Optical metrology for directed self-assembly patterning using Mueller matrix spectroscopic ellipsometry based scatterometry

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Optical Metrology for Directed Self-assembly
Patterning Using Mueller Matrix Spectroscopic Ellipsometry Based Scatterometry

by
Dhairya J. Dixit

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
2015
Optical Metrology for Directed Self-assembly

Patterning Using Mueller Matrix Spectroscopic

Ellipsometry Based Scatterometry

by

Dhairya J. Dixit

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Dedicated to my parents, all my relatives, and friends.
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The semiconductor industry continues to drive patterning solutions that enable devices with higher memory storage capacity, faster computing performance, lower cost per transistors, and higher transistor density. These developments in the field of semiconductor manufacturing along with the overall minimization of the size of transistors require cutting-edge metrology tools for characterization.

Directed self-assembly (DSA) patterning process can be used to fabricate nanoscale line-space patterns and contact holes via thermodynamically driven micro-phase separation of block copolymer (BCP) films with boundary constraints from guiding templates. Its main advantages are high pattern resolution (~10 nm), high throughput, no requirement of a high-resolution mask, and compatibility with standard fab-equipment and processes. Although research into DSA patterning has demonstrated a high potential as a nanoscale patterning process, there are critical challenges that must be overcome before transferring DSA into high volume manufacturing, including achievement of low defect density and high process stability. For this, advances in critical dimension (CD) and overlay measurement as well as rapid defect characterization are required. Both scatterometry and critical dimension-scanning electron microscopy (CD-SEM) are routinely used for inline dimensional metrology. CD-SEM inspection is limited, as it does not easily provide detailed line-shape information, whereas scatterometry has the capability of measuring important feature dimensions including: line-width, line-shape, sidewall-angle, and thickness of the patterned samples quickly and non-destructively.

The present work describes the application of Mueller matrix spectroscopic
ellipsometry (MMSE) based scatterometry to optically characterize DSA patterned line-space grating and contact hole structures fabricated with phase-separated polystyrene-\textit{b}-polymethylmethacrylate (PS-\textit{b}-PMMA) at various integration steps of BCP DSA based patterning process. This work focuses on understanding the efficacy of MMSE base scatterometry for characterizing complex DSA structures. For example, the use of symmetry-antisymmetry properties associated with Mueller matrix (MM) elements to understand the topography of the periodic nanostructures and measure defectivity. Simulations (the forward problem approach of scatterometry) are used to investigate MM elements’ sensitivity to changes in DSA structure such as one vs. two contact hole patterns and predict sensitivity to dimensional changes. A regression-based approach is used to extract feature shape parameters of the DSA structures by fitting simulated optical spectra to experimental optical spectra. Detection of the DSA defects is a key to reducing defect density for eventual manufacturability and production use of DSA process. Simulations of optical models of structures containing defects are used to evaluate the sensitivity of MM elements to DSA defects. This study describes the application of MMSE to determine the DSA pattern defectivity via spectral comparisons based on optical anisotropy and depolarization. The use of depolarization and optical anisotropy for characterization of experimental MMSE data is a very recent development in scatterometry. In addition, reconstructed scatterometry models are used to calculate line edge roughness in 28 nm pitch Si fins fabricated using DSA patterning process.
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Chapter I

Directing the self-assembly of block copolymers

1.1 Overview: Nanofabrication techniques

The rising demand for nanoscale fabrication methods, combined with the resolution limit of optical lithography caused by diffraction, the drawbacks like high cost and low throughput of scanning beam techniques such as electron beam lithography (EB) or focused ion beam lithography (FIBL), and delay in the development of extreme ultraviolet lithography (EUVL) have motivated researchers in academia and industry to explore nonconventional nanoscale fabrication techniques. There are several general requirements that need to be satisfied for a volume nanoscale manufacturing process. For example, the method should be able to pattern high-resolution features, it must be cost effective; it must allow large-area patterning; and the alignment of the patterns should be possible. Throughput must be high and the defect density must be low.¹

Several alternative approaches for nanoscale fabrication have been exploited in the past 25 years, without resorting to expensive tools such as those required in EUVL and EBL. These techniques include nano-imprint lithography (NIL),² scanning-probe-based techniques (for example, atomic force microscope (AFM) lithography),³ self-assembly block copolymer patterning,⁴ and dip-pen lithography.⁵ In particular, the directed self-assembly (DSA) of the micro domains of block copolymers (BCP) within lithographically defined templates to create high resolution patterns with long range order has attracted considerable attention. This is due to the scalability of the self-assembled
features, regularity, and cost-effectiveness of the process.\textsuperscript{6} Table 1.1 shows the comparison between the performances of different nanofabrication techniques.

<table>
<thead>
<tr>
<th>Technique</th>
<th>Cost</th>
<th>Resolution</th>
<th>Throughput</th>
<th>Defects</th>
<th>Overlay</th>
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<td>Optical</td>
<td>High</td>
<td>Moderate</td>
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<td>Low</td>
<td>High</td>
<td>High</td>
<td>Moderate</td>
<td>Poor</td>
</tr>
</tbody>
</table>

In spite of the critical challenges like achievement of low defect density and high process stability that must be overcome before transferring DSA patterning into high volume manufacturing, it is a particularly attractive choice for semiconductor patterning applications. BCP films are similar to conventional polymer photoresist patterning materials used in semiconductor fabrication and thus DSA patterning process has compatibility with standard fab-equipment and processes.\textsuperscript{8} In addition, BCP can autonomously form regular patterns at dimensions not achievable by lithographic means (i.e., high resolution can be achieved without the use of a high-resolution mask). In addition, the throughput of the DSA patterning process is reasonably high. The idea of using polystyrene-\textit{b}-polybutadiene (PS-\textit{b}-PB) BCP thin films for patterning was first proposed by Mansky et al. in 1995.\textsuperscript{9} The orientation control of BCP micro domains with nanoscale chemical patterns was introduced by Russell et al. in 1997,\textsuperscript{10} and the first defect-free DSA nanoscale fabrication integrated with top-down lithography was demonstrated by Kim et al. in 2003.\textsuperscript{11} Microelectronic devices such as field effect
transistors, capacitors, flash memory cells, biosensors, and photovoltaics, made using block copolymer patterning have been proposed and demonstrated. The detailed pattern formation mechanism of BCP is described in sections 1.2 and 1.3.

1.2 Self-assembly of block copolymers

A copolymer is composed of two or more different monomer units. In copolymers, the repeating units can be placed randomly (random copolymer), alternating (alternating copolymer), or in blocks (BCP) as seen in figure 1.1. BCPs are made up of blocks of different polymerized monomers, i.e. they are composed of two (di-block copolymer) or more (multi-block copolymer) chemically distinct and immiscible polymer units covalently bound together.


Figure 1.1 Different types of copolymers (A and B are the two different monomers)

Thermodynamic incompatibility between the A and B blocks drives a collection of A–B di-block molecules to self-organize through a minimization of free energy process known as microphase separation in which the contact between similar and dissimilar blocks are maximized and minimized, respectively. For example, when soap or detergent (soap molecules-nonpolar tail) is added to water (polar solvent) bubbles or micelles are formed due to surfactants (amphiphile). The microphase separation is driven by chemical incompatibilities between the different blocks that make up the di-block molecules. For example, polystyrene (PS) is nonpolar and polymethylmethacrylate (PMMA) is polar in
PS-\(b\)-PMMA BCP. Two opposing effects: entropy and enthalpy, govern the thermodynamics of such a BCP composed of mutually incompatible blocks. At a lower temperature, enthalpy effect drives the blocks to phase-separate, while at a higher temperature, entropy effects result in a homogeneous mixture of chains.\(^{13}\) In the case of a mixture of two polymerized monomers (homopolymer), phase-separation is thermodynamically favorable only when the Gibbs free energy of mixing is greater than 0. The free energy is given by the following equation:

\[
\Delta G_m = RT \left[ n_A \ln f_A + n_B \ln f_B + n_A f_B \chi_{AB} \right],
\]

where \(f\) and \(n\) are the volume fraction and the number of moles of each homopolymer, and \(\chi_{AB}\) is the Flory-Huggins interaction (FHI) parameter. The FHI parameter is the energy required to interdisperse polymer A and B, and is related to the enthalpic contribution for phase-separation dominated by the incompatibility of monomer units. The FHI parameter is given by the following expression:

\[
\chi_{AB} = \frac{z \Delta w}{kT},
\]

where \(z\) is the coordination number (the number of nearest monomers for a lattice site) and \(\Delta w\) is the energy change or the free energy cost per A-B interaction compared to A-A and B-B interaction. It is given by the following expression:

\[
\Delta w = w_{AB} - \frac{1}{2} \left( w_{AA} + w_{BB} \right),
\]

where \(w_{AB}\) is the change in internal energy from mixing. All these parameters are useful in defining the dimensionless, \(\chi_{AB}\) parameter, which is inversely related to temperature but independent of composition. When the \(\chi_{AB}\) value is positive there is a net repulsion between homopolymers A and B, while a negative \(\chi_{AB}\) value indicates a free energy drive
towards mixing of A and B polymer species.

The strength of repulsive interaction between copolymer blocks is given by, $\chi_{AB} N$ (where $N$ is the number of monomers in di-BCP). $\chi_{AB} N$ takes into account both the enthalpic and entropic contributions.\textsuperscript{14} Theoretically, if $\chi_{AB} N$ is smaller than 10.5 for a given composition value, then the polymerized monomer chains are intermixed, morphology is disordered and microphase separation is not possible. If the $\chi_{AB} N$ value is greater than 10.5, then di-block copolymer will form repeating self-assembled domains via microphase separation process (Figure 1.2).\textsuperscript{15} In a typical BCP, the dimension of the domains ranges from 10 nm to 100 nm. The width of one repeating unit ($L_0$ - natural period) is given by the following expression:

$$L_0 \approx a \chi^{1/6} N^{2/3},$$  \hspace{1cm} (1.4)

where $a$ is the monomer size, $\chi$ is the FHI parameter and $N$ is total number of monomers in di-block copolymer. The natural period ($L_0$) for a particular di-BCP can be controlled by changing the overall molecular weight of the macromolecule. For example, the natural period of PS-$b$-PMMA ranges from $\sim 25$ - 80 nm.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1_2.png}
\caption{Microphase separation of BCPs.}
\end{figure}
The self-assembled domain shapes can be tuned by adjusting the relative volume fraction of each block (f), FHI parameter (χ), and the degree of polymerization (N) as seen in the calculated phase diagram of di-BCP (figure 1.3). If the strength of repulsive interaction (χ_{AB}N) is much greater than 10.5, then the ordered phase can have body-centered spheres (S), closed-packed spheres (CPS), hexagonally packed cylinders (HC), lamellae (L), double-gyroid phase (G), and disordered structure depending upon the composition and χ_{AB}N value. For example, in the case of PS-\textit{b}-PMMA, upon self-assembly the 50:50 (PS:PMMA) composition and 70:30 (PS:PMMA) composition forms a thin film of alternating two-dimensional lamellae patterns and one-dimensional close-packed cylinder patterns, respectively. The calculated phase-diagram is symmetric due to the assumption of symmetric chains. Experimentally determined phase diagrams often show significant asymmetry due to the differences in sizes and shapes of repeating units and so they are more complex and distorted. BCP structures described in the phase diagram are schematically seen in Figure 1.4.

![Figure 1.3](image)

**Figure 1.3** Theoretical phase-diagram of di-BCPs calculated by self-consistent mean field theory. Figure from [14], used with permission from Elsevier.
The degree of long-range order and orientation of these domains can be controlled by a variety of factors, such as the interaction of the BCP molecules with the substrate, the film thickness, and the post-deposition annealing procedures.\textsuperscript{14,15} For example, if the BCP film thickness is similar to its natural period ($L_0$), smooth and uniform thin films with lamellae planes aligned parallel with the substrate are obtained. However, if the BCP film thickness is much less than its natural period, micro-domain formation is constrained, resulting in slow phase separation. If the BCP film thickness is much greater than its natural period, layers of micro-domains with different surface topography are obtained. BCP thin film morphologies are influenced by the surface boundary conditions (interfacial energy) at interfaces such as polymer/substrate and polymer/air. Figure 1.5 presents possible morphologies of lamellar BCP films with different substrate properties.

\textbf{Figure 1.4} Different morphologies of diblock copolymers with varying minority volume fractions. Figure from [14], used with permission from Elsevier.

\textbf{Figure 1.5} Orientations of BCP films with different interfacial properties of the substrate.
1.3 Directing the self-assembly of block copolymers

As seen in section 1.2, many different micro-phase morphologies are possible from different BCP compositions, but the cylinder-forming and lamella-forming compositions are the most relevant morphologies for semiconductor manufacturing industry. The self-assembly of BCP can be used to create short-range order. Patterning over very large areas and aligning patterns with existing features of the underlying substrate are the major goals of any process with respect to the nanoscale fabrication. Hence it is important to direct the self-assembly of di-BCP to achieve patterns that are useful in semiconductor manufacturing.

DSA techniques can be divided into two main categories: namely; field-guided self-assembly and template-guided self-assembly. Some of the field-guided self-assembly techniques that are pursued in order to increase the length scale over which the domains in BCP films are desirably oriented and ordered include in-plane electric fields, temperature gradients (zone annealing), directional solidification, directional mechanical shear stress and solvent evaporation. However, these techniques cannot be used to align the new patterns with the existing patterns of the underlying substrate. On the other hand, both patterning over large areas and aligning patterns with existing underlying features can be achieved through template guided self-assembly. According to the nature of the guiding structures the template-guided self-assembly techniques can be roughly divided into two categories: graphoepitaxy and chemoepitaxy.

Graphoepitaxy DSA refers to topographic guide structures that align the BCP pattern through a combination of physical confinement and preferential wetting of the
topographic surfaces. The topographic guide structure with controlled dimensions form a set of confinement wells. The selective wetting of a particular BCP component at the trench side walls enforces the lateral ordering of the self-assembled BCP nano domains along the trenches and thereby the BCP patterns are formed within the confinement wells. Kramer et al. first demonstrated the use of graphoepitaxy DSA to obtain patterns with high resolution in 2001.16

On the other hand, in chemoepitaxy DSA is induced by changing the surface properties of the substrate. The substrate is rendered neutral toward the components of the BCP and a chemical guide pattern that has little topography guides the BCP phase behavior via chemical interaction with the BCP. Kim et al. demonstrated the first defect-free DSA nanoscale patterns obtained using chemical guide patterns fabricated with top-down lithography in 2003.11

Both chemoepitaxy and graphoepitaxy methods are competing for line-space patterning applications together with EUV lithography and other multi-patterning techniques such as self-aligned double patterning (SADP)17 and self-aligned quadruple patterning (SAQP).18 While graphoepitaxy has a significant advantage in terms of design flexibility (to create off-grid non-periodic arrays), the guide structure used in graphoepitaxy DSA is a part of the final pattern. In addition, the roughness associated with the guide structures is transferred to the DSA pattern. On the other hand chemoepitaxy is currently limited only to long-range periodic patterns. In chemoepitaxy, the chemical guide patterns are coated with the BCP and hence the guide patterns are not an active part in the final DSA pattern. Consequently, chemoepitaxy DSA is best suited for forming large areas of repeating patterns.6
While current multiple patterning strategies such as double and triple patterning lithography can be used to pattern narrower lines with smaller pitch, challenges remain for patterning contact holes. DSA assisted contact hole shrink process can be used to fabricate nanoscale holes. A. Gharbi et al. successfully demonstrated the use of DSA graphoepitaxy contact hole shrink process to fabricate vias with a minimum CD of 15 nm and an over-lay accuracy of 1 nm, using 100 nm CD contact hole guide structures. For contact-hole arrays, the graphoepitaxy shrink approach has emerged as the preferred choice due to relatively simple processing requirements, reduced number of patterning steps by eliminating multiple vias or using cut-mask schemes, possible rectification of contact edge roughness, improved placement errors and most importantly because of the opportunity for pitch multiplication without the need for double/triple patterning. For example, a larger template can be used to guide the formation of multiple DSA contact holes with same CD and center-to-center distance. Yu Bao et al. demonstrated the use of these topographical templates to fabricate contact holes for SRAM, DRAM, and NAND circuits.

This work focuses largely on optical metrology of template-guided DSA of PS-\textit{b}-PMMA materials. Many other block copolymer choices are possible and may ultimately prove better suited for use in nanoscale fabrication. 28 nm pitch and 14 nm CD DSA PS-\textit{b}-PMMA patterns and PS line-space patterns (post PMMA etch) fabricated using chemoepitaxy resist trim and neutral brush (RTNB) process, 28 nm pitch and 14 nm Si fins fabricated using chemoepitaxy neutral layer lift off (NLLO) process, and 15 nm CD contact holes fabricated using DSA graphoepitaxy contact hole shrink process are optically characterized using Mueller matrix ellipsometry based scatterometry. DSA PS-
b-PMMA patterns, PS line-space patterns, and Si fin wafers are provided by GLOBALFOUNDRIES and DSA contact hole wafers are provided by TEL.

The chemoepitaxy RTNB is based on a process that was first described by Liu et al.\textsuperscript{22} As seen in figure 1.6, the processing begins by depositing an 11 nm thick coating of silicon nitride on silicon substrate using an atomic layer deposition (ALD) process. The substrate is then spin-coated with a 5 - 7 nm thick PS layer, which is then cross-linked by baking in a nitrogen atmosphere for 5 minutes. This is followed by a general photolithography step (coating, exposing, and etching) on another positive resist to create 84 nm (3x\(L_o\)) pitch x-PS grating patterns. The random copolymer is grafted to form a polymer brush on the exposed portions of the nitride surface, thereby completing the formation of a RTNB chemical guide surface.\textsuperscript{6}

![Figure 1.6 Outline of the chemoepitaxy resist trim and neutral brush method (RTNB).](image)

The chemoepitaxy NLLO chemoepitaxy process is based on a process that was first described by Cheng et al.\textsuperscript{23} As seen in figure 1.7, the processing begins with spin coating of a photoresist on a conventional anti-reflective coating (ARC) stack, followed by resist patterning using a conventional photolithography technique (coating, exposing and etching). The resist features thus formed are then exposed and hard-baked, which renders the features soluble in aqueous base and stable toward the subsequent coating, completing the formation of a NLLO chemical guide pattern.\textsuperscript{6}
The DSA patterning process is then performed by spin-coating PS-b-PMMA (with composition ratio PS:PMMA ~50:50 and $L_0$ ~ 28 nm) of thickness around 28 - 35 nm is spin-coated on to the chemical guide surface and then annealed (baked) at a temperature of 250 - 255 °C for 5 minutes to induce self-assembly. Finally, the patterns are transferred onto bulk silicon to form Si fins. Several key differences can be observed in the two methods. For example, the x-PS patterns in RTNB guides are attractive (pinning) toward the PS component in the BCP while in the NLLO the exposed portions of the ARC are attractive toward the PMMA component of the BCP. From the perspective of process simplicity and cost, the NLLO method has advantages over the current RTNB processing. Both processes have demonstrated capability for patterning 300 mm wafers with high-resolution line-space structures.

The graphoepitaxy flow for contact hole shrink process is schematically depicted in the figure 1.8. A silicon substrate wafer is coated with a typical tri-layer stack consisting of organic planarizing layer (OPL), Si-ARC and photoresist (PR). Contact hole guide structures with 60 nm CD and 90 nm pitch is transferred into the OPL/Si-ARC stack using conventional optical lithography patterning (coating, exposing and etching). PS-b-PMMA (of composition ratio PS:PMMA ~70:30) is coated on to the topographical guide structure resulting in partial conformal coating of the template topography. Annealing of the BCP results in phase separation of the blocks and forms the desired contact hole
structures.

Figure 1.8 Outline of the DSA grappo-epitaxy contact hole shrink process.

In summary, DSA process is a bridge between the bottom-up approach and the top-down approach as conventional top-down lithography is used to fabricate patterned guide structures that allow the bottom-up growth of high-resolution patterns through self-assembly. The DSA patterning step, as an extension of current state-of-the-art photolithography, has demonstrated the capability for patterning with a variety of potential benefits, such as high-resolution molecular scale pattern precision, and cost effectiveness beyond the capability of other techniques. In order to integrate the DSA patterning step into a robust process for fabricating device layers, researchers in academia (IMEC, University of Chicago, etc.) and industry (GF, IBM, TEL, Applied Materials, Intel, etc.) have devoted a considerable amount of research effort on the optimization of the DSA process, development of relevant materials, analysis of defect sources, reduction defect density, reduction of line edge roughness and development of a robust pattern transfer step. For a detailed analysis report, the reader is referred to the following publications.²⁴-²⁸
1.4 Motivation and statement of thesis

The technology node beyond 20 nm marks the beginning of a major transition from conventional scaling-driven planar devices to complex 3D transistor architectures, redefining future needs for lithographic metrology solutions for high-volume manufacturing. New complex processes and materials, shrinking design rules, and reduced process tolerances require accurate CD and profile metrology.\textsuperscript{29,30}

As seen in table 1.2,\textsuperscript{29} a wide variety of CD metrology techniques are available, but no single technology solves all CD metrology needs. For example, use of CD-scanning electron microscopy (CD-SEM) for CD variation and roughness, and optical critical dimension (OCD) scatterometry for average line-width and 3D profile of the structure. However in their present forms, they are beginning to reach physical limitations in usefulness for some applications. For example, correlation between geometric parameters and variation in materials’ optical properties limits scatterometry metrology. Similarly, charging effect and profile variations negatively impact measurement performance of the CD-SEM toolset. CD-AFM suffers from issues such as tip wear, tip characterization, low throughput, and inaccuracy in measuring dense structures and at the bottom of the profile. To address these challenges, a robust metrology strategy should encompass the extendibility of conventional techniques that are approaching their fundamental limits, as well as the development of new technologies.
Scatterometry measurements are carried out by comparing measured spectra of the diffracted light from a periodic array of nanostructures to simulated spectra. Scatterometry is sensitive to the pitch, optical properties, critical dimensions (CD), height, side-wall angle (SWA) structure or rounding of the line-space patterns as well as thickness and optical properties of underlying layers. The feature dimensions can be extracted from the measured signal as long as the variation of the feature size causes detectable change on the response signal. Scatterometry is applicable to a number of processes involved in the production of microelectronic devices for in situ and ex situ metrology. The modern manufacturing operations require extensive statistical information to perform routine checks on the process quality. Since, the scatterometry measurements are fast and non-destructive, statistical variation across the wafer, wafer-to-wafer, and lot-to-lot can be measured with ease. Second and third chapter presents an elaborate discussion on theory, hardware, and software aspects of ellipsometry and scatterometry techniques, respectively.

<table>
<thead>
<tr>
<th>Method</th>
<th>Scatterometry</th>
<th>AFM</th>
<th>CD-SEM</th>
<th>TEM/ X-SEM</th>
<th>CD-SAXS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measuring</td>
<td>CD, 3D profile, material properties</td>
<td>CD, LER/LWR, 3D profile</td>
<td>CD, LER/LWR</td>
<td>CD, 3D profile</td>
<td>CD, 3D profile</td>
</tr>
<tr>
<td>Sample Specification</td>
<td>Periodic grating</td>
<td>Any</td>
<td>Any</td>
<td>Any</td>
<td>Periodic grating</td>
</tr>
<tr>
<td>Measurement time</td>
<td>Seconds</td>
<td>Minutes</td>
<td>Seconds</td>
<td>Days</td>
<td>Minutes</td>
</tr>
<tr>
<td>Analysis/Time</td>
<td>Days to weeks</td>
<td>Hours</td>
<td>Minutes</td>
<td>Hours to days</td>
<td>Days to weeks</td>
</tr>
<tr>
<td>Destructive</td>
<td>Negligible</td>
<td>No</td>
<td>Minor (Resist)</td>
<td>Yes</td>
<td>Negligible</td>
</tr>
<tr>
<td>Strengths</td>
<td>Fast, most profile info</td>
<td>Accuracy, profile info</td>
<td>Quick setup, fast, qualitative information</td>
<td>Full profile info, high accuracy, high resolution</td>
<td>Excellent precision, capability improves in future nodes.</td>
</tr>
<tr>
<td>Limitations</td>
<td>Model based, periodic grating, varying optical properties</td>
<td>Tip wear, low throughput, probe dimensions/shape limit measurements</td>
<td>No profile info, local measurement i.e more sampling required</td>
<td>Limited sampling, resist shrinkage, sample preparation required</td>
<td>Large spot size, slow simulator software, insensitive at large depths</td>
</tr>
</tbody>
</table>

Table 1.2 Comparison between different CD metrology techniques.\textsuperscript{29,30}

15
Along with the advantages, there are some potential limitations and challenges of the scatterometry technique. With the new complex 3D architectures, more parameters must be solved in order to measure the feature dimensions and the parameter correlation issues increases with complexity in structure. The more parameters floating in the model, it is more likely to capture all real variations of the structure (better accuracy) at the expense of inter-parameter correlation (worse repeatability). Furthermore, scatterometry can only measure specific periodic grating structures. The spot size of the light beam used for scatterometry measurements is typically several millimeters and hence these measurements have low spatial resolution - the parameter results are statistically representative of average values for many features within that incident spot. Extending scatterometry to measure the position of local process induced defectivity is extremely challenging- it cannot measure discrete or truly isolated features, and has difficulty measuring within grating feature-to-feature variation and random line edge roughness (LER) or the power spectrum of roughness. In addition, scatterometry models generally rely on the assumption that the optical properties of materials present in grating are approximately equal to that of thin films and constant. This assumption holds true for the majority of cases but fails when optical properties change due to dimensional confinement or strain effects and use of either bulk optical properties in models would result in a significant inaccuracy of the extracted parameters. These changes are very dependent on the dimensions and geometry of the features or thickness of the blanket films and it is important to incorporate these changes in the optical scatterometry models.

Most of recent hardware and software developments in the scatterometry tools, potentially address many of the challenges above by further reducing uncertainties for
some parameters and improving sensitivity to others. For example, modern ellipsometers that incorporate compensators can operate over long wavelength range and data acquisition at multiple angles can be carried out in seconds.\textsuperscript{32} Multiple incident angle scatterometry analysis improves precision and accuracy and has been demonstrated to improve sensitivity to feature parameters. Multiple azimuthal angle scatterometry analysis increases the amount of information content in the data for analysis. Currently, the optical scatterometry is based on conventional spectroscopic ellipsometry (SE) and spectroscopic reflectometry (SR) measurements, but generalized ellipsometry, or MMSE data provides additional information about complex structures that exhibit anisotropy and depolarization effects.\textsuperscript{33} In addition, it has greater sensitivity to changes in structural parameters when compared to conventional ellipsometry data. Mueller based scatterometry is still evolving and limited research has been done understanding the advantages and disadvantages of this new methodology. In addition, focusing optics with appropriate optical elements are now available to decrease the spot size of ellipsometers. Scatterometry tools with spot size as low as \(~15\ \mu\text{m}\) are now available commercially.\textsuperscript{34} However, there is a trade-off between smaller spot size and amount of noise in experimental data acquired. For this, a new laser-pumped plasma source has also been reported which promises an improvement factor of 30 in signal to noise ratio for scatterometry measurements.\textsuperscript{35} These advances along with the unique characteristics makes optical scatterometry a potential candidate for future metrology needs because of the unique characteristics and its advancements.

Table 1.3 shows a general classification system of application families for CD metrology, with the different possible applications and challenges, as described by
Bunday et al. in 2013. Bunday et al. designated DSA patterning process as another application family. However, the CD metrology applications and possible challenges for the DSA patterning technique was not defined in this work.

Table 1.3 Main CD metrology application families. Table from [30], used with permission.
The present work describes the application of MMSE based scatterometry to optically characterize DSA patterned line-space grating and contact hole structures fabricated with phase-separated PS-\textit{b}-PMMA at various integration steps of BCP DSA based patterning process. This work focuses on understanding the efficacies of MM elements using a systematic approach and optimizing MMSE based scatterometry to characterize complex DSA structures. DSA induced defects like missing vias, bridges, and overlay inaccuracy are incorporated in scatterometry models with a much larger field of view are created and simulations are carried out for the sensitivity study of MM elements to these unique DSA induced defects. In addition, reconstructed scatterometry models are used to calculate line edge roughness in 28 nm pitch Si fins fabricated using DSA patterning process. Depolarization and anisotropy values obtained from MM elements and symmetry properties associated with MM elements are used to increase the sensitivity to defects and to extend scatterometry to measure the position of local process induced defectivity via spectral comparisons based on anisotropy and depolarization.

1.5 References


Chapter II

An Introduction to Ellipsometry

2.1 Optics and Maxwell’s equations

2.1.1 Electric field and displacement

For a polarized dielectric material of the permanent or induced electric polarization \( P \), the electric displacement vector \( D \) is given by the expression:

\[
D = \varepsilon_0 E + P,
\]

(2.1)

where \( \varepsilon_0 \) is the electric permittivity of vacuum, and \( P \) is permanent or induced electric polarization which occurs in response to the applied electric field \( E \). For a linear and isotropic dielectric medium, the polarization is given by the expression:

\[
P = \varepsilon_0 \chi_e E,
\]

(2.2)

where \( \chi_e \) is the electric susceptibility. The relationship between electric field vector and electric displacement vector is given by the expression:

\[
D = \varepsilon E = \varepsilon_0 (1 + \chi_e) E,
\]

(2.3)

where \( \varepsilon \) is the electric permittivity of the medium.

2.1.2 Maxwell’s equations

The electric field and electric displacement vectors together with the magnetic field and magnetic flux density vectors, classically describe an electromagnetic wave. These vectors are related by Maxwell’s equations.\(^1\) Maxwell showed that light has electromagnetic properties with wave like form consisting of mutually perpendicular oscillating electric and magnetic fields propagating with a characteristic frequency. Maxwell’s equations also describe the interaction of light with a medium.\(^2\)
Mathematically, the differential form of the time varying Maxwell’s equations are given by:1,3

\[ \nabla \times E(r,t) = -\frac{\partial B(r,t)}{\partial t} , \]

\[ \nabla \times H(r,t) = J(r,t) + \frac{\partial D(r,t)}{\partial t} , \]

\[ \nabla \cdot E(r,t) = \rho(r,t) , \]

\[ \nabla \cdot B(r,t) = 0 , \] (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.

### 2.1.3 The wave equation

The wave equation is one of the most important results of Maxwell’s equations. From Maxwell’s equation and the relations described in equations 2.1 to 2.3 and we obtain the following wave equation for the electric field:1,3

\[ \nabla^2 E = \frac{\varepsilon \mu}{c^2} \frac{\partial^2 E}{\partial t^2} + \frac{4\pi \sigma \mu}{c^2} \frac{\partial E}{\partial t} , \] (2.5)

where \( c \) is the speed of light, \( \sigma \) is the conductivity in the medium, and \( \mu \) is the magnetic permeability of the medium. The solution to the equation is a sinusoidal function and the resulting \( x \)-component of the electric field the is given by the equation:1,3

\[ E_x(r,t) = E_0 e^{i(kr - \omega t)} , \] (2.6)

where \( \omega \) is the frequency of light and \( k \) is the complex propagation constant.

### 2.1.4 Optical constants

The real part and imaginary parts of \( K \) are the wave vector and attenuation of light in the material respectively. Substituting equation 2.6 into the wave equation 2.5 and assuming
that the imaginary part of $K$ (attenuation of light in the material) to be negligible, we obtain:\(^3\)
\[
\text{Re}(K) = \frac{\omega}{c} \sqrt{\varepsilon_{\text{complex}} \mu},
\]  
(2.7)
where $\varepsilon_{\text{complex}}$ is the complex dielectric constant of the medium and is given by the expression:\(^3\)
\[
\varepsilon_{\text{complex}} = \varepsilon + \frac{i(4\pi\sigma)}{\omega} = \varepsilon_1 + i\varepsilon_2 = N^2,
\]  
(2.8)
where $\varepsilon_1$ and $\varepsilon_2$ are the real and imaginary parts of the relative complex dielectric function of the medium, respectively and $N$ is the complex refractive index of the medium. For non-magnetic materials, the complex refractive index of the medium is given by the expression:
\[
N = \sqrt{\varepsilon_{\text{complex}}} = n + ik,
\]  
(2.9)
where $n$ is the refractive index and $k$ is the extinction coefficient. The relationships between optical constants are listed in Table 2.1.\(^4\) In equations 2.5 and 2.6 the phase of the electromagnetic waves is expressed using $\left(kr - \omega t\right)$. However, if the equations 2.5 and 2.6 are expanded using the phase $\left(\omega t - kr\right)$, the complex refractive index and complex dielectric functions are defined by these expressions:\(^1\)
\[
N = n - ik \quad \text{and} \quad \varepsilon = \varepsilon_1 - i\varepsilon_2.
\]  
(2.10)

When substrates are optically isotropic, the definition of $N = n - ik$ can also be used for defining the ellipsometer parameters by replacing $-i$ with $i$.\(^1\) However, this procedure cannot be used in defining the cross-polarization effects present in the ellipsometry parameters of the anisotropic substrates\(^1\) and, therefore, the convention of $N = n + ik$ has been used throughout this report.
Spectroscopic ellipsometry (SE) is a rapid, high precision, and non-destructive optical measurement technique that measures the change in state of polarization of an incident polarized light beam after reflection (or transmission) from a sample surface. Typically, ellipsometry is done only in the reflection setup. Paul Drude performed the first ellipsometric measurements in the late 19th century. Drude used the phase shift induced between mutually perpendicular components of polarized light to measure film thicknesses. When the mutually perpendicular components of polarized light are out of phase, the light is said to be elliptically polarized; and hence the technique that evolved from Drudes’ early measurements came to be known as ellipsometry.

While the fundamentals behind ellipsometry have been known for some time, the use of ellipsometry as an important surface and thin film characterization technique did not occur until the availability of digital computers. Until the early 1970s, most ellipsometry measurements were carried out only at a single wavelength, were operated manually, and this was very time consuming. However during the last quarter of the 20th century, SE evolved significantly. These developments not only improved the measurement time but

<table>
<thead>
<tr>
<th>Optical Constant (symbol)</th>
<th>Real part</th>
<th>Imaginary part</th>
</tr>
</thead>
<tbody>
<tr>
<td>conductivity (σ = σ₁ + iσ₂)</td>
<td>σ₁ = ωε₀ε₂</td>
<td>σ₂ = -ωε₀(ε₁ - 1)</td>
</tr>
<tr>
<td>dielectric function (ε = ε₁ + iε₂)</td>
<td>ε₁ = 1 - σ₂/(ωε₀)</td>
<td>ε₂ = σ₁/(ωε₀)</td>
</tr>
<tr>
<td>refractive index (N = n + ik)</td>
<td>n = (ε₁ + 2ε₂)/2</td>
<td>k = (−ε₁ + 2ε₂)/2</td>
</tr>
<tr>
<td></td>
<td>n = ε₂/(2k)</td>
<td>k = ε₂/(2n)</td>
</tr>
</tbody>
</table>

Table 2.1 Relationship between optical constants.
also the measurement precision significantly. The use of completely automated SE measurements was demonstrated first by Aspnes et al. in 1975,\textsuperscript{5} and the use of ellipsometry for real-time monitoring was reported first by Muller and Farmer in 1984.\textsuperscript{2}

Some of the recent developments in the field of ellipsometry involves incorporation of improved optics and use of compensators, development of variable angle of incidence and generalized SE, extensions to rotating compensator and dual rotating compensator configurations, increases in spectral range, development of imaging ellipsometry, and improvement of spectroscopic ellipsometry for real time applications.\textsuperscript{2} In the recent past, several books have been published which provide comprehensive information about the concepts and applications of SE.\textsuperscript{1,2,6,7} Ellipsometric systems integrated with several other instruments such as high-temperature stages, cryogenic stages, deposition chambers, gas adsorption systems, liquid cells, etc., are now capable of characterizing a wide variety of samples using appropriate optical models. These optical models can be used to determine the optical properties and thickness of the thin films from the ellipsometric data as well as the band gap of materials, alloy compositions, growth processes, evolution of microstructure, phase, and grain size, carrier concentration, optical conductivity, mobility, porosity, pore size, coefficient of thermal expansion, glass transition temperature, Young’s modulus, and anisotropic properties.\textsuperscript{8-14}

\textbf{2.3 Features of traditional ellipsometry}

The states of polarization of incident and reflected light waves are described by the coordinates of the parallel and perpendicular (p-component and s-component) components of electric field. The vectors $E_{ip}$ and $E_{is}$ represent the incident electric field
parallel and perpendicular components of incident light as seen in figure 2.1. The amplitudes of $E_{ip}$ and $E_{is}$ are the same and the phase difference between the components is zero ($\delta_i = 0$) i.e. the incident light is linearly polarized oriented at $+45^\circ$ relative to the plane of incidence. Upon reflection from a sample, p- and s-components show different changes in amplitude and phase resulting in elliptically polarized light as seen in figure 2.1. Ellipsometry measures the two parameters that express the amplitude ratio ($\Psi$) and phase difference ($\Delta$) between p- and s-components, respectively. These two ellipsometry parameters can be determined directly from the Fresnel reflection coefficients. This is the basic principle of an ellipsometry measurement.

![Figure 2.1 Measurement principle of ellipsometry. Here the incident light is linearly polarized i.e. $\delta_{ip} - \delta_{is} = 0$.](image)

Both, linearly polarized light or elliptically polarized incident light can be used as a probe. The induced ellipticity or change in ellipticity can be measured in terms of two ellipsometry parameters - change in the phase difference ($\Delta$) and the amplitude ratio ($\Psi$). For an incident elliptical polarization, $\Delta$ is the difference between the phase difference of parallel ($\delta_{ip}$) and perpendicular ($\delta_{is}$) components of the incoming wave and the phase difference between the parallel ($\delta_{rp}$) and perpendicular ($\delta_{rs}$) components of the reflected wave. This equality is seen in the expression:

$$
\Delta = \left[ (\delta_{rp}) - (\delta_{rs}) \right] - \left[ (\delta_{ip}) - (\delta_{is}) \right].
$$

(2.11)
The ratio of the amplitude of parallel and perpendicular components of Fresnel reflection coefficients (\(r_p\) and \(r_s\)) is given by equation:\(^1\)

\[
\rho = \frac{r_p}{r_s} = \frac{E_{rp}}{E_{ip}} = \frac{E_{rs}}{E_{is}} = \tan \Psi e^{-i\Delta},
\]  

(2.12)

from which the \(\Psi\) is derived, and is seen in equation:\(^1\)

\[
\Psi = \tan^{-1}(\rho) = \tan^{-1}\left(\frac{|r_p|}{|r_s|}\right).
\]  

(2.13)

**Figure 2.2** Characterization of physical properties by spectroscopic ellipsometry.

The complete reflection ellipsometry measurement includes the four following steps: (1) generation of an incident light beam with a known polarization state through instrument calibration, (2) specular reflection of the beam from a sample surface-producing a reflected beam with an altered polarization state, (3) determination of beam/sample interaction parameters, i.e. the ellipsometric angles (\(\Psi\), \(\Delta\)) from the information on the incident and reflected beam polarization states again relying on instrument calibration information, and (4) computation of optical and structural information for the sample such as optical constants and thicknesses by using the measured values \(\Psi\) and \(\Delta\) in various equations and algorithms to produce a model that describes the interaction of light with the sample. In general, the interpretation of
measurement results is rather difficult from the raw values of $\Psi$ and $\Delta$. Thus, construction of an optical model is required for data analysis to extract the physical properties of the sample. Figure 2.2 shows various physical properties that can be determined from SE.¹

2.4 Data analysis and applications

There are multiple advantages of SE measurements over single wavelength measurements. Firstly, it is the easiest way to improve the performance of an ellipsometer and helps to provide a unique answer. Each new wavelength contains information about the sample properties. In the early days of ellipsometry, a laser was used to collect data at a single wavelength. With two known values ($\Psi$ and $\Delta$), only two unknown sample properties could be determined. Even in a simple case of transparent film (k=0), film thickness and refractive index could not be uniquely determined from a single layered film. On the other hand, spectroscopic measurement with 200 wavelength steps produce 400 known parameters ($\Psi$ and $\Delta$ at each wavelength), with only 201 unknowns (The index of refraction (n) at each wavelength and the thickness of the film). For example, the $\Psi$ values for all the three HfO₂ samples with 100 nm, 200 nm, and 300 nm thickness are identical at the single-wavelength of ~390 nm, while the calculated spectral response for each sample is entirely unique as see in figure 2.3

![Figure 2.3 Calculated optical spectra of $\Psi$ for HfO₂ thin film with varying thickness on Si.](image)
In general, SE measurement is carried out in the ultraviolet (UV) and visible region, but measurement in the infrared (IR) region is also common. SE Data in UV/visible region is generally used to determine film thickness, electronic transitions (inter-band transitions) and band structure of the material.\textsuperscript{7,13,14} The band-gap ($E_g$) can be deduced from the variation of absorption coefficient ($\alpha$) with respect to photon energy of incident light. The band structure varies with alloy composition, phase structure, and crystal grain size. Hence these properties can also be determined from the spectral analysis of optical constants. For example, the absorption shape of silicon films in UV spectra can be used to determine the layer crystallinity as seen in figure 2.4. If the film is amorphous, the absorption is broadened with no critical point features and as crystallinity increases the absorption features in the ultraviolet become more distinct.

In the IR wavelength region, free carrier absorption is induced by free electrons (or holes) in solids (only for metals and solids with a metallic character, it is not true for dielectrics and undoped semiconductors). When carrier concentration is high, electrical properties such as carrier mobility, carrier concentration, and conductivity can be obtained.\textsuperscript{9} Molecular bonding information can also be obtained. For many applications, optical properties are desired at specific wavelengths. For example, lithography in semiconductor manufacturing requires ellipsometry measurements in the UV region (157 nm, 193 nm, 248 nm, etc.). Hence an ellipsometer with a broad spectral range offers an incredible flexibility that can meet almost all the application requirements.
Ellipsometry is typically used for films whose thickness ranges from angstroms to microns. The film thickness affects the path length of light traveling through the film, and the optical properties of the material affect the light waves' velocity and refracted angle. Data analysis for thickness measurements must be carried out in the spectral region with lower absorption. For example, an organic film may strongly absorb UV and IR light, but remain transparent in the visible wavelength - thickness determination should be carried out using visible wavelengths for such samples.

SE data provides information about the thickness based on the position and number of interference oscillations as seen in figure 2.5. As the film becomes thicker, the large number of data oscillations become difficult to resolve at shorter wavelengths and are better separated at longer wavelengths. So the upper thickness limit measurable by SE depends on the probing wavelength and the samples’ optical properties. For example, thickness determination of metal films using SE has been one of the major challenges in optical metrology and the maximum thickness determination by SE is typically in the range of 100 nm.

Figure 2.4 Real and imaginary part of dielectric functions ($\varepsilon_1$ and $\varepsilon_2$) for amorphous, polycrystalline, and crystalline Si.
Thickness measurement requires that a portion of the light travel through the entire film and return to the surface. For example, the sensitivity of SE to thickness of Cu thin films on Si substrates reduces significantly for 50 nm or thicker Cu films as seen in figure 2.6. The imaginary part of the dielectric function of thin metal films is non-zero in a wide optical range (0.01 - 10 eV) due to the absorption of light from far IR frequency to the plasma frequency by free and bound electrons in metals. However, the interference enhancement method can be used to characterize absorbing films. The absorbing film must be deposited over a thick dielectric layer, which significantly enhances the interaction between light and the absorbing film.

Data from multiple thin film stacks could be analyzed very rapidly to yield thin film thickness measurements that compares favorably to cross-sectional transmission electron microscopy and as the ellipsometry measurement takes only a few seconds, real-time
observation and feedback control of processing can be performed relatively easily. For example, ellipsometry recipes are created to calculate the etch rate for InGaAs, InP and GaAs thin films. Experimental data acquired from the multiple thin film stack of InGaAs/InP/GaAs/Si, InP/GaAs/Si, and GaAs/Si can be seen in figure 2.7.

![Figure 2.7](image1.png)

**Figure 2.7** Experimental optical spectra of $\Psi$ and $\Delta$ for InGaAs/InP/GaAs/Si, InP/GaAs/Si, and GaAs/Si samples. These samples are provided by TEL.

SE measurements can be used for real-time monitoring and characterization of thin-film growth while it is deposited by different deposition techniques like CVD, ALD, etc. The changes in acquired experimental data and the optical properties of the material can be due to the varying amount of strain, grain size, homogeneity, or porosity in the deposited thin film. For example, SE data from different SiN samples deposited with varying process conditions is analyzed to understand the effect of the varying conditions on the optical properties. The optical properties of SiN samples varied with the changes in process conditions as seen in figure 2.8.

![Figure 2.8](image2.png)

**Figure 2.8** Refractive index ($n$) and extinction coefficient ($k$) of SiN samples deposited with varying process conditions. These samples are provided by CNSE.
Changes in real and imaginary part of the dielectric functions as well as the optical band gap of the material with alloy concentrations can be measured using SE analysis. SE can be used as the inline metrology tool for accurate process control to characterize composition, thickness, and optical properties during the deposition process in order to improve the efficiency of solar cells and product yield. Deposition of copper indium-gallium di-selenide thin film photovoltaic absorber (CuIn$_{1-x}$Ga$_x$Se$_2$; CIGS) is done through a thermal 3-stage co-evaporation process as it yields highest efficiency solar cell devices. Dielectric functions determined for samples stopped after each deposition stage of the three-stage co-evaporation process show that the direct band gap increases from 1.2 - 1.6 eV with increase in concentration ratio of Ga/In+Ga after each stage as seen in figure 2.9.

All this research work shows the importance of SE in the characterization of materials and highlights the necessity of consideration of the material thickness, concentration, and process parameters for SE data analysis. However, SE has its limitations. The spot size of the light beam used for spectroscopic ellipsometry is typically several millimeters and hence ellipsometers have low spatial resolution. SE data analysis requires use of an optical model; this indirect method of characterization tends to become complicated for samples with high absorption coefficients. SE cannot be used to measure scattering effects i.e. it cannot be used to characterize gratings or line-space patterns and thin films with high roughness as it causes depolarization and affects the reflected light intensity.
severely. SE measurement errors generally increase when the size of surface roughness exceeds $\sim 30\%$ of the measurement wavelength. In addition, the SE approach is highly satisfactory for characterization of conventional isotropic samples, but cannot be used to characterize anisotropic samples. Thus, most recent ellipsometry advances are in the development of ellipsometry instruments. For example, in the early days ellipsometry measurements were typically performed at oblique angles near the Brewster angle because sensitivity to structural parameters and optical properties is highest at this position. Acquiring data at the Brewster angle is much less important for modern ellipsometers that incorporate compensators. Advanced ellipsometers with compensator can operate over a long wavelength range, which allows for quick and accurate measurement of samples with depolarization or anisotropy, and data acquisition at multiple angles can be carried out in seconds. In order to improve spatial resolution, focusing optics with appropriate optical elements are used to decrease the spot size of ellipsometers. Ellipsometers with spot size as small as $\sim 15\, \mu\text{m}$ are now available commercially. In addition, optically anisotropic materials have been studied extensively by applying generalized SE or Mueller matrix SE (MMSE) that allows for complete characterization of asymmetric samples.

### 2.5 Generalized ellipsometry: Jones and Stokes-Mueller formalism

In order to quickly and accurately model and simulate ellipsometry measurements, matrix algebra is necessary. The principle of traditional SE can be described by the Jones matrix formalism as seen in the equation:

$$\vec{j}_r = J \vec{j}_i,$$

which describes the interaction of incoming electrical fields with the sample. The 2x1
Jones vectors contain the complex electrical field vectors in p- and s-orientation for the incoming and reflected light respectively, as seen in equations:\textsuperscript{1}

\[
\begin{bmatrix}
E_{rp} \\
E_{rs}
\end{bmatrix}
= \begin{bmatrix}
    r_{pp} & 0 \\
    0 & r_{ss}
\end{bmatrix}
\begin{bmatrix}
E_{ip} \\
E_{is}
\end{bmatrix}
\]

\[
J = r_{ss}
\begin{bmatrix}
    r_{pp}/r_{ss} & 0 \\
    0 & 1
\end{bmatrix},
\tag{2.15}
\]

\[
\begin{bmatrix}
E_{rp} \\
E_{rs}
\end{bmatrix}
= \begin{bmatrix}
    r_{pp} & r_{ps} \\
    r_{sp} & r_{ss}
\end{bmatrix}
\begin{bmatrix}
E_{ip} \\
E_{is}
\end{bmatrix}
\]

\[
J_{ani} = \begin{bmatrix}
    r_{pp} & r_{ps} \\
    r_{sp} & r_{ss}
\end{bmatrix}, \tag{2.16}
\]

where $E_p$ and $E_s$ are the complex electric field vectors of incoming and reflected light and the 2x2 Jones matrix ($J$) is a transformation matrix representing the interaction of incoming light based on the optical properties of the material. The Jones matrix in equation 2.15 represents the light reflection by an optically isotropic sample.\textsuperscript{1} In the case of an isotropic sample, the s- and p-components are the only eigenmodes of reflection, and hence the cross-polarization reflection coefficients $r_{sp}$ and $r_{ps}$ are zero and the diagonal elements of the Jones matrix can be expressed in terms of $\Psi$ and $\Delta$, which are defined in equation 2.12.\textsuperscript{2}

The Jones matrix in equation 2.16 describes a sample with anisotropic optical properties.\textsuperscript{1} The off-diagonal terms here refer to light that exits with a polarization orthogonal to the input polarization. For example, $r_{sp}$ represents input p-component of light that reflects off as output sp-component of light. Incorporating cross-polarization effects into standard ellipsometry - is the foundation of generalized ellipsometry. For an anisotropic sample, the ellipsometry response can be defined by seven independent parameters and they can be obtained by dividing each term in the Jones matrix of the anisotropic sample by $r_{ss}$ as seen in equation:
where $\rho$, $\rho_{sp}$, and $\rho_{ps}$ are complex quantities that are related to the six classical ellipsometry angles and are given by:

$$\rho_{pp} = \frac{r_{pp}}{r_{ps}} = \frac{E_{rp}}{E_{ip}} \left( \frac{E_{rs}}{E_{is}} \right) = \tan \Psi_{pp} e^{-i \Delta_{pp}},$$

$$\rho_{ps} = \frac{r_{ps}}{r_{ss}} = \frac{E_{rp}}{E_{ps}} \left( \frac{E_{rs}}{E_{is}} \right) = \tan \Psi_{ps} e^{-i \Delta_{ps}} \text{, and}$$

$$\rho_{sp} = \frac{r_{sp}}{r_{ss}} = \frac{E_{rs}}{E_{sp}} \left( \frac{E_{rs}}{E_{is}} \right) = \tan \Psi_{sp} e^{-i \Delta_{sp}}. \quad (2.18)$$

Here,

$$\Psi_{pp} = \tan^{-1}(\rho_{pp}) = \tan^{-1} \left( \frac{r_{pp}}{r_{ps}} \right), \quad \Delta_{pp} = (\delta_{rp} - \delta_{ip}) - (\delta_{rs} - \delta_{is}),$$

$$\Psi_{ps} = \tan^{-1}(\rho_{ps}) = \tan^{-1} \left( \frac{r_{ps}}{r_{ss}} \right), \quad \Delta_{ps} = (\delta_{rp} - \delta_{is}) - (\delta_{rs} - \delta_{is}),$$

$$\Psi_{sp} = \tan^{-1}(\rho_{sp}) = \tan^{-1} \left( \frac{r_{sp}}{r_{ss}} \right), \quad \Delta_{sp} = (\delta_{ps} - \delta_{rp}) - (\delta_{rs} - \delta_{is}), \quad (2.19)$$

where $\delta_{ip}$ and $\delta_{is}$ are the phase of parallel and perpendicular components of the reflected wave, respectively. $\delta_{rp}$ and $\delta_{rs}$ are the phase of parallel and perpendicular components of the incoming wave, respectively. The sample reflectivity is the seventh parameter and is given by:

$$R = \left( r_{pp} r_{pp}^* + r_{ps} r_{ps}^* + r_{sp} r_{sp}^* + r_{ss} r_{ss}^* \right) / 2. \quad (2.20)$$

Characterization of anisotropic samples using 2 x 2 Jones matrix generally is complicated in general. In addition, the Jones formalism assumes that the light is fully polarized, i.e. the formalism is only valid for non-depolarizing samples. Depolarization
can be present either in the sample or the system itself. Stokes-Mueller formalism can describe linearly polarized, circularly polarized, partially polarized, as well as depolarized light. MM is a transformation matrix for the stoke vectors of incoming and outgoing light as seen in the equation:\(^1\)

\[
\vec{S}_r = M \vec{S}_i .
\]

Here,

\[
\vec{S} = \begin{bmatrix}
S_1 \\
S_2 \\
S_3 \\
S_4 \\
\end{bmatrix} = \begin{bmatrix}
I_x + I_y \\
I_x - I_y \\
I_{+45^\circ} + I_{-45^\circ} \\
I_R - I_L \\
\end{bmatrix} = \begin{bmatrix}
E_x E_x^* + E_y E_y^* \\
E_x E_y^* - E_y E_x^* \\
E_x E_y^* + E_y E_x^* \\
i \left(E_x E_y^* - E_y E_x^*\right) \\
\end{bmatrix}, \quad \text{and}
\]

\[
M = \begin{bmatrix}
M_{11} & M_{12} & M_{13} & M_{14} \\
M_{21} & M_{22} & M_{23} & M_{24} \\
M_{31} & M_{32} & M_{33} & M_{34} \\
M_{41} & M_{42} & M_{43} & M_{44} \\
\end{bmatrix} .
\]

The 4 x 1 Stokes vector (S) and the 4x4 Mueller matrix (MM) in equation 2.22 represents incoming and outgoing light beams and the interaction of light with the sample, respectively. The Stokes vector is described by the intensities or electric fields of p, s, +45° and -45°, right and left handed circularly polarized light components as seen in equation 2.22. The MM completely specifies the interaction of light with a specular sample.\(^20\) For the past several years, MMSE has been used to address some of the shortcomings of conventional SE.\(^20-23\)

The MM is an appropriate formalism for characterizing polarization measurements because it contains within its elements all of the polarization properties: diattenuation, retardance, depolarization, and their form: linear, circular, or elliptical.\(^24\) Diattenuation is the property of an optical element or system whereby the intensity transmittance or
reflectance of the exiting beam depends on the polarization state of the incident beam.\textsuperscript{25} Dichroism is the material property of displaying diattenuation during propagation. For each direction of propagation, dichroic media have two modes of propagation with different absorption coefficients. Retardance is a polarization-dependent phase change property of the material.\textsuperscript{24} A sample with retardation properties that vary rapidly with wavelength may induce depolarization if the system collects spectroscopic data rather than a single wavelength. Since retardation is proportional to the inverse of the wavelength, spectroscopic measurements from a sample gives different retardation value for each wavelength, resulting in partially polarized light.\textsuperscript{24} For more detailed description of polarimetric properties of a sample the reader is referred to this book chapter.\textsuperscript{25}

The MM does not provide additional information about an isotropic sample compared to standard ellipsometry. The 8 off-block diagonal elements are zero, whereas the on-block diagonal elements can be calculated from the standard ellipsometry values $\Psi$ and $\Delta$ as seen in equation 2.12.\textsuperscript{1} MM take a very simple and symmetric form for reflection from isotropic samples. The isotropic sample MM in the NSC representation is given by:\textsuperscript{2}

\[
M = \begin{bmatrix}
1 & -N & 0 & 0 \\
-N & 1 & 0 & 0 \\
0 & 0 & C & S \\
0 & 0 & -S & C \\
\end{bmatrix}
\]

Here, 
\[N = \cos(2\Psi),\]
\[C = \sin(2\Psi)\cos(\Delta),\]
and 
\[S = \sin(2\Psi)\sin(\Delta).\] \hspace{1cm} (2.23) \hspace{1cm} (2.24)

However, for anisotropic samples such as in the case of cross-polarization effects caused due to light scattering in the near-specular reflection, uniaxial or biaxial anisotropic samples, symmetric patterned structures, and less ideal surfaces (rough, non-homogenous, etc.), the off-diagonal elements of the MM may be non-zero and the resulting MM is seen in equation 2.25.\textsuperscript{2} For example, in the less ideal surfaces, the change in intensity arises from the fact that the rough surface geometry produces several
different polarization states in the reflected beam simultaneously, which is interpreted as an unpolarized component by the ellipsometer. In the ideal smooth surface case, a p-polarized input component reflects as a p-polarized output (and s-polarized input reflects as a s-polarized output). However for rough surfaces reflected light comprises of both p- and s-polarized components. If there is no symmetry along the direction of propagation of incoming light of one component (p or s) relative to the sample's in-plane characteristic vectors, the resulting reflection will be composed of both p and s-components as seen in figure 2.10 (r_p and r_s for p-polarized incident light, or r_a and r_ps for s-polarized incident light). This effect is known as cross-polarization. The light before reflection can be projected onto the sample vectors that have different refractive indices in general. After reflection, this results in differing optical response between the components which produces a composite reflected vector with both p and s-components. The anisotropic sample MM in the NSC representation is given by:  

\[
M = \begin{bmatrix}
1 & -N - \alpha_{ps} & C_{sp} + \xi_1 & S_{sp} + \xi_2 \\
-N - \alpha_{sp} & 1 - \alpha_{sp} - \alpha_{ps} & -C_{sp} + \xi_1 & -S_{sp} + \xi_2 \\
C_{ps} + \xi_1 & -C_{ps} + \xi_1 & C_{pp} + \beta_1 & S_{pp} + \beta_2 \\
-S_{ps} + \xi_2 & S_{ps} + \xi_2 & -S_{pp} + \beta_2 & C_{pp} - \beta_1
\end{bmatrix}
\]  

(2.25)

Here,  

\[
N = \left[1 - \tan^2(\Psi_{pp}) - \tan^2(\Psi_{ps}) - \tan^2(\Psi_{sp})\right] / D, \quad \xi_1 = \left(D / 2\right)\left(C_{ps} + S_{ps}\right), \\
D = \left[1 + \tan^2(\Psi_{pp}) + \tan^2(\Psi_{ps}) + \tan^2(\Psi_{sp})\right], \quad \xi_2 = \left(D / 2\right)\left(C_{sp} - S_{sp}\right), \\
C = 2\tan(\Psi_{pp})\cos(\Delta_{pp}) / D, \quad \xi_1 = \left(D / 2\right)\left(C_{sp} + S_{sp}\right), \\
S = 2\tan(\Psi_{pp})\sin(\Delta_{pp}) / D, \quad \xi_2 = \left(D / 2\right)\left(C_{sp} - S_{sp}\right), \\
S_{ij} = 2\tan(\Psi_{ij})\sin(\Delta_{ij}) / D, \quad \beta_1 = \left(D / 2\right)\left(C_{ps} + C_{sp} + S_{ps} \cdot S_{sp}\right), \text{ and} \\
C_{ij} = 2\tan(\Psi_{ij})\cos(\Delta_{ij}) / D, \quad \beta_2 = \left(D / 2\right)\left(C_{ps} C_{sp} - S_{ps} S_{sp}\right).
\]  

(2.26)
It is possible to calculate Jones matrix from a non-depolarizing MM using analytical equations. However, a measured MM is never perfectly non-depolarizing. In addition, the three contributions are mixed together in a MM, causing that every MM element corresponds to more than one type of polarization change. Generally all 15 MM elements are required for complete characterization of the reflected beam. When no matrix symmetries apply all 15 MM elements are non-vanishing and different between them. However, the number of independent MM elements may vary according to the
crystal structure of the material and direction of propagation of the incident light.\textsuperscript{26}

Optical behavior of solids with different crystal systems is seen in table 2.2.

<table>
<thead>
<tr>
<th>Crystal Systems</th>
<th>Index ellipsoid</th>
<th>Optical behavior</th>
<th>Optical axes</th>
<th>Variation with ($\lambda$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>Sphere</td>
<td>Isotropic</td>
<td></td>
<td>n will change</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Spheroid</td>
<td>Uniaxial</td>
<td>Optic axis parallel to c</td>
<td>$n_o$ and $n_e$ will vary</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>Spheroid</td>
<td>Uniaxial</td>
<td>Optic axis parallel to c</td>
<td>$n_o$ and $n_e$ will vary</td>
</tr>
<tr>
<td>Trigonal</td>
<td>Spheroid</td>
<td>Uniaxial</td>
<td>Optic axis parallel to c</td>
<td>$n_o$ and $n_e$ will vary</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>Ellipsoid</td>
<td>Biaxial</td>
<td>Optic axial plane parallel to $ab$, $bc$, or $ca$; optical axes along $a$, $b$, and $c$</td>
<td>$n_x$, $n_y$, and $n_z$ will vary</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>Ellipsoid</td>
<td>Biaxial</td>
<td>Optic axial plane either parallel or perpendicular to $b$, One axis parallel to $b$, other two perpendicular to $b$</td>
<td>unspecified</td>
</tr>
<tr>
<td>Triclinic</td>
<td>Ellipsoid</td>
<td>Biaxial</td>
<td>Optic axes in unspecified directions</td>
<td>unspecified</td>
</tr>
</tbody>
</table>

($a, b, c$) designate the principal crystallographic axes which are aligned with the principal dielectric axes $(x, y, z)$ for crystals. $n_x, n_y,$ and $n_z$ are the principal indices of refraction. For biaxial crystals, ($n_x < n_y < n_z$). For uniaxial crystals, $n_o = n_x = n_y$ is the ordinary index of refraction, and $n_e = n_z$ is the extraordinary index of refraction.

The index ellipsoids and symmetry relations of the MM elements for isotropic, uniaxial, and orthorhombic crystal families are seen in figure 2.11 and table 2.3, respectively.\textsuperscript{2,22,26} Certain crystal orientations with respect to direction of propagation of light result in matrix symmetry. The MM for a sample is a function of the direction of propagation and wavelength $\lambda$. For example, in the case of an uniaxial system the off-diagonal block MM elements are non-zero if the direction of propagation of the incident light is neither parallel nor perpendicular to the optic axis of the crystal.\textsuperscript{22} In addition, the optical spectra of Mueller element pairs M12 and M21, M14 and M41, M24 and M42, and M33 and M44 are symmetric while Mueller element pairs M13 and M31, M23 and M32, and M34 and M43 are anti-symmetric. On the contrary for an isotropic sample the off-diagonal Mueller elements are always zero as seen in equation 2.24. For more
information on MM symmetries the reader is referred to these journal articles.\textsuperscript{22,26}

![Image of MM symmetries](image)

**Figure 2.11** Index ellipsoids of (a) isotropic material ($n_x = n_y = n_z$) (b) uniaxial material ($n_x = n_y < n_z$), and (c) biaxial material ($n_x < n_y < n_z$).\textsuperscript{1}

**Table 2.3** MM symmetries in different medias with respect to its optical axes and direction of propagation of the incident light.\textsuperscript{26} Figure from [26], used with permission.

<table>
<thead>
<tr>
<th>Mueller symmetry</th>
<th>Types of media and direction of propagation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M = \begin{bmatrix} 1 &amp; M_{12} &amp; 0 &amp; 0 \ M_{12} &amp; 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; M_{33} &amp; M_{34} \ 0 &amp; 0 &amp; -M_{14} &amp; M_{13} \end{bmatrix}$</td>
<td>Plane of incidence (POI)</td>
</tr>
<tr>
<td>Isotropic</td>
<td>Optic axis (OA)</td>
</tr>
<tr>
<td></td>
<td>1. OA perpendicular to surface</td>
</tr>
<tr>
<td></td>
<td>2. OA contained in POI (parallel)</td>
</tr>
<tr>
<td></td>
<td>3. OA perpendicular to POI</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1. One OA perpendicular to the surface</td>
</tr>
<tr>
<td></td>
<td>2. One OA perpendicular to POI</td>
</tr>
<tr>
<td>$M = \begin{bmatrix} 1 &amp; M_{12} &amp; M_{13} &amp; M_{14} \ M_{12} &amp; 1 &amp; M_{23} &amp; M_{24} \ -M_{13} &amp; -M_{23} &amp; M_{33} &amp; M_{34} \ M_{14} &amp; M_{24} &amp; -M_{14} &amp; M_{13} \end{bmatrix}$</td>
<td>Biaxial: One OA contained in the POI</td>
</tr>
<tr>
<td></td>
<td>Uniaxial: OA parallel to sample surface</td>
</tr>
</tbody>
</table>

Traditional ellipsometry functions; $\Psi$ and $\Delta$ for both planar and conical diffraction modes can be calculated from MM elements by equation:\textsuperscript{21}

\[
\Psi = 0.5 \cos^{-1} \left[ \frac{(-MM_{12} - MM_{21})}{2} \right] \\
\Delta = \tan^{-1} \left[ \frac{(MM_{33} - MM_{43})/(MM_{33} + MM_{44})}{MM_{11}} \right].
\] (2.27)

The scattered light intensity in parallel ($R_p$) and perpendicular ($R_s$) direction after reflection from the sample are measured in spectroscopic reflectometry (SR)
measurements. The reflectometry functions, \( R_p \) and \( R_s \) can also be calculated from MM elements by equation:\(^{27}\)

\[
R_p = \frac{(MM_{11} + MM_{12} + MM_{21} + MM_{22})}{2}
\]

\[
R_s = \frac{(MM_{11} - MM_{12} - MM_{21} + MM_{22})}{2}.
\]  \(\text{(2.28)}\)

Hence it can be said that SE and SR functions are subsets of MM elements. Though MMSE provides a lot more information than the conventional SE data and is a powerful technique for the study of complex systems, the optics community has been very slow to adopt MM for the testing of optical components and optical systems, delaying a broad understanding of how real polarization elements actually perform.\(^{24}\) The widespread acceptance of Mueller matrices for polarization element qualification is deterred because the polarization properties associated with a MM (the diattenuation, retardance, and depolarization) are not easily extracted from the matrix.\(^{24}\) Thus, while the operational definition of the MM (equation 2.7) is straightforward, determining the diattenuation, retardance, and depolarization from an experimentally determined MM is a complex process.\(^{26}\) On decomposition of a MM the following matrix element pairs indicate the presence of the various forms of diattenuation and retardance:\(^{28,29}\)

\[
M = M_\Delta M_R M_D \Rightarrow \begin{bmatrix}
0 & M_{12} & M_{13} & M_{14} \\
M_{21} & 0 & M_{23} & M_{24} \\
M_{31} & M_{32} & 0 & M_{34} \\
M_{41} & M_{42} & M_{43} & 0
\end{bmatrix} = \begin{bmatrix}
0 & a & b & c \\
a & 0 & -d & -e \\
b & d & 0 & -f \\
c & e & f & 0
\end{bmatrix}.
\]  \(\text{(2.29)}\)

where \( M_\Delta \) is the decomposed depolarizing matrix, \( M_R \) is the decomposed retardance matrix, and \( M_D \) is the decomposed diattenuation matrix.\(^{29}\) Each pair of matrix element is related to the following properties: ‘a’ is linear diattenuation oriented at 0° or 90°, ‘b’ is linear diattenuation oriented at 45° or 135°, ‘c’ is circular diattenuation, d is linear
retardance oriented at 0° or 90°, ‘e’ is linear retardance oriented at 45° or 135°, ‘f’ is circular retardance. For small amounts of these properties, the MM elements indicated are linear in diattenuation or retardance. Antisymmetry in a, b, or c or symmetry in d, e, or f, indicate the presence of depolarization and inhomogeneity.  

Depolarization is caused by the incoherent superposition of the optical responses from different sample regions within the probe beam due to surface roughness, inhomogeneity, film-thickness variation, target etch effects, probe beam angular spread, and finite spectral bandwidth.  

The depolarization provides an excellent metric for the degree of defectivity in samples. A depolarization coefficient (D) can be calculated from experimental MMSE data by using the following mathematical expression:

\[ D = M_{11} - \sqrt{\frac{\text{trace}(M \cdot M^t) - (M_{11})^2}{3}}, \]  

where M is Mueller matrix and M\(^t\) is Transpose of Mueller matrix. The value for Depolarization coefficient (D) ranges from 0 (non-depolarizing) to 1 (perfectly depolarizing).

Non-depolarizing MMSE data can be retrieved from the experimental MMSE data by using decomposition methods. Calculation of anisotropy coefficients (\(\alpha\), \(\beta\), and \(\gamma\)) from experimental depolarization free MMSE data is very simple and straightforward. \(\alpha\), \(\beta\), and \(\gamma\) are described respectively as the ratios of 90° linear anisotropy, 45° linear anisotropy, and circular anisotropy. The coefficients are not quantitatively equivalent to the absolute magnitudes of the anisotropies but rather they are ratios of the given type of anisotropy to the global anisotropy. Anisotropy coefficients can be calculated by using the following mathematical expressions:
For a perfectly non-depolarizing sample, anisotropy coefficients are related to each other by: $\alpha^2 + \beta^2 + \gamma^2 = 1$. The values of anisotropy coefficients for linear horizontal anisotropy are, $\alpha = 1$, $\beta = 0$, and $\gamma = 0$, for 45° linear anisotropy are, $\alpha = 0$, $\beta = 1$, and $\gamma = 0$, and for circular anisotropy are, $\alpha = 0$, $\beta = 0$, and $\gamma = 1$.

### 2.6 Instrumentation

In the present work, SE and MMSE data are collected using a dual rotating compensator ellipsometer (RC2®) and vacuum ultraviolet - variable angle spectroscopic ellipsometer (VUV-VASE®) of J. A. Woollam. The optical configurations of both the ellipsometers are seen in figure 2.12.

![Figure 2.12 Optical configuration of the Woollam RC2® and VUV-VASE® ellipsometer.](image)

The RC2® is configured with a polarizer, two rotating compensators, and an analyzer that measure the change in polarization of light. The tool is equipped with a quartz tungsten halogen (QTH) lamp and a xenon (Xe) arc lamp to cover a spectroscopic optical
range of 245 - 1700 nm. Si and InGaAs charge-coupled device (CCD) detectors are used to detect the UV/visible and near IR wavelengths, respectively. A computer-controlled software Complete EASE® is used to align, calibrate, and collect data from the ellipsometer. Typically, the data acquisition time for a single spectrum at one angle of incidence (at one azimuth) is 5 - 15 seconds. The spot size of the incident beam is ~ 3 mm x 5 mm depending upon the selected angle of incidence. However focusing optics can be used to reduce the spot size of the incident beam to ~200 μm x 450 μm.

The VUV-VASE® is configured with a polarizer, an auto retarder, and an analyzer that measure the change in polarization of light. The tool is equipped with a deuterium arc lamp (D₂) and a Xe arc lamp sources to cover a spectroscopic optical range of 150 - 1000 nm. The wavelength of this ellipsometer is extended to 150 nm by using a nitrogen purge, as air containing oxygen and water vapor have absorption bands below 190 nm. A computer-controlled software (WVASE®) is used to align, calibrate, and collect data from the ellipsometer. Typically, the data acquisition time for a single spectrum at one angle of incidence (at one azimuth angle) is 4 - 5 hours. The spot size of the incident beam is ~5 mm x 8 mm, depending upon the selected angle of incidence.

For detailed description of different types of ellipsometric hardware configurations the reader is referred to the following books.¹ ² ⁶ ⁷ Each configuration has its advantages and limitations. For example, the VUV-VASE® ellipsometer allows data acquisition in VUV wavelengths (up to 150 nm), while the RC²® ellipsometer allows quick data acquisition (all 16 MM elements) with a relatively smaller spot size. The optical properties (figure 2.13) of various materials used in the DSA stack such as PS, PMMA, OPL, Si-ARC, TiN, and SiN materials are obtained using traditional ellipsometric analysis of their respective
blanket films using both the RC2® and VUV-VASE® ellipsometers.

![Figure 2.13](image)

**Figure 2.13** Refractive index (n) and extinction coefficient (k) of OPL, TiN, PMMA, PS, Si-ARC, and SiN samples.

## 2.7 References


Chapter III

An Introduction to Scatterometry

3.1 History and future developments

Diffraction has long been used to characterize periodic grating structures, evolving into the metrology technique called scatterometry. In 1978, Kleinknecht and Meier used light diffraction from a photoresist grating to measure line-widths on photomasks and monitor the etch rate of an underlying SiO$_2$ layer using Fraunhofer diffraction theory.\textsuperscript{1} Due to limitations in the scalar diffraction model, both of these applications were limited to specific grating geometries.\textsuperscript{2}

In 1981, Moharam and Gaylord were able to calculate the diffraction from a one-dimensional periodic grating structure by solving Maxwell’s equation of electromagnetic radiation.\textsuperscript{3} Their method is called rigorous coupled wave approximation (RCWA) and still remains the foundation of the modern scatterometry optimization software.\textsuperscript{4} Later, the first scatterometer was developed in 1987 at the University of New Mexico and this angle resolved laser scattering technique has been used in many applications for dimensional measurements of periodic grating structures.\textsuperscript{5} J. R. McNeil, S. Naqvi, and coworkers demonstrated improved sensitivity to small variations in line-width of grating structures and presented theoretical and experimental results that illustrated the use of ellipsometry based scatterometry for optical metrology of grating structures.\textsuperscript{5,6} Subsequently, several other research groups illustrated that measurement of diffracted light from grating structures could be analyzed with accurate diffraction modeling...
algorithms to yield accurate and repeatable dimensional information with sub-wavelength resolution.\(^7\)\(^9\) This technique has moved rapidly from initial demonstrations to significant in situ and ex situ industrial applications. The emergence of this approach is directly analogous to evolution of better optical hardware and faster computing capabilities and most of the recent scatterometry studies have been made on methods to increase sensitivity of scatterometry to various complex-grating structures.

There are a wide variety of tool configurations, such as single wavelength-multiple angle and varying wavelength-fixed angle, or varying wavelength-varying angle analyzing changes in the amplitude, phase difference, or the intensity of the light scattered by a periodic grating structure. In the early days, scatterometry measurements were carried out at different incidence angles using a single wavelength He-Ne laser at 442 nm and 633 nm. Simulated data from the model is fitted to extract feature dimensions like line-width, line-shape, and periodicity or pitch.\(^5\) In contrast to conventional scatterometry tools, modern SE (figure 3.1) and normal incidence SR based scatterometry is designed for measurements at a fixed incident angle or multiple incident angles and the wavelength of the sources might range from extreme ultra violet through the visible and to infrared region.\(^10\) Generally, smaller wavelengths provide data for characterizing samples that have structures of smaller dimensions.\(^2\) In addition, a variable angle scatterometry setup can measure higher diffraction orders. Many simulation studies and experimental results have shown that better sensitivity to feature dimensions and more accurate measurements can be made using varying angle spectroscopy.\(^10\)
Over the past several years, the evolution of device architectures has increased the complexity of the integrated circuits’ geometries. This dramatically increased the number of floating parameters as well as the correlation between these parameters in optical scatterometry model. Increase in correlation affects the statistical robustness or accuracy of the model. Ideally, scatterometry models should be such that there exists no correlation between the floating parameters. Several researchers have reported the advantages of Mueller based scatterometry over the conventional SE and SR based scatterometry and performed simulation and experimental studies showing improvement in sensitivity to changes in feature shape parameters using additional information obtained from MM elements. In 2005 Novikova, Martino and coworkers demonstrated the first theoretical evaluation of MM-based scatterometry simulations describing the benefits of MM for overlay measurement. Later, they successfully implemented MM based OCD studies on a photo-resist grating on a silicon substrate to extract the feature dimensions and demonstrated the precision and accuracy of this method by a comparison study of MM-based scatterometry with other metrology methods (CD-SEM and 3D-AFM).

3.2 Features of Scatterometry

Scatterometry is an optical diffraction-based metrology technique used for measuring
the feature dimensions of complex grating structures. It is based on ellipsometric measurements coupled with highly advance modeling and fitting algorithms used to deduce feature dimensions from the phase and amplitude difference of the reflected beam. In general terms, scatterometry can be defined as the measurement and characterization of light diffracted from periodic structures. The scattered light consists of distinct diffraction orders at angular locations specified by the following expression:

\[ \sin \theta_i + \sin \theta_n = n \frac{\lambda}{d}, \]

where \( \theta_i \) is the angle of incidence, \( \theta_n \) is the angular location of the nth diffraction order, \( \lambda \) is the wavelength of incident light, and \( d \) is the spatial period (pitch) of the structure. The fraction of incident light diffracted into any order is very sensitive to the shape and dimensional parameters of the diffracting structure, and thus can be used to characterize that structure itself.

Figure 3.2 Overview of the scatterometry method.

There are two main procedures in optical scatterometry (figure 3.2). The first procedure- forward problem approach involves generation of an optical response signal using rigorous coupled-wave analysis (RCWA), finite element method (FEM), boundary
element method (BEM), finite difference time domain (FDTD) method, or Chandezon method for a given grating structure with the help of a theoretical diffraction model where the complete stack information is fed to the optical simulator.\textsuperscript{21-24} Regardless of the diffraction model used, the theoretical data will only be as useful as the degree to which it reflects accurately the physical composition of the stack being measured in the forward problem. Out of all the methods listed above, in the last decade the rigorous coupled wave analysis (RCWA) algorithm proved to be an efficient approach for the accurate simulation of electromagnetic wave diffraction on periodic gratings.\textsuperscript{3,4,12} In the present work, the optical response for the scatterometry model systems are generated using Nanodiffract\textsuperscript{®} software, which contains a RCWA optical response simulator.

Figure 3.3 A schematic illustration of the RCWA method in which the one-dimensional grating is sliced into a series of rectangular subdomains.

RCWA is a mathematical algorithm that calculates the direct solution of the diffracted electromagnetic fields by utilizing Maxwell’s equations in vector differential form and by applying boundary conditions at all interfaces (See Appendix I for a more detailed description of the RCWA method). It is based on certain assumptions that the optical properties of the substrate and grating material are isotropic and homogeneous (i.e. optical properties are varying only along the horizontal axis (x-axis) and not the vertical
axis (z-axis)) and grating structure is uniformly extended from \(-\infty\) to \(+\infty\) along the grating axis (y-axis).\(^{23}\) The periodic one-dimensional grating is sliced into a series of rectangular subdomains as seen in figure 3.3. The grating can be viewed as a one-dimensional modulation of the dielectric function along the horizontal axis (x-axis) and the effective dielectric function of the periodic grating \((\varepsilon(x))\) can be expanded as a Fourier series:\(^9\)

\[
\varepsilon(x) = \sum_h \varepsilon_h \exp \left( j \frac{2\pi h}{p} x \right),
\]

where \(h\) is the spatial expansion parameter and \(p\) is the pitch of the grating patterns. This Fourier series expansion of the dielectric function is carried out for all the subdomains and the scattered or diffracted electromagnetic fields can be determined by matching the solutions at each subdomain. The exact solution of diffraction of light from the grating structure can be achieved by increasing the number of subdomains.\(^{23}\) However, this is computationally difficult and time consuming. An approximate solution is obtained by assuming finite number of subdomains with spatial orders, which works very well for a majority of the scatterometry problems. Typically, the number of subdomains varies from 1 to 50 based on the number of the spatial orders, the grating structure, and its dielectric function.\(^9\)

Although this approach is conceptually relatively simple, special attention must be paid to the numerical stability of this technique and to the convergence of its solutions with varying field harmonics and truncation values which characterize the approximation.\(^{12}\) Also RCWA results in large matrix eigenvalue solutions and presents a very significant computational time problem.\(^9\) Due to advances in both the hardware and software capabilities of computers practical use of this method is now possible.
The second procedure is the inverse problem that involves extraction of the structural profile of the periodic grating structure from the acquired experimental data using regression based data analysis to find a profile whose theoretical optical response coincides with the experimental data. To solve the inverse problem in optical scatterometry, several linear and non-linear regression methods have been reported.\textsuperscript{26,27} The linear and non-linear regression methods are very time-consuming as the structural profile is achieved through an iterative procedure that computes the forward optical spectra at each step. The library search method has been demonstrated to be an effective approach for improved scatterometry time to solution and has been commonly used in industry.\textsuperscript{28} In this method, a library of optical responses is generated using simulations prior to the measurement, and then an algorithm is used to find a best match between the simulated and measured optical spectra. Although the off-line generation of the signature library is time consuming, the search itself during the in-line measurement can be done quickly. A lot of memory space is used to store the signatures, and having a large size signature library reduces the speed of this method. However, some algorithms based on sensitivity analysis can be developed to reduce the size of the signature library.\textsuperscript{27}

3.3 Data analysis and applications

The optical response contains the scattered light information from the structure, and it can be in the form of reflectance, traditional ellipsometry parameters, or MM elements. However, as explained earlier Mueller measurements provide important additional information and have better sensitivities with respect to minute structural changes than traditional SE and SR measurements.\textsuperscript{11-20} The MM for a sample is a function of the
direction of propagation and wavelength $\lambda$. The direction of incident light is defined by both the incidence angle and the azimuthal angle. The azimuthal angle is the angle between the grating direction and angle of incidence as seen in figure 3.4. In addition, the optical spectra of each MM element change significantly with the angle of incidence and azimuthal angle. Different experimental MM optical spectra acquired at each azimuthal angle and incident angle for a given grating structure are very useful in de-correlating several feature parameters and each MM data set provides its own best fit (MSE value) to the structural model. The standard deviation of these different MSE values of parameters can then be used to provide more robust solutions and profile parameters.

If the periodic structures are perpendicular to the plane of incidence, all diffracted orders of reflected light beam are within the plane of incidence. This phenomenon is called planar diffraction. For planar diffraction, cross-polarization is absent and mirror symmetry about the incidence plane leaves the parallel components of electric fields invariant while the perpendicular components of electric field change sign.\textsuperscript{12} As a result, the intensity of off-diagonal MM elements is zero. From the above discussion it follows that for cylindrical contact hole structures at $0^\circ$, $45^\circ$, and $90^\circ$ azimuthal angles and for

Figure 3.4 A schematic illustration of acquiring scatterometry data at multiple configurations by changing the angle of incidence and rotating the sample.
line-space patterns at 0° and 90° azimuthal angles the off-diagonal blocks of the MM of the grating will vanish as seen in figure 3.5.

![Graph showing Mueller matrix elements for different azimuths](image)

**Figure 3.5** Experimental spectroscopic Mueller matrix data of Si & SiGe line space patterns at azimuths = 0°, 90° (Planar diffraction mode), and 45° (conical diffraction mode). Mueller matrix of the structure in planar diffraction mode has simple symmetrical structure with zero 2 x 2 upper right and bottom left sub-matrices. Figure from [15], used with permission.

On the other hand if periodic structures are not perpendicular to the plane of incidence or if there is no mirror symmetry, cross-polarization of parallel and perpendicular components of electric field is present. Hence, MM of diffracting structure has non-zero values for the off-diagonal MM elements as in the case of azimuthal angles other than 0°, 45°, and 90° for cylindrical contact hole structures and 0° and 90° for the line-space patterns. This phenomenon is called conical diffraction. MMSE based scatterometry carried out in conical diffraction mode provides more information which can be used to increase the sensitivity to various feature parameters and reduce the correlation between them. In the case of a perfectly symmetrical structure; there are only seven independent MM elements in experimental or theoretically generated optical spectra. There is symmetry between Mueller elements M12 and M21, M14 and M41, M24 and M42, and M33 and M44 and anti-symmetry between Mueller elements M13 and M31, M23 and M32, and M34 and M43. The symmetry-antisymmetry properties associated with MM
provide an excellent means of measuring and understanding any asymmetry present in the structure.\textsuperscript{20}

*Figure 3.6 (a) Generated MM12 optical spectra for Si fin structures with varying top CD values (from 10 nm to 22 nm) and scatterometry Si fin model with top CD value = 10 nm and 22nm.*

*Figure 3.6 (b) Generated MM12 optical spectra for Si fin structures with varying bottom CD values (from 14 nm to 26 nm) and scatterometry Si fin model with top CD value = 14 nm and 26nm.*

*Figure 3.6 (c) Generated MM12 optical spectra for Si fin structures with varying amount of rounding (from 0 % to 90 %) and scatterometry model of Si fins with top rounding = 30 % and 90 %.*

*Figure 3.6 Generated MM optical spectra for 28 nm pitch Si fin structures with varying (a) top CD values (b) bottom CD values (c) rounding. (65° angle of incidence and 45° azimuth)*

The feature dimensions can be extracted from the measured signal as long as the variation of the feature shape or size causes a detectable change in the response signal. For example, the MM12 spectral peak shifts when either bottom or top CD values are varied in the Si fin model as seen in figure 3.6. It is important to note that only one of the parameters in the model is being varied at a time for the sensitivity analysis. For example,
the change in the optical spectra of the element MM34 is due to increase in amount of rounding of the Si fins as seen in figure 3.6.

Systematic analysis of focus-exposure matrix (FEM) data is vital to the accurate determination of the process window. A process engineer must perform process window analysis to find the maximum two-dimensional (dose and focus) region where the interested parameter of the printed feature is within tolerance. Process window analysis is very important for robustness of lithography and the etching process. The process window analysis to achieve the target CD can be carried out by plotting Bossung curves from CD-SEM images of FEM wafer as well as using scatterometry analysis for data measured at different locations across the wafer. The comparison of the Bossung curve obtained using CD-SEM images and scatterometry measurements of macros in a FEM wafer (used in the present work) with varying guide CD macros (for a constant focus value and changing exposure values) is seen in figure 3.7.

Figure 3.7 The Bossung curve for constant focus value of 0.040 and varying exposure values from 69 to 89 mJ/cm², obtained using CD-SEM images and scatterometry measurements.

In semiconductor manufacturing scatterometry is used as an inline statistical process control (SPC) method, to simply monitor effective focus and exposure settings, plot
Bossung curves, to extract the best line spacing regime, and halt the equipment in the case of an excursion. Scatterometry is also used as an advanced process control (APC) method, to correct dose and focus settings on a run-by-run basis. A variety of factors like mask errors, mask tilt, astigmatism, chuck flatness, lens aberrations, scanner illumination variations, wafer edge effects, post-exposure bake (PEB) temperature non-uniformity, and plasma etch rate non-uniformity contribute to overall CD variation. Scatterometry is used for calibration of all these critical lithography parameters for CD uniformity across the wafer. In addition to the primary parameters of interest associated with gratings, such as thickness and line-width, more complex structural shapes such as rounded corners or non-rectangular profiles, scatterometry has been further used to characterize process induced defects like the amplitude of line edge roughness, pitch walking, and overlay errors.

In scatterometry the total time required for measurements is mainly due to time spent creating an optical and geometric model of the measurement target. A new approach known as Signal Response Metrology (SRM) has been demonstrated by Pandev et al., that uses optical response signals for measuring targets and reduces the time to solution from weeks to only a few hours by eliminating the need for complex 3D structure modeling and substantial computing resources. The fundamental concepts of SRM and the process of developing and using SRM recipe for CD, focus and dose measurements has been well demonstrated in the referenced work.
3.4 References


Chapter IV

Optical CD Metrology of PS-\textit{b}-PMMA and PS Line-space Patterns Fabricated Using DSA Patterning

This report is a study on Mueller matrix spectroscopic ellipsometry (MMSE) scatterometry measurements of 28 nm pitch directly self-assembled (DSA) patterns consisting of polystyrene-\textit{block}-polymethylmethacrylate (PS-\textit{b}-PMMA) block copolymer sample fabricated using a chemical epitaxy process. Scatterometry is used to evaluate defectivity in DSA patterns and calculate thickness of the underlying layers, line-widths, line-shapes, sidewall-angle (SWA) of the DSA patterns by fitting experimental data to measured data.

4.1 Design of the experiment

The polymer samples (PS-\textit{b}-PMMA patterns and PS line-space patterns with a lamellae period of $L_o \sim 28$ nm) are fabricated by the RTNB chemoepitaxy method as seen in figure 1.6. The focus and exposure conditions are systematically varied across the wafer (referred to as a focus exposure matrix or FEM wafer in this paper) as seen in figure 4.1. The process window is varied with dose increments of 2 mJ/cm$^2$ and focus steps of 30 nm with a center dose of 30 mJ/cm$^2$ for 84 nm ($3L_o$) guide pattern pitch and 25 mJ/cm$^2$ for 112 nm ($4L_o$), 140 nm ($5L_o$), and 168nm ($6L_o$) guide pattern pitch and with a center focus of -30 nm. BCP DSA patterning performance is dependent on underlying pre-pattern pitch, guide strip CD, variation in chemistry of background materials, and block copolymer film thickness. At optimum conditions, parallel defect
free DSA PS-b-PMMA patterns are obtained. However, as the conditions deviate from optimal the defectivity and disorder are present in the DSA patterns. The DSA process window response to the photolithography FEM is then characterized by acquiring CD-SEM images at each focus-exposure condition.

**Figure 4.1** Across-wafer lithography with focus-exposure variation.

MMSE data is collected from various different guide pattern pitch macros ((3x$L_o$), (4x$L_o$), (5x$L_o$), and (6x$L_o$)) at each focus-exposure condition at various azimuthal angles (0°, 45°, and 90°) over a spectral range from 245 to 1700 nm using a J.A. Woollam RC2® spectroscopic ellipsometer for scatterometry analysis. The azimuthal angle is the angle between the grating direction and angle of incidence as seen in figure 4.2. The angle of incidence for all the measurements is fixed at 65° for focusing probe measurements. Focusing optics and camera are used to center the incident beam spot (~200 μm x 450 μm) inside a 2 mm x 2 mm square macro. Collecting multiple measurements from the same structure at different azimuthal angles enhances the amount of spectral information for modeling. Prior to this, optical properties (refractive index and extinction coefficient) and thicknesses of SiN, PS, and PMMA are measured at an earlier process step using SE.
These parameters are injected into the final structure model to reduce the number of floating parameters in the model. The precision and accuracy of the MMSE results depend on the model utilized and parameters’ sensitivity. Optical response of the DSA structure is generated using the forward problem approach based on RCWA- rigorous coupled wave analysis and using regression based inverse problem approach the generated optical response is fit to the experimentally measured optical spectra using three-dimensional multi-parameter models to extract feature dimensions like CD, height, side-wall angle and line shape.

**Figure 4.2** Overview of the scatterometry method used to calculate the feature dimensions.²,³

In order to confirm the results, a repeatability analysis is carried out; MMSE data is collected at nine different spots from each chemical guide pitch macro within several fields at 0°, 45°, and 90° azimuthal angles. Additionally the current work represents a unique application of using MSE, anisotropy, and depolarization values as a method to judge the degree of alignment of the DSA patterns across wafer. The MSE is used as the criteria to estimate the degree of mismatch between experimental and model-generated MM data and is calculated from:
\[
MSE = \frac{1}{(N - M)} \sum_{i=1}^{N} (y_i - y(x_i))^2,
\]

where, \(y_i\) is the experimental MMSE data, \(y(x_i)\) is the generated MMSE data, \(N\) is the number of data points, and \(M\) is the number of floating parameters. Depolarization and anisotropy coefficients are calculated from experimental data using equations 2.30 and 2.31, respectively.

4.2 Data analysis and results

4.2.1 Analysis for PS-b-PMMA patterns

There is a nearly indiscernible difference in the optical spectra of \(\Psi\), \(\Delta\), and the MM elements between the different chemical guide pitch samples for perfectly oriