more information than conventional SE or SR based techniques especially for complex structures with anisotropy.
Several researchers have reported the advantages of MM over the conventional SE based scatterometry and performed simulated studies to understand its sensitivity to changes in feature dimensions [5–12]. Novikova et al. presented the first theoretical evaluation of MM based scatterometry and used simulation to demonstrate the benefits of MM for overlay measurement [5]. Later, they successfully implemented MM based OCD (Wavelength range used 450nm-700nm) on a photo-resist grating on a silicon substrate to extract the feature dimensions [6]. Martino et al. reported a comparison study of MM based scatterometry with other metrology methods (CD-SEM and 3D-AFM) demonstrating precision and accuracy of the method [13]. Nerbø et al. successfully characterized inclined GaSb pillars grown on a commercially available GaSb (100) wafer by MM scatterometry measurements over a spectral range of 450nm-850nm [10]. The optical properties of complex GaSb pillars were calculated using a graded uniaxial anisotropic effective medium approximation [10]. Ma et al. reported MM simulations on a simple 2D symmetric grating model and demonstrated that different geometric parameters show variable sensitivities under fixed measurement configurations and more information is achieved by changing the measurement configuration [11]. Previous studies extracted feature dimensions using a wavelength region limited to visible region and restricted analysis to simple 1D and 2D symmetric structures. MM data has complex dependence on the feature shape, orientation of the structure, depolarization and optical properties associated with the grating and underlying layers [12]. Explicit understanding of the effect of shape, asymmetry and anisotropy on MM is of great interest to the metrology community and helps pave the way for improving the characterization capabilities. The present study focuses on investigating the impact of lateral complexity.
on full MM over a wide wavelength range (245nm-1700nm). A comparison between
conventional SE based and MM based scatterometry is also provided.

4.2 Mueller properties: Stokes-Mueller formalism

The working principle is based on Stoke-Mueller formalism where the sample is defined
by a 4x4 Mueller matrix (M), which is a transformation matrix relating the incident and
reflected polarized light represented in terms of the Stokes vector. Unlike the Jones
formalism, MM can completely characterize the reflection (or transmission) by a sample
and hence, are used to describe samples which exhibit depolarization\cite{5,14}. MM
elements are represented by means of experimentally measured quantities, which make it
useful in accurate characterization of the sample. The general expression relating the
incoming and the emergent polarized light (Stokes-Mueller Formalism) is written as,

\[
\begin{bmatrix}
S_1^o \\
S_2^o \\
S_3^o \\
S_4^o
\end{bmatrix}
= 
\begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} \\
M_{21} & M_{22} & M_{23} & M_{24} \\
M_{31} & M_{32} & M_{33} & M_{34} \\
M_{41} & M_{42} & M_{43} & M_{44}
\end{bmatrix}
\begin{bmatrix}
S_1^i \\
S_2^i \\
S_3^i \\
S_4^i
\end{bmatrix},
\]

(4.1)

where superscripts ‘o’ and ‘i’ refers to the emergent and incident Stokes vector
representation of light (S), which further is expressed in terms of intensities of polarized
light in various forms and is shown below,

\[
\begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4
\end{bmatrix}
= 
\begin{bmatrix}
I_x + I_y \\
I_x - I_y \\
I_{45^o} - I_{45^o} \\
I_L + I_R
\end{bmatrix},
\]

(4.2)
where,

$I_x$, $I_y$ : Intensity of linearly polarized light oscillating parallel to X and Y axes respectively,

$I_{45^\circ}$, $I_{-45^\circ}$: Intensity of polarized light oscillating at angles $45^\circ$ and $135^\circ$ respectively and

$I_L$, $I_R$ : Intensity of left circularly and right circularly polarized light respectively.

For non-depolarizing samples, both Jones matrix (JM) and MM are related and MM can be calculated from JM using the expression defined in equation (2.58) [14]. JM is a transformation matrix relating the electric field vectors of incident and reflected polarized light and is expressed by following equation,

$$
\begin{bmatrix}
E_s^r \\
E_p^r
\end{bmatrix} =
\begin{bmatrix}
J_{11} & J_{12} \\
J_{21} & J_{22}
\end{bmatrix}
\begin{bmatrix}
E_s^i \\
E_p^i
\end{bmatrix},
$$

(4.3)

where subscript ‘s’ and ‘p’ refers to the perpendicular and parallel components of electric field ‘E’ with reference to the plane of incidence and superscript ‘i’ and ‘r’ refers to the incident and reflected polarized light respectively.

Mueller matrix data from periodic structures reflect the symmetry of the structure. The angle between the grating direction and the plane of incidence is referred to as azimuthal angle or azimuth ($\Phi$). MM depend on the mirror symmetric properties of the structure[8]. At a specific azimuth, the 2x2 off-diagonal block elements of MM vanish when the grating structure shows mirror symmetry about the plane of incidence. This is generally observed when $\Phi$ is either 0 or 90 degrees i.e. the off-diagonal elements of MM disappear when a 1D grating structure is either parallel or perpendicular to the plane of incidence[15]. Due to mirror symmetry, reflection about plane of incidence leaves the parallel components of the electric field invariant and perpendicular components change
This optical configuration is called planar diffraction and elements obtained in planar diffraction can be expressed in terms of conventional spectroscopic ellipsometric parameters $\Psi$ and $\Delta$ (which are generally used to characterize isotropic surfaces) and are expressed as follows,

$$\frac{J_{11}}{J_{22}} = \tan \psi \exp(i\Delta),$$

(4.4)

$$J = J_{22}\begin{bmatrix} \tan \psi \exp(i\Delta) & 0 \\ 0 & 1 \end{bmatrix}.$$  

(4.5)

Likewise, MM for a non-depolarizing isotropic sample (M) can be expressed in terms of $\Psi$ and $\Delta$ [3],

$$M = \frac{1}{2}\left( |J_{11}|^2 + |J_{22}|^2 \right) \begin{bmatrix} 1 & -\cos 2\psi & 0 & 0 \\ -\cos 2\psi & 1 & 0 & 0 \\ 0 & 0 & \sin 2\psi \cos \Delta & \sin 2\psi \sin \Delta \\ 0 & 0 & -\sin 2\psi \sin \Delta & \sin 2\psi \cos \Delta \end{bmatrix}.$$  

(4.6)

The normalizing multiplication factor in the above equation is referred to as sample reflectivity ($\tau$).

MM elements also depend on spot size (i.e. area of the spot enclosing the periodic structure) and anisotropic optical properties of the sample. Spot size larger than the area of periodic structure results in incoherent scattered reflection leading to depolarization[9]. Other factors like roughness, thickness non-uniformity, angular spread and finite spectral bandwidth also cause depolarization. Depolarization associated with a sample is calculated from MM elements with the following expression,

$$P_D(M) = \sqrt{\frac{\sum_{j,l} M_{jl}^2 - M_{11}^2}{3M_{11}^2}},$$

(4.7)
where $P_D(M)$ is called the depolarization index with values ranging from 0 (Perfect depolarizer) to 1 (Non-depolarizing). MM data obtained from a sample that depolarizes some of the reflected light can still be used to extract feature dimensions. A non-depolarizing MM data can be retrieved using known mathematical decomposition techniques[16].

In summary, MM exhibit model-independent simple symmetries, which may prove valuable to assess the accuracy of measurements themselves. Also, raw data changes drastically with azimuth. As a result, Mueller spectrum taken at each individual azimuth is already sufficient to reconstruct the profile by fitting data with simple model; a significant assessment of the model validity can be performed by spectra obtained at different azimuths[12].

### 4.3 Experimental details: Sample fabrication & measurement

In order to investigate the complex dependence of MM, several nano-structures were fabricated on Si (100) substrate using E-beam lithography. The structures fabricated for this study have increasing lateral complexity. Schematic picture of the layouts of all the structures are shown in figure 4.1. Clearly, the asymmetry associated with structures increases from lines to L-shaped structures and this asymmetry was expected to become visible in the off diagonal MM data.

The pattern layout required for e-beam patterning was designed using Layout editor software and transferred onto Vistec™ 300 e-beam direct-write tool. A negative resist (trade name XR-1541 Dow Corning™) was spin coated on a 3” Si (100) wafer and was transferred on to the Vistec™ 300 for patterning. The approximate thickness of the
resist ranged from 40-60 nm for all the samples. After exposure, the patterned wafer was developed in 2-3% TMAH (Tetra Methyl Ammonium Hydroxide) solvent at a temperature of 40°C for 1 minute and baked for about 1-2 minutes. Several doses of charge density were employed to find the optimum process conditions to get the desired pattern. Die size for each pattern is 1mm x 1mm. The negative resist employed is chemically similar to silicon oxide and is very stable once the resist was patterned. Also, it is capable of achieving structures of dimension around 10-20nm of resolution with minimal line edge roughness.

Figure 4.1: Schematic diagram of various periodic grating structures.
Spectroscopic MM data over a wavelength region of 245nm-1700nm was collected in planar diffraction mode using a J.A.Woollam dual-rotating compensator ellipsometer (RC2™). The angle of incidence for all the measurements was fixed at 65°. A computer controlled rotational stage was used to vary azimuth for sample alignment and the tolerance is about a fraction of a degree. Focusing optics (Numerical Aperture, NA =0.04) and camera were used to center the spot (200 microns) inside the 1mm x 1mm pattern. Negligible depolarization (less than 1%) was observed for all the samples and was not included in analysis. Presence of dual rotating compensators in the ellipsometer made it possible to measure all the 16 MM elements simultaneously. MM data collected is accurate and reproducible to an order of magnitude of 10⁻⁴. Along with MM, conventional SE data (Ψ & Δ) was simultaneously collected. Experimental data was modeled using a commercial scatterometry software (NanoDiffract™) provided by Nanometrics Inc. and is based on the well-known rigorous coupled wave analysis (RCWA) for periodic gratings[2]. Three dimensional model strategies were built and a regression based fit procedure was employed to match experimental data for determining the critical dimensions of the grating. SEM imaging was performed using Hitachi 4800™ SEM on all the samples to test the uniformity of the grating and was also used as a complimentary technique to compare the results obtained from scatterometry. The tops down micrographs of above-mentioned structures are shown in figure 4.2.
Figure 4.2: SEM micrographs of all the grating structures.

CD ≈ 31nm, Pitch ≈ 91nm

CD_x ≈ 98nm, CD_y = 95nm,
Space ≈ 100nm

CD ≈ 197nm, CD_y = 100nm,
Space ≈ 200nm

CD_x ≈ 114nm, CD_y = 107nm,
Offset ≈ 100nm, Space ≈ 100nm

CD_x ≈ 190nm, CD_y = 115nm,
Offset ≈ 200nm, Space ≈ 200nm

CD ≈ 210nm, CD_y = 102nm,
Angle ≈ 45°, Space ≈ 100nm

CD_x ≈ 83nm, CD_y = 81nm,
CD_x ≈ 377nm, CD_y = 305nm,
Space ≈ 325nm
4.4 Scatterometry analysis: Results & discussion

Spectroscopic MM (unique elements) data for all the gratings are shown in figure 4.3. Several key features are observed in the spectra and are presented below.

- Off-diagonal block elements for ‘Lines’ grating are almost zero. Since the measurement was performed in planar diffraction mode, these elements should not have values for any wavelength. However, azimuth misalignment would result in significant non-zero off-diagonal values. Hence, azimuth was also included as one of the floating parameter in the regression analysis and the offset from experimental azimuth was found to be less than fraction of a degree for all the grating structures.

- ‘Squares’ and ‘Rectangles’ gratings show similar off-diagonal behavior as the ‘Lines’ except in the region close to 245nm. The values around 245nm are above the instrument noise level. This non-zero behavior corresponds to azimuth offset and was accounted in the model.

- ‘Squares with offset’ and ‘Rectangles with offset’ gratings show a unique spectral peak around 312nm and 400nm in all the off-diagonal block elements (M13, M31, M14, M41, M23, M32, M24 and M42) respectively. This peak was absent for the grating structures without offset. The specificity of the wavelength of this spectral feature allows one to determine which sample is being analyzed in the ellipsometer without the use of high magnification images.

- ‘Parallelogram’ gratings show significant enhancement in all the off-diagonal MM elements. Lack of mirror symmetry about the plane of incidence is the reason for these non-zero values.
• The trends in the MM data for the 'L-Shaped' grating structures are similar to that of the 'Rectangles' below 300 nm. However, they have small MM values.

Figure 4.3: Scatterometry Model fit to the experimental data for all the structures. (Only unique MM elements are presented)
Floating parameters:
CD (X & Y-direction),
Resist Height
Spectroscopic ellipsometric data for all the gratings is shown in figure 4.4. Unlike MM data, SE illustrates relatively small changes in the optical spectra collected for all the gratings. Specifically, regarding the structures with offset & without offset, intensity changes seen in the SE data are small and hence, the difficulty in removing the correlation between model variables is increased. Other complementary information has to be used to improve the accuracy and sensitivity of the model. A comparison plot showing M13 values of selected grating structures with SE data are shown in figure 4.5. It is evident from figure 4.5 that MM spectra from these samples show distinct intensity variations between structures. Also, directionality of asymmetry can be predicted using this data.
As mentioned earlier, change in azimuth has a significant effect on the magnitude and sign of the MM elements. Optimal azimuthal angles that achieve the maximum signal from off-diagonal elements can be found by design of experiments. An example plot showing the effect of change in azimuthal angle over M13 element is shown in figure 4.6. MM data obtained at this specific orientation can be coupled with the data obtained in planar-diffraction to improve the robustness of the model and resolve some of the correlation between OCD parameters.

Figure 4.4: Spectroscopic ellipsometric parameters of various laterally complex grating structures fabricated using E-beam lithography.
Stitching errors are a common problem during e-beam patterning of large area structures. Some of the patterns fabricated in this study showed both stitching errors at boundaries between sub-patterns and non-uniformity at the edges of the grating structure. These samples were used to collect MM and depolarization data. A SEM micrograph of square array with stitching error is shown in figure 4.7. A comparison plot of depolarization for ‘Squares’ grating with and without stitching error is also included. Both depolarization and off-diagonal elements were significant proving the sensitivity of MM data to pattern imperfections. These errors were absent from subsequent gratings as was the signal observed in the MM and depolarization data. This was an interesting observation and was later used to identify any defects caused by e-beam lithography and change the process of fabrication accordingly eliminating some of the need for SEM imaging.
Optical constants of the resist layer were extracted by ellipsometric analysis of non-patterned resist samples. It was assumed that the grating had identical optical properties to that of a blanket film. Silicon substrate optical constants were taken from
the optical library provided in J.A Woollam Complete EASE™ software. Then, three-dimensional models were created in NanoDiffract™ using the nominal dimensions of the structures of interest. Since MM is symmetric, only unique MM elements were selected in the analysis. This enabled faster regression. Regression analysis was started with nominal structural dimensions as initial guess values and later selected parameters were floated to reduce the mean square error (MSE) between experimental and model generated data. Pitches in X and Y direction were kept constant during regression. Also, sidewall angles for all the grating structures were fixed at $90^\circ$. These values are selected based on SEM measurements. Optical spectra were sensitive to pitch values and model robustness deteriorated when used as floating parameters. The height of the grating structure is highly correlated with top CD in X and Y directions. In order to reduce the correlation, SE analysis was performed on the blanket wafer (before lithography step) to extract the thickness of resist and was used as the nominal height. No side wall angle variation was taken into consideration, as the SEM images show little to negligible rounding of the edges on the grating structure.

Off-diagonal MM elements played a crucial role in distinguishing ‘Rectangles’ and ‘Parallelogram’ grating structures. The diagonal MM elements of both the gratings are almost equal (CD values for both ‘Rectangles’ and ‘Parallelograms’ are approximately equal) and hence, it becomes difficult to distinguish ‘Parallelograms’ and ‘Rectangles’ with SE based scatterometry. The diagonal elements are representative of the critical dimensions of the structure and off-diagonal block elements are representative of the orientation of the grating. The sign of off-diagonal block elements was useful in extracting the orientation of the structure. The angle between the edges of the structure in
X and Y-direction is kept constant at 45° in the model analysis of the 'parallelogram' grating structures. For L-Shaped structures, additional floating parameters were introduced to define the complete shape during simulation (shown in figure 4.3), and careful adjustment of initial starting parameters allowed convergence to the final solution.

The typical mean squared error (MSE) in all the models was less than 0.001, validating the assumptions used in the regression analysis. The results obtained from the model fit procedure described above are shown in table 4.1. Figure 4.3 shows the individual MM elements comparing the measured and model-generated spectra. All the fits appear to be excellent, and this is validated by the root mean square (RMS) values. RMS values obtained in the regression analysis are acceptable and reasonable based on assumptions used in creating the model.
Table 4.1: Comparison of mean CD values obtained from MM scatterometry and CD-SEM.

<table>
<thead>
<tr>
<th></th>
<th>X-dimension (nm)</th>
<th>Y-dimension (nm)</th>
<th>Z-dimension (nm)</th>
<th>X-Pitch* (nm)</th>
<th>Y-Pitch* (nm)</th>
<th>RMS (Root mean square)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lines</td>
<td>33.1 31</td>
<td>-</td>
<td>-</td>
<td>52.3 55</td>
<td>90 90</td>
<td>0.017</td>
</tr>
<tr>
<td>Squares</td>
<td>107.0 98</td>
<td>104.0 95</td>
<td>57.6 60</td>
<td>200 197</td>
<td>200 207</td>
<td>0.012</td>
</tr>
<tr>
<td>Squares with offset</td>
<td>140.2 114</td>
<td>135.7 107</td>
<td>47.1 53</td>
<td>300 300</td>
<td>300 300</td>
<td>0.013</td>
</tr>
<tr>
<td>Rectangles</td>
<td>209.0 197</td>
<td>107.6 100</td>
<td>60.3 60</td>
<td>400 400</td>
<td>200 200</td>
<td>0.013</td>
</tr>
<tr>
<td>Rectangles with offset</td>
<td>176.9 190</td>
<td>136.4 115</td>
<td>54.9 59</td>
<td>350 350</td>
<td>415 415</td>
<td>0.015</td>
</tr>
<tr>
<td>Parallelograms</td>
<td>212.1 210</td>
<td>114.1 100</td>
<td>58.6 60</td>
<td>400 400</td>
<td>200 200</td>
<td>0.025</td>
</tr>
<tr>
<td>L-Shaped</td>
<td>301.2 310</td>
<td>365.1 375</td>
<td>50.7 53</td>
<td>600 600</td>
<td>700 700</td>
<td>0.013</td>
</tr>
</tbody>
</table>

*X-Pitch & Y-Pitch were not used as floating parameters in the analysis, but were manually varied to get the best possible solution during the RCWA analysis by NanoDiffraction™. CD-SEM values shown above are an average of five measurements performed at random locations on the grating structure.

Standard deviation (σ) and mean values (x_M) for each grating were calculated based on a series of fifteen measurements done at the same location with each measurement taking 10 seconds. Shorter measurement times are possible. Standard deviation (σ) associated for a given data set of measurements for a particular grating structure is calculated by the following expression[17],

\[ \sigma = \sqrt{\frac{\sum_{i=1}^{N}(x_i - x_M)^2}{N-1}}. \] (4.8)

Low standard deviations were observed (Table 4.2) for all the critical dimensions extracted indicating good precision. We expect long-term repeatability σ values for the measurements will not be significantly different than those of the short-term data. Table 4.1 also shows the comparison of values obtained from CD-SEM and MM OCD analysis.
There is discrepancy in the values obtained from both the tools. Multiple factors were responsible for these deviations. The resist used to pattern exhibited charging effects and could contribute to errors in measurement. Also, it should be noted that, OCD results are average values of the grating critical dimension parameters confined in the measurement spot, whereas the SEM data is localized and are expected to change as you move the measurement spot. Overall CD-SEM and MM OCD results show reasonable correlation based on the assumptions used in the scatterometry models.

Table 4.2: Mean & Standard deviation of critical dimensions extracted from \textit{NanoDiffraclTM}

<table>
<thead>
<tr>
<th>Grating structure</th>
<th>CD-Z (nm) (Resist Height)</th>
<th>CD-X (nm)</th>
<th>CD-Y (nm)</th>
<th>Pitch X (nm)</th>
<th>Pitch Y (nm)</th>
<th>RMS (Root mean square)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Mean ± 1σ</td>
<td>Mean ± 1σ</td>
<td>Mean ± 1σ</td>
<td>Mean ± 1σ</td>
<td>Mean ± 1σ</td>
<td>Mean ± 1σ</td>
</tr>
<tr>
<td>Lines</td>
<td>52.3 ± 0.04</td>
<td>33.1 ± 0.03</td>
<td>- ± -</td>
<td>90 ± -</td>
<td>- ± -</td>
<td>0.017 ± -</td>
</tr>
<tr>
<td>Squares</td>
<td>57.6 ± 0.00</td>
<td>107.0 ± 0.12</td>
<td>104.0 ± 0.21</td>
<td>200 ± 200</td>
<td>0.012 ± -</td>
<td></td>
</tr>
<tr>
<td>Squares with offset</td>
<td>47.1 ± 0.04</td>
<td>140.2 ± 0.21</td>
<td>135.7 ± 0.19</td>
<td>300 ± 300</td>
<td>0.013 ± -</td>
<td></td>
</tr>
<tr>
<td>Rectangles</td>
<td>60.3 ± 0.07</td>
<td>209.0 ± 0.17</td>
<td>107.6 ± 0.28</td>
<td>400 ± 400</td>
<td>0.013 ± -</td>
<td></td>
</tr>
<tr>
<td>Rectangles with offset</td>
<td>54.9 ± 0.06</td>
<td>176.9 ± 0.53</td>
<td>136.4 ± 0.60</td>
<td>350 ± 350</td>
<td>0.015 ± -</td>
<td></td>
</tr>
<tr>
<td>Parallelograms</td>
<td>58.6 ± 0.08</td>
<td>212.1 ± 0.49</td>
<td>114.1 ± 0.43</td>
<td>400 ± 400</td>
<td>0.025 ± -</td>
<td></td>
</tr>
<tr>
<td>L-Shaped</td>
<td>50.7 ± 0.20</td>
<td>301.2 ± 1.18</td>
<td>365.1 ± 1.46</td>
<td>600 ± 600</td>
<td>0.013 ± -</td>
<td></td>
</tr>
<tr>
<td>L-Width</td>
<td>114.2 ± 0.33</td>
<td>175.0 ± 2.45</td>
<td>700 ± 700</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

4.5 Summary

Mueller properties were investigated for several nanoscale complex grating structures fabricated using e-beam lithography. Experimental Mueller and ellipsometric data were collected using a dual rotating compensator ellipsometer over a wide wavelength range of
245-1700nm. Critical observations regarding the effect of symmetry on experimental Mueller data was presented. Also the importance of off-diagonal elements for characterizing complex structures was discussed. Key comparisons with ellipsometric data were also presented. Finally, a detailed analysis on the results obtained from regression based Mueller scatterometry and its added advantage over conventional scatterometry was discussed.
4.6 References


The use of strained channels became prevalent at the 65 nm node and has continued to be a large part of logic device performance improvements in every technology generation. These material and integration innovations will continue to be important in sub-22nm devices, and are already being applied in finFET devices where total available in-channel strains are potentially higher. The measurement of structures containing these materials is complicated by the intrinsic correlation of the measured optical thickness and variation of optical properties with strain, as well as the dramatic reduction in total volume of the device. Optical scatterometry has enabled characterization of the feature shape and dimensions of complex 3D structures, including non-planar transistors and memory structures. Ellipsometric methods have been successfully applied to the measurement of thin films of SiGe and related strained structures. A direction for research is validating that the thin film stress results can be extended into the much more physically complex 3D shape. There are clear challenges in this: the stress in a SiGe fin is constrained to match the underlying Si along one axis, but the sides and top are free, leading to very large strain gradients both along the fin width and height. Practical utilization of optical techniques as a development tool is often limited by the complexity of the scatterometry model and setup, and this added material complexity presents a new challenge. In this chapter, a detailed discussion of generalized spectroscopic Mueller based scatterometry measurements of strained gratings was presented, in parallel with reference cross sectional and top down SEM data. The measurements were modeled for both anisotropy...
calculations, as well as full scatterometry calculations, extracting the critical dimensions of the grating structure. The degree to which strain and CD can be quickly quantified in an optical model is discussed. Sum decomposition method has been implemented to extract the effective anisotropic coefficients and a discussion on the effect of anisotropy towards modeling is presented. Mueller based sensitivity analysis was performed to understand the relative optical sensitivities of various critical dimensions of the grating structure. Finally, errors in the scatterometry measurement are analyzed, and the relative strengths and limitations of these optical measurements were compared.

5.1 Strained FinFET metrology: Challenges

Optical scatterometry is a fast, accurate, non-destructive and model-based metrology technique used for measuring the feature dimensions of complex grating structures. The technique is rooted in high precision ellipsometric measurements, coupled to highly advance modeling and fitting algorithms. With the introduction of 3D finFETs and incorporation of strain into the channel materials, the complexity associated with modeling poses several technical challenges. First, scatterometry models generally rely on the assumption that the optical properties of materials present in grating are isotropic and constant. This assumption holds true for the majority of cases but fails when optical properties change due to dimensional confinement, or when the optical properties are sufficiently anisotropic. Several studies demonstrated the effect of strain on optical properties and use of either bulk or thin properties in models would result in a significant inaccuracy of the extracted parameters[1–3]. Second, high correlation between feature
dimensions and optical properties (which changes with strain in the 3D structures) makes it extremely difficult to build robust physical scatterometry models.

For the past several years, Mueller matrix based scatterometry has been used to address some of the short-comings of conventional ellipsometric based modeling[4–6]. MM provides the complete information of reflection/transmission intensity changes of polarized light of a sample, and in particular any anisotropic behaviors in materials. MM can be also used to calculate complex dielectric tensor of anisotropic materials by means of transmission or reflection ellipsometric measurements. Stachakovsky et al. measured the anisotropy associated with flexible polymeric sheets by combination of phase modulated spectroscopic ellipsometry and liquid crystal Mueller matrix measurements in both reflection and transmission configurations[7]. Oriol and co-workers were able to extract the two independent components of gyration tensor and the optical activity of quartz crystal by oblique incidence transmission generalized ellipsometry[8]. Nervo et al. characterized inclined GaSb pillars both ex situ and in situ to extract feature dimensions using Mueller matrix ellipsometry. They described the optical properties of the medium by assuming effective medium approximation model and incorporating uniaxial and biaxial anisotropic behavior to GaSb pillars[9,10].

Depolarization and other systematic uncertainties strongly affect the experimentally measured MM resulting in a depolarized MM[11]. Careful filtering of MM enables the user to interpret anisotropic and depolarizing properties of a sample. Several decomposition methods have been developed based on optical path and its interaction of light with the sample media[12]. In the present study, we implement the Cloude sum decomposition method[12] to understand strained grating structures. This
method is based on Eigen value decomposition and works well for systems with low depolarization effects (typically less than 15%). Also, Mueller based scatterometry was used to measure feature dimensions of these strained structures by using optical methods developed prior to this study and details can be found elsewhere[1].

5.2 Depolarization effects: Sum decomposition method

Cloude[15,16] introduced an algorithm to decompose experimental MM that removes measurement uncertainties as well as depolarization using a spectral decomposition (also called Eigen decomposition) technique and can be well represented by an equivalent Mueller-Jones matrix. The calculated Eigen value spectrum from experimental MM is degenerated for the case of noise and can be used to distinguish between random noise effects and true system depolarization effects, though systematic sources of variation are not normalized out. For an experimental MM, a representative coherency matrix can be calculated by the following expression,

\[ H = \frac{1}{2} \sum_{i=0}^{3} \sum_{j=0}^{3} M_{ij} (\sigma_i \otimes \sigma_j), \]  
(5.1)

where \( \sigma_{i,j} \) are the 2x2 Pauli matrices defined as,

\[ \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \sigma_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \]

(5.2)

The coherency matrix calculated from experimental MM is Hermitian by construction and can be spectral decomposed. After decomposition, \( H \) can be expressed as

\[ H = W A W^*, \]  
(5.3)
where $\Lambda$ is a real diagonal matrix having Eigen values $(\lambda_{k,k}, k=1,2,3,4)$ of the coherency matrix $(H)$ with $|\lambda_{4,4}| \leq |\lambda_{3,3}| \leq |\lambda_{2,2}| \leq |\lambda_{1,1}|$. $W$ is the corresponding unitary matrix formed by its Eigen vectors. Further, $M$ can be expressed as a linear summation of the product of the calculated Eigen values and its corresponding non-depolarizing Mueller-Jones matrices $(MJ_i)$. Mathematically, it can be represented by the following equation,

$$M = \lambda_{11}MJ_1 + \lambda_{22}MJ_2 + \lambda_{33}MJ_3 + \lambda_{44}MJ_4,$$ \hspace{1cm} (5.4)

where $MJ_i$ can be derived from the following Jones matrices and by using equation (2.56):

$$j_{11}^k = \psi_1^k + \psi_2^k, j_{12}^k = \psi_3^k - i\psi_4^k, \hspace{1cm} j_{21}^k = \psi_3^k + i\psi_4^k, j_{22}^k = \psi_1^k - i\psi_3^k,$$ \hspace{1cm} (5.5)

where $\psi^k = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ is the $k^{th}$ Eigen vector of the coherency matrix $(H)$. When $M$ is not a Mueller-Jones matrix and trace of coherency matrix is approximately equal to $2M_{11}$ and three of the Eigen values $(\lambda_{k,k}, k=2,3,4)$ are close to zero, then an estimated Mueller-Jones matrix $(MJ_1)$ representative of the experimental MM can be calculated using equations (5.4) and (5.5)[15].

A perfectly non-depolarizing MM can be described using eight independent parameters. Six of these parameters depend on the state of the polarization of light. Among these six parameters, two describe linear horizontal anisotropy; the other two define $45^0$ linear anisotropy and the rest account for the circular anisotropy of light beam with respect to the sample. Both dispersion and absorption anisotropies are also distributed in these parameters. As a result, it is possible to define Mueller matrices for three special cases of anisotropy with only two independent parameters and can be represented as,
• Linear horizontal anisotropy Mueller matrix ($M_L$),

$$M_L = \begin{bmatrix}
1 & M_{12} & 0 & 0 \\
M_{21} & 1 & 0 & 0 \\
0 & 0 & M_{33} & M_{34} \\
0 & 0 & M_{43} & M_{44}
\end{bmatrix}, \quad (5.6)$$

where $M_{12} = M_{21}$, $M_{33} = M_{44}$, $M_{34} = -M_{43}$ and $M_{12}^2 + M_{33}^2 + M_{34}^2 = 1$.

• $45^0$ Linear horizontal anisotropy Mueller matrix ($M_P$),

$$M_P = \begin{bmatrix}
1 & 0 & M_{13} & 0 \\
0 & M_{22} & 0 & M_{24} \\
M_{31} & 0 & 1 & 0 \\
0 & M_{42} & 0 & M_{44}
\end{bmatrix}, \quad (5.7)$$

where $M_{22} = M_{44}$, $M_{13} = M_{31}$, $M_{24} = -M_{42}$ and $M_{22}^2 + M_{13}^2 + M_{24}^2 = 1$.

• Circular anisotropy Mueller matrix ($M_C$),

$$M_C = \begin{bmatrix}
1 & 0 & 0 & M_{14} \\
0 & M_{22} & M_{23} & 0 \\
0 & M_{32} & M_{33} & 0 \\
M_{41} & 0 & 0 & 1
\end{bmatrix}, \quad (5.8)$$

where $M_{22} = M_{33}$, $M_{14} = M_{41}$, $M_{23} = -M_{32}$ and $M_{22}^2 + M_{14}^2 + M_{23}^2 = 1$.

Clearly from equations (5.6) to (5.8), $M_L$, $M_P$ and $M_C$ anisotropy Mueller matrices have only two independent parameters. Further, any perfectly non-depolarizing Mueller-Jones (MJ) matrix can be decomposed (or parameterized) into a matrix product of these anisotropic representative matrices ($M_L$, $M_P$ and $M_C$). For perfect anisotropic crystals, the analysis described above can provide information regarding the magnitude and direction of anisotropy.
For a general case, MM is not as straightforward as $M_L$, $M_P$ or $M_C$, rather has a complicated structure. However, it is still possible to define approximate relations describing the anisotropic response from a sample. Using Stokes-Mueller formalism, different kinds of anisotropies observed, depend on certain Mueller elements. Mueller elements $\left(M_{12} + M_{21}\right)$ and $\left(M_{34} - M_{43}\right)$ account for linear horizontal anisotropy; $\left(M_{13} + M_{31}\right)$, $\left(M_{24} - M_{42}\right)$ correspond to $45^0$ linear anisotropy while $\left(M_{14} + M_{41}\right)$, $\left(M_{23} - M_{32}\right)$ account for circular anisotropy. This unique proportionality of Mueller elements to different kinds of anisotropies enables the determination of the effective anisotropic behavior of a sample with respect to polarized light.

Once experimental MM data is filtered to remove depolarization and systematic uncertainties, effective anisotropy coefficients $(\alpha, \beta, \gamma)$ can be calculated using the following expressions described in reference [17].

\[
\begin{align*}
\alpha &= \sqrt{\frac{\left(M_{12} + M_{21}\right)^2 + \left(M_{34} - M_{43}\right)^2}{\sum}} \\
\beta &= \sqrt{\frac{\left(M_{13} + M_{31}\right)^2 + \left(M_{24} - M_{42}\right)^2}{\sum}} \\
\gamma &= \sqrt{\frac{\left(M_{14} + M_{41}\right)^2 + \left(M_{23} - M_{32}\right)^2}{\sum}},
\end{align*}
\]

(5.9)

where

\[
\sum = 3M_{11}^2 - \left(M_{22}^2 + M_{33}^2 + M_{44}^2\right) + 2\Delta
\]

(5.10)

\[
\Delta = M_{12}M_{21} + M_{13}M_{31} + M_{14}M_{41} - \left(M_{34}M_{43} + M_{24}M_{42} + M_{23}M_{32}\right).
\]

Here $\alpha, \beta, \gamma$ are described respectively as the ratios of $90^0$ linear anisotropy, $45^0$ linear anisotropy and circular anisotropy with respect to the total global anisotropy of the
medium. Also, anisotropy coefficients for a perfectly non-depolarizing MM are related by the following expression:

$$\alpha^2 + \beta^2 + \gamma^2 = 1. \quad (5.11)$$

For the special cases of anisotropy described using equations (5.6) to (5.8), the effective anisotropic coefficients can be calculated using equation (5.9) and are given by,

For linear horizontal anisotropy \( (M_L) \), \( \alpha = 1, \beta = 0, \gamma = 0 \),

For 45° linear anisotropy \( (M_r) \), \( \alpha = 0, \beta = 1, \gamma = 0 \),

For circular anisotropy \( (M_c) \), \( \alpha = 0, \beta = 0, \gamma = 1 \).

It is important to note that these anisotropy coefficients are not quantitatively equivalent to the actual magnitude of anisotropy but are rather proportional. Using the above-discussed approach, one can calculate the effective anisotropic behavior of a medium directly from the experimentally measured MM. They are much more convenient than the Mueller elements directly, which are not always symmetric.

### 5.3 Scatterometry analysis

Ellipsometric measurements were obtained using a dual rotating compensator ellipsometer (J. A. Woollam RC2) capable of collecting all the 16 Mueller elements in reflection or transmission mode over a wide wavelength region of 245-1700nm. The angle of incidence for all the measurements was fixed at 65° for focusing probe measurements. A computer controlled rotational stage was used to vary azimuth (0°, 45°, 90°, 135°, 180°, 225°, 270°, 315°).
& 90°) and the tolerance in alignment is about a fraction of a degree. Focusing optics (Numerical Aperture (NA) = 0.04) and camera were used to center the spot (200 microns) inside a square die of approximately 1 cm. Mueller data collected is accurate and reproducible to an order of magnitude of 10⁻⁴. Regular calibrations of the tool and measurements with a standard of 250 Å SiO₂ on Si were performed periodically to ensure accuracy. Etched grating fin structures made of Si & SiGe alloy on a 12” silicon substrate wafer were used as test samples for measuring spectroscopic Mueller data. These fins are partially strained along the length. Strain and concentration of germanium were confirmed using reciprocal space maps and high-resolution X-ray diffraction measurements. A schematic diagram showing the 3D fin structure is shown in figure 5.1.

Figure 5.1: Schematic diagram of the grating structures used in MM analysis
A key aspect of using the measured MM data is to understand the key experimental sources of error. Our goal is to measure the composition, strain and shape of these structures. The experimental methods used to calculate MM always involve systematic and random errors. Important fundamental sources for systematic error are presence of a finite numerical aperture, finite spectral source-width, and offset in sample alignment to ellipsometer and sample variation over the spot size. A calibration procedure of the polarization components of the optical system allows the reduction of systematic errors and the estimation of measurement uncertainties in MM. Beyond these; it is also vital to understand any items that may bias the measurements. Any errors in assumption about the structure used to build the 3D optical model and offsets in the true optical properties from the real would also affect the results. More subtly, there are correlations between different measurements. These can be spectral, where the spectral changes caused by one measurement are substantially similar to those caused by another. And there are physical correlations, due to the physical nature of the process measured. Thin film performance is an excellent proxy for real optical behavior- but in cases where there is significant dimensional confinement, nucleation, or high degree of deposited variation, the offset in these optical properties can be very large.

For this experiment, gratings of SiGe and Si were measured using ellipsometer to collect the full Mueller data over a spectral range of 245nm-1700nm. Data above 1000nm was not included in the analysis to restrict the effects of incoherent backside reflections of Si. The average strain properties were calibrated using the x-ray diffraction system using dense reciprocal space maps near the 224 and 004 Si peaks. In all cases, the stress state was partially relaxed for SiGe grating structure. Also a series of Mueller data
simulations were performed using commercial RCWA based software engine (NanoDiffract™) for varying conditions of pitch walking and azimuth offset. Both strained and relaxed SiGe thin film properties were used in the simulations [1]. Strain alters the critical energy points of the alloy material and optical constants of the strained layer were extracted using spectroscopic ellipsometry. More information on the characterization of strained Si$_{1-X}$Ge$_X$ ($0 \leq X \leq 0.75$) thin films can be found elsewhere[1]. Later, sum decomposition method was implemented to extract the effective anisotropic coefficients for both experimental and calculated Mueller data.

5.4 MM simulations: Results & discussion

Normalized experimental spectroscopic Mueller data taken at three different azimuths is shown in figure 5.2. The degree of depolarization was determined using equation (2.59) at these optical configurations is plotted in figure 5.3. Depolarization and measurement noise makes it difficult to interpret the effective anisotropic behavior of the fin structures. A sum decomposition method discussed in the earlier section was used to filter a representative Mueller-Jones matrix of the sample.
Figure 5.2: Experimental spectroscopic Mueller matrix data of Si & SiGe alloy grating structures at azimuths = 0°, 45° & 90°.

Azimuth = 0°

Azimuth = 45°
Figure 5.3: Percentage degree of depolarization calculated at various azimuths from experimental MM data of SiGe grating structure.
Regression based optimization process (discussed in section 2.8) was implemented to extract the critical dimensions of both Si and SiGe grating structures. RCWA based commercial software (NanoDiffraction™) provided by Nanometrics Inc., was used to execute the optimization process. Cross-section scanning electron microscopy (XSEM) was used as a complementary technique for comparison with scatterometry results. Three-dimensional optical models shown in figure 5.1 were developed using nominal dimensions provided by the industrial partner. Only unique Mueller elements were considered during the optimization process. This enables efficient and faster convergence to experimental data. The critical dimensions floated to match the experimental Mueller data are shown in table 5.1 (Si fins) and table 5.2 (SiGe fins). Pitch and concentration of Ge were not included in the table due to confidentiality agreements with the sample provider. Since, it is difficult to get samples with systematically varying dimensions, simulations based sensitivity analysis was performed and the results obtained were discussed in the subsequent section. Both scatterometry and XSEM data shows good correlation validating the optical model developed. Best fits to experimental Mueller data for both Si and SiGe grating structures at various azimuths is shown in figure 5.4. The mean square error (MSE) was used the metric to calculate the degree of mismatch between experimental and model-generated Mueller data. A series of ten experimental data sets were collected at the same spot on both the samples and were used to calculate the average values. Tables 5.1 and 5.2 show the average MSE values along with the mean critical dimensions obtained after the optimization process.

Unlike the scatterometry results obtained from Si fin Mueller data, the mean squared error obtained for SiGe fins at azimuth 45° is slightly higher compared to the fits
at azimuth 0° and 90°. This raises a question regarding the effect of strain and anisotropy of optical properties for these structures. Mueller anisotropy analysis discussed earlier in this chapter was used to understand the important effects of strain, pitch walking of these grating structures.

Table 5.1: Mueller based scatterometry results extracted using NanoDiffract™ for Si grating structure.

<table>
<thead>
<tr>
<th>Mean OCD values</th>
<th>Azimuth 0°</th>
<th>Azimuth 45°</th>
<th>Azimuth 90°</th>
<th>Coupled Multi-azimuth Regression</th>
<th>XSEM (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom CD (nm)</td>
<td>29.3 1σ=0.01</td>
<td>32.4 1σ=0.01</td>
<td>31.3 1σ=0.03</td>
<td>30.9</td>
<td>27.6</td>
</tr>
<tr>
<td>Top CD (nm)</td>
<td>11.7 1σ=0.01</td>
<td>12.7 1σ=0.01</td>
<td>12.3 1σ=0.01</td>
<td>11.4</td>
<td>14.8</td>
</tr>
<tr>
<td>Height (nm)</td>
<td>65.5 1σ=0.07</td>
<td>66.3 1σ=0.02</td>
<td>67.5 1σ=0.01</td>
<td>65.9</td>
<td>62.3</td>
</tr>
<tr>
<td>MSE</td>
<td>0.03</td>
<td>0.06</td>
<td>0.04</td>
<td>0.04</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.2: Mueller based scatterometry results extracted using NanoDiffract™ for SiGe grating structure.

<table>
<thead>
<tr>
<th>Mean OCD values</th>
<th>Azimuth 0°</th>
<th>Azimuth 45°</th>
<th>Azimuth 90°</th>
<th>Coupled Multi-azimuth Regression</th>
<th>XSEM (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom CD (nm)</td>
<td>24.2 1σ=0.03</td>
<td>29.2 1σ=0.03</td>
<td>26.2 1σ=0.02</td>
<td>24.5 1σ=0.03</td>
<td>28</td>
</tr>
<tr>
<td>Top CD (nm)</td>
<td>11.8 1σ=0.01</td>
<td>14.6 1σ=0.01</td>
<td>12.1 1σ=0.01</td>
<td>14.8 1σ=0.01</td>
<td>12</td>
</tr>
<tr>
<td>SiGe Height (nm)</td>
<td>35.1 1σ=0.02</td>
<td>35.3 1σ=0.03</td>
<td>36.2 1σ=0.03</td>
<td>36.7 1σ=0.02</td>
<td>32</td>
</tr>
<tr>
<td>MSE</td>
<td>0.09</td>
<td>0.18</td>
<td>0.06</td>
<td>0.15</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5.4: RCWA based regression fits to experimental Mueller data for Si and SiGe grating structures at azimuths = 0°, 45° & 90°. (Only unique MM elements (7) are shown)
Si grating at azimuth = 90°

SiGe grating at azimuth = 0°

SiGe grating at azimuth = 45°
SiGe grating at azimuth = 90°

MM of symmetric periodic grating structures at azimuth orientations of 0° and 90° result in zero off-diagonal Mueller elements [4]. Mirror symmetry of sample reflection about the plane of incidence leaves the parallel components of the electric field invariant and the perpendicular components change sign resulting in zero off-diagonal MM response. Typically the anisotropic coefficients $\alpha$, $\beta$ and $\gamma$ of a grating structure show a response similar to that of isotropic thin film at these azimuth orientations having the values for $\alpha$, $\beta$, $\gamma$ at 1, 0 and 0 respectively. However, any offset in azimuth alignment would cause them to deviate from this behavior. This can be observed from the anisotropic coefficients extracted from experimental MM data for azimuth 0° shown in figure 5.5. It also includes the best fits for azimuth achieved during scatterometry analysis of these structures. A fraction of degree misalignment in azimuth orientation would translate to these coefficients. This is due to the enhanced non-zero off-diagonal response from the sample. Different values for azimuth offset were obtained when strained and relaxed
SiGe optical properties were used. This can be due to correlation between strain in the material and feature dimensions or offset itself.

Figure 5.5: Effective anisotropy coefficients extracted from experimental MM data for both Si and SiGe alloy grating structures at azimuth = 0° & 45°. Also included are the best fits for azimuth calculated using NanoDiffract™ showing offset in azimuth alignment.

In order to further understand the effects of strain on these coefficients, MM simulations were performed for Si and SiGe grating structures with strained and relaxed optical properties but identical feature dimensions. Pitch walking is another important feature dimension of interest and Mueller calculations were performed for two conditions of 1 nm and 3nm. Figure 5.6 shows the anisotropic coefficients calculated for Si and SiGe grating at 45° azimuth orientation and significant deviation can be observed between them. This is due to the unique optical properties of each constituent material present in
the grating structure. As predicted from theory, $\alpha$, $\beta$ and $\gamma$ calculated at azimuths of $0^0$ and $90^0$ show values of 1, 0 and 0 respectively and is shown in figure 5.7. Pitch walking and the choice of optical properties used for SiGe did not change this response.

Figure 5.6: Effective anisotropy coefficients extracted from simulated MM data for Si and SiGe alloy grating structures using relaxed and strained thin film optical properties at azimuth = $45^0$ for pitch walking (PW) = 0 nm

Azimuth orientation at $45^0$ breaks the mirror symmetry in Mueller response from the grating and maximizes the off-diagonal values. Two Mueller elements M12 (on-diagonal) and M13 (off-diagonal) calculated for SiGe grating were plotted for various pitch walking conditions for both relaxed and strained optical constants and is shown is figure 5.8. Largest and smallest deviations in M12 were observed at $90^0$ and $0^0$ azimuths respectively whereas M13 shows a behavior contrary to M12. Also pitch walking seems to have minimal effect as compared to strain. Although M13 show deviations at $0^0$ azimuths, these are close to the measurement noise limit in the tool and this makes it extremely difficult to measure. Magnitudes of deviations observed due to strain in M12 and M13 at azimuth orientation of $45^0$ are in measurable range of the tool. It is difficult to
extract pitch walking due to correlation from other feature dimensions. Similar behavior is observed in the effective anisotropic behavior of these gratings and is shown in figure 5.9. Nevertheless, these calculations provide an insight into effect of strain on the Mueller response.

Figure 5.7: Effective anisotropy coefficients extracted from simulated MM data for SiGe alloy grating structures using relaxed and strained thin film optical properties at azimuth = 0° & 90°. Pitch walking was assumed to be zero.
Figure 5.8: Calculated $M_{12}$ (On-diagonal block element) & $M_{13}$ (Off-diagonal block element) for Si and SiGe alloy grating structures using relaxed and strained thin film optical properties at azimuth = $0^0$, $45^0$ & $90^0$ for pitch walking (PW) = 0 nm & 3 nm over a wavelength region of 245 nm to 600 nm.

Figure 5.9: Effective anisotropy coefficients extracted from simulated MM data for SiGe alloy grating structures using relaxed and strained thin film optical properties at azimuth = $45^0$ for pitch walking (PW) = 0 nm and 3 nm.
5.5 Sensitivity analysis: Optical critical dimensions of FinFET

A systematic simulation process was employed to understand the effect of the change in the critical dimensions on the optical spectra. The spectroscopic ellipsometer used in current work is capable of measuring Mueller elements accurately with an order of magnitude of $10^{-3}$. A critical dimensional parameter is said to be optically sensitive when the largest difference in magnitude of intensities observed to change in dimensions is greater than the detectable limits of the tool. Consolidated reports showing the sensitivity spectra to changes in various important critical dimensions for both Si and SiGe gratings are shown in table 5.3 and 5.4. In order to simplify the interpretation process, only one off-diagonal (M13) and one on-diagonal (M34) Mueller elements are presented in the tables. These elements were selected as they showed relatively larger sensitivity compared to other Mueller components.

Optical sensitivity analysis for both Si and SiGe grating structures showed some interesting observation and are listed below,

- Mueller data at $45^0$ azimuth improved sensitivity to all the critical dimensions (BCD, TCD, Height of the fin). This is due to enhanced non-zero off-diagonal behavior of Mueller elements.

- On-diagonal Mueller data at $0^0$ azimuth for changes in BCD, TCD & height of Si fin showed relatively larger sensitivity compared to the data at $90^0$ azimuth. Only BCD of SiGe fin showed similar behavior. TCD and height of SiGe fin showed relatively higher sensitivity at $90^0$ azimuth.
- Off-diagonal Mueller data at both $0^\circ$ and $90^\circ$ azimuth showed zero sensitivity to changes in critical dimensions. This zero off-diagonal behavior is due to mirror symmetry property of MM about the plane of incidence.

- Optical sensitivity to critical dimensions was observed to increase with decrease in wavelength of the incident light.

In summary, Mueller data at various azimuths show unique behavior to the changes in critical dimensions and can be used to improve the statistical robustness of the optical model as well as reduce correlation between parameters.
Table 5.3: Optical sensitivity of various critical dimensions of Si grating structure.

<table>
<thead>
<tr>
<th>Critical Dimensions</th>
<th>Calculated M34 (On-diagonal) and M13 (Off-diagonal) elements for Si grating structure</th>
</tr>
</thead>
</table>
| **Varied:** BCD=29nm, 27nm, 25nm, 23nm  
  Fixed: TCD=10nm  
  Height = 37nm | ![Graphs showing optical sensitivity](image) |
| **Varied:** TCD=8nm, 10nm, 12nm, 14nm  
  Fixed: BCD=27nm  
  Height = 37nm | ![Graphs showing optical sensitivity](image) |
| **Varied:** Height=35nm, 37nm, 39nm, 41nm  
  Fixed: TCD=10nm, BCD = 27nm | ![Graphs showing optical sensitivity](image) |
Table 5.4: Optical sensitivity of various critical dimensions of Si grating structure.

<table>
<thead>
<tr>
<th>Critical Dimensions</th>
<th>Calculated M34 (On-diagonal) and M13 (Off-diagonal) elements for SiGe grating structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Varied: BCD=26nm, 24nm, 22nm, 20nm</td>
<td><img src="image1" alt="Graphs showing optical sensitivity for varying BCD values with M34 and M13 elements indicated." /></td>
</tr>
<tr>
<td>Fixed: TCD=10nm, Height Si = 35nm, Height SiGe = 37nm</td>
<td><img src="image2" alt="Graphs showing optical sensitivity for fixed TCD values with M34 and M13 elements indicated." /></td>
</tr>
<tr>
<td>Varied: TCD=8nm, 10nm, 12nm, 14nm</td>
<td><img src="image3" alt="Graphs showing optical sensitivity for varying TCD values with M34 and M13 elements indicated." /></td>
</tr>
<tr>
<td>Fixed: BCD=24nm Height Si = 35nm, Height SiGe= 37nm</td>
<td><img src="image4" alt="Graphs showing optical sensitivity for fixed BCD values with M34 and M13 elements indicated." /></td>
</tr>
<tr>
<td>Varied: Height Si =33nm, 35nm, 37nm, 39nm</td>
<td><img src="image5" alt="Graphs showing optical sensitivity for varying Height Si values with M34 and M13 elements indicated." /></td>
</tr>
<tr>
<td>Fixed: BCD=24nm TCD= 10nm, Height SiGe= 37nm</td>
<td><img src="image6" alt="Graphs showing optical sensitivity for fixed BCD and TCD values with M34 and M13 elements indicated." /></td>
</tr>
</tbody>
</table>
5.6 Summary

Spectroscopic 4x4 Mueller data was collected on Si and SiGe fin grating structure using a dual rotating compensator ellipsometer over a wide wavelength range of 245-1000nm. Experimental MM data was filtered using Cloude sum decomposition method to filter depolarization and measurement noise. A detailed mathematical approach providing the basis for extracting the effective anisotropy using Mueller elements was presented. Effective anisotropic coefficients were calculated for a representative Mueller-Jones matrix of the sample and a discussion on the effect of strain and pitch walking on anisotropic response was discussed. Regression based optimization process was used to extract the critical dimensions and a comparison with XSEM data was presented. Best fits to experimental Mueller data along with the mean squared error showing the degree of mismatch were presented. Further, simulations were carried to out to analyze anisotropic behavior and optical sensitivity. Important observations regarding sensitivity to various critical dimensions were also discussed.
5.7 References


Case Study: Optical metrology of 3D SOI Fins

Silicon on insulator (SOI) technology uses a layered silicon-oxide-silicon substrate instead of the conventional bulk silicon in semiconductor nano-electronics manufacturing. The critical advantage of this technology is the reduction of parasitic capacitance of the fabricated devices, thereby significantly improving device performance [1]. IBM was the first company to industrially implement SOI technology in semiconductor manufacturing (1998) [2]. It is widely believed that SOI technology is a potential alternative to 3D FinFET technology and can serve the needs to follow the trend of Moore’s law for 22nm technology node and beyond [3].

Optical metrology of SOI thin films and 3D structures is extremely important for efficient process control for optical lithography, etching and other processes. The current chapter focuses on Mueller based scatterometry of 3D silicon fins fabricated on SOI (provided by SEMATECH, Albany, NY) and a critical comparison with the conventional ellipsometry-based scatterometry. Further, scanning electron microscopy was used as a complementary technique to compare the results from scatterometry. Sensitivity analysis was performed to study the effect of various critical dimensions of the SOI fins.

6.1 Optical metrology: Scatterometry of SOI fins

A schematic diagram illustrating silicon fins on SOI along with the gate stack is shown in figure 6.1. The samples set used in current study were fins with 10nm nominal CD and
65nm pitch fabricated on a 300mm (100) bulk silicon wafer using double-patterning lithography. Scatterometry analysis of silicon fins with gate stack was not included in this chapter.

Optical scatterometry requires the knowledge of the dielectric function and conventional approach assumes the bulk properties to these nano-scale structures [4]. It has been studied that quantum and dimensional confinement affects the optical properties of material and it is extremely critical to understand these non-ideal consequences. For the case of silicon, these effects were proved to be prominent for dimensions less than 8-10 nm and were expected to be absent in the current scatterometry work. Full spectroscopic Mueller matrix elements (16) and ellipsometric parameters (ψ, Δ) were collected on these samples using a dual rotating compensator ellipsometer (J. A. Woollam RC²) over a spectral range of 245nm-1700nm. RCWA based optimization software provided by Nanometrics Inc., (NanoDiffract) was used for scatterometry analysis. A detailed explanation of the hardware and software can be found in chapter 2. Mueller and ellipsometric data was collected at three different azimuth rotations (0°, 45° & 90°) and regression analysis was performed for all the data sets. Experimental Mueller data at various azimuths for both SOI fins with and without gate stack is shown in figure 6.2.

Three-dimensional optical models (figure 6.1) were built using the nominal dimensions provided by SEMATECH. Regression based approach was implemented for both ellipsometric and Mueller data sets. The starting point for regression process was identical for both the data sets. This was done to eliminate any artifacts during the optimization process and care was taken to avoid local minima. Top CD, Bottom CD,
height of SOI fins and buried oxide thickness were used as floating regression parameters. Once a good fit was obtained with the experimental data, pitch was manually varied to get the best possible fit. Pitch is highly correlated with other critical dimensions and this approach was needed to improve convergence process.

**Figure 6.1: Schematic diagram of 3D silicon fins with gate on SOI**
Figure 6.2: Experimental MM of Si fins on SOI versus fins with gates on SOI at azimuths = $0^\circ$, $45^\circ$, $90^\circ$. (Samples provided by SEMATECH)

Azimuth = $0^\circ$

Azimuth = $45^\circ$
At azimuthal angles of $0^\circ$ and $90^\circ$, differences in the diagonal MM elements are clearly distinctive. At azimuthal angles of $45^\circ$, the off-diagonal MM elements are significantly different. This is expected since the off-diagonal MM elements are sensitive to feature shape changes. Because we were unable to obtain thin film samples of the gate stack materials, we were unable to develop the optical models necessary for scatterometry simulations of the samples with gates. In summary, Figure 6.2 shows that the MMSE is strongly sensitive to the extra diffraction caused by the gate stack structure.
6.2 Mueller Vs. SE based Scatterometry

Experimental Mueller data (MM) and the regression fits for SOI fins at various azimuths are shown in figure 6.3, and the SE data with best fits are shown in figure 6.4. Table 6.1 summarizes the obtained results comparing the scatterometry values for CD and pitch with cross-sectional SEM data. Table 6.1 also compares MM and traditional SE ($\Psi, \Delta$) based scatterometry. Although spectroscopic $\Psi$ and $\Delta$ data is easy to model, it lacks the necessary information content for modeling the 3D shape and dimensions of the fins fabricated from SOI. Scatterometry analysis of MM data at azimuth = 90$^\circ$ gave the best model fit to experimental data. SE based scatterometry fits at all the azimuthal angles gave similar mean square error (MSE) values (but higher than Muller based scatterometry) showing that SE is not as sensitive as MM to feature dimensions or azimuth. MMSE scatterometry simulations were well within the range of bottom and top CD values measured by CD-SEM while the feature dimensions (bottom and top CD) from SE scatterometry simulations were too small. As an overview, here are some of the important observations regarding Mueller and SE based scatterometry analysis,

- Unlike SE based scatterometry, azimuth misalignment can be easily calculated during MM based optimization process to a fraction of degree (typically to an order of magnitude of $1/3^{rd}$ of a degree). This is extremely useful to calibrate the process and include non-ideal effects in the optical model.

- Coupling of MM data at multiple azimuths should help resolve correlation between some of the critical floating parameters. This is crucial in improving the robustness of the optical model and also eliminates non-physical optical
strategies. This strategy does not work with SE data as no additional data is added at multiple azimuths.

- SE based regression approach converges in less time than MM based scatterometry analysis. The fundamental reason being that MM based analysis requires evaluation of considerably more data. One way around is using unique non-zero Mueller elements and restricting the spectral region with largest sensitivity. This resolves the problem to maximum possible extent.

Table 6.1: Mean critical dimensions of silicon fins on SOI extracted by MM & SE Scatterometry.

<table>
<thead>
<tr>
<th>Mean OCD values</th>
<th>Mueller Analysis</th>
<th>SE Analysis</th>
<th>XSEM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Azimuth</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0°</td>
<td>45°</td>
<td>90°</td>
</tr>
<tr>
<td>Fin Height (nm)</td>
<td>18.5</td>
<td>20.1</td>
<td>20.5</td>
</tr>
<tr>
<td>Pitch (nm)</td>
<td>65</td>
<td>65</td>
<td>65</td>
</tr>
<tr>
<td>Bottom CD (nm)</td>
<td>16.9</td>
<td>17.1</td>
<td>18.4</td>
</tr>
<tr>
<td>Top CD (nm)</td>
<td>12.9</td>
<td>11.9</td>
<td>13.3</td>
</tr>
<tr>
<td>BOX thickness (nm)</td>
<td>147.8</td>
<td>147.2</td>
<td>143.9</td>
</tr>
<tr>
<td>Azimuth</td>
<td>179.8°</td>
<td>133.4°</td>
<td>90.3°</td>
</tr>
<tr>
<td>MSE</td>
<td>1.7</td>
<td>1.1</td>
<td>0.6</td>
</tr>
</tbody>
</table>
Figure 6.3: Regression fits to experimental Mueller elements at azimuths = 0°, 45° & 90° optimized using NanoDiffraction™. Only unique MM elements are shown.

Azimuth = 0°

Azimuth = 45°

Azimuth = 90°
Figure 6.4: Regression fits to experimental ellipsometric parameters at azimuths = $0^\circ$, $45^\circ$ & $90^\circ$ optimized using NanoDiffract$^\text{TM}$.

Azimuth = $0^\circ$

Azimuth = $45^\circ$

Azimuth = $90^\circ$
6.3  Sensitivity analysis: Critical dimensions of SOI fins

Since fabrication of structures with changes in pitch and film stack was not possible, simulations provided a window into measurement sensitivity. The pitch of the silicon fins was fixed (occasionally varied to check the fit quality) at 65 nm for most of the simulations. The starting film stack dimensions are Fin Height = 19 nm, Top CD = 13 nm, Bottom CD = 17 nm, Pitch=65 nm, and buried oxide thickness = 143 nm. Only M34 (On-diagonal) and M24 (Off-diagonal) elements are shown and can be assumed to be representative of the full MM (SOI fin grating structure). An order of magnitude change of $10^{-3}$ is generally detectable by the dual rotating compensator ellipsometer used in the study. Sensitivity here represents the maximum change in the difference of intensities of two spectra. For example, an order of magnitude change of $10^{-2}$ is observed in M24 at azimuth = 45° for change in 2 nm of fin height between 17nm and 19nm. In other words, the fit parameter “Fin height” is said to be sensitive and it is likely that differences of 2 nm in fin height can be measured.

Simulations of the sensitivity to changes in buried oxide (BOX) thickness, fins sidewall angle, fin height, and bottom fin CD are shown in figure 6.5. The simulations are sensitive to the thickness of the BOX layer, and that sensitivity is observed in both on and off diagonal MM elements at an azimuthal angle of 45° and 90°. The simulations indicate that there is little sensitivity to sidewall angle for fins on SOI for any azimuthal angle. The fin height can be measured at any angle, but the off diagonal MM elements show greatly enhanced sensitivity to fin height at an azimuthal angle of 45°. Sensitivity to changes in the bottom CD for Fin (BW) = 15, 17, 19, 21 nm in the on diagonal MM elements is enhanced at 45° and 90°, and is enhanced for the off-diagonal MM elements
at only 45°. There are many advantages to using an azimuthal angle of 45°. The availability of additional information aids in decoupling the effects of changes in CD from changes in shape and film stack thickness variations.

**Figure 6.5: Sensitivity analysis performed for various critical dimensions of SOI Fins.**

*Azimuth = 0°* Thickness sensitivity for BOX = 140, 142, 144, 146 nm
Azimuth = 0°. Sensitivity for side wall angle, SWA = 81, 82, 83, 84 degrees

Azimuth = 0°. Sensitivity for fin height = 17, 19, 21, 23 nm
Azimuth = $0^\circ$. Sensitivity for CD fin Bottom width, Fin (BW) = 15, 17, 19, 21 nm

Azimuth = $45^\circ$. Sensitivity for SOI Thickness = 140, 142, 144, 146 nm
Azimuth = 45°. Sensitivity for side wall angle, SWA = 81, 82, 83, 84 degrees

Azimuth = 45°. Sensitivity for Fin height = 17, 19, 21, 23 nm
Azimuth = 45° Sensitivity for Bottom width, Fin (BW) = 15, 17, 19, 21 nm

Azimuth = 90° Sensitivity for SOI Thickness = 140, 142, 144, 146 nm
Azimuth = 90° Sensitivity for side wall angle, SWA = 81, 82, 83, 84 degrees

Azimuth = 90° Sensitivity for Fin height = 17, 19, 21, 23 nm
6.4 Summary

Silicon fins fabricated on SOI were used as the test case sample set for comparing Mueller to SE based scatterometry analysis. A regression based optimization approach was executed to extract the critical dimensions of the fins. An overview of key advantages of using Mueller elements in the optimization process was discussed. Regression fits for both SE and Mueller data at three different azimuths were presented.
Also a comparison was made with the results obtained from XSEM data. Finally, sensitivity analysis was performed to understand the impact of changes in critical dimension on the scatterometry optimization process.
6.5 References


CHAPTER 7

Conclusions

7.1 Summary of work

The following list gives a brief summary of the work discussed in the thesis,

- An overview of the history and development of scatterometry technology was discussed. A comparison of several commonly used optical metrology techniques were presented. An insight into some of the key challenges in metrology in modern semiconductor manufacturing was provided and few of the potential solutions were discussed.

- A detailed description of the theory and nomenclature used in scatterometry was presented. Mathematical foundation to understand scatterometry in terms of Jones & Mueller matrices was provided. Software and hardware components with different variants used for data collection were thoroughly discussed. Optimization processes employed in scatterometry were reviewed.

- The importance of dielectric function (or optical properties) of a material in the development of optical model was demonstrated. The effect of stress on the dielectric function of a strained SiGe film was investigated using spectroscopic ellipsometry. Optical models were built to extract the dielectric function of fully strained Si(1-x)Ge(x), 0<x<0.75 thin films grown on silicon substrate. Further,
direct space analysis was performed to extract the critical points and elastic theory was used to compare the results from the experiments.

- A systematic investigation of Mueller properties of several complex nanostructures fabricated using e-beam lithography was presented. The advantages of using Mueller matrix data over ellipsometric parameters were discussed. A comparison of scatterometry results with XSEM was reviewed. The effect of stitching errors, commonly observed in lithography, in terms of depolarization was investigated.

- Regression and Mueller based scatterometry optimization process was implemented to extract critical dimension and profile information of 3D Si and SiGe FinFET grating structures. Theoretical foundation required to extract the degree of anisotropy in terms of the effective anisotropic coefficients was introduced. Later, an algorithm (Sum decomposition method) was used to filter depolarization from the experimental Mueller matrices was presented. The effect of strain, azimuth misalignment and pitch walking on anisotropic coefficients was presented. The results obtained from Mueller based scatterometry was compared with XSEM data. Finally, sensitivity analysis was performed using simulations to understand the impact of critical dimensions.

- A case study comparison of ellipsometry and Mueller based scatterometry techniques was performed using silicon fin grating structures fabricated on SOI substrate. Several key advantages of using Mueller based approach were reviewed. Regression fits for both ellipsometric and Mueller data were provided. Also, data from XSEM data was used to compare results obtained from both the
scatterometry approaches. Finally, optical sensitivity analysis was performed using Mueller simulations to understand the effect of various critical dimensions.

7.2 Suggestions for future work

Block co-polymer (BCP) and EUV lithography are currently in development and are considered critical for meeting challenges for the future technology nodes. Optical metrology is extremely crucial to analyze and implement these technologies in high-volume manufacturing. Mueller based scatterometry is one of the potential solutions for in-line metrology of these complicated nanostructures. Investigation of Mueller and optical properties of BCP and EUV samples is of technological importance. Also, limited research has been performed on IR (Infrared) based Mueller scatterometry. Metals and some of the alloy semiconductor materials are transparent in IR region and it alters the Mueller properties. A feasibility study of IR based Mueller analysis would be useful for back end of line manufacturing operations.
APPENDIX I

The real $\varepsilon_1$ and imaginary $\varepsilon_2$ parts of the dielectric function for pseudomorphic $\text{Si}_{1-x}\text{Ge}_x$ alloys.

<table>
<thead>
<tr>
<th>$\varepsilon_2$, $\varepsilon_1$</th>
<th>$X$ =0.05</th>
<th>$X$ =0.10</th>
<th>$X$ =0.14</th>
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<td>5.0</td>
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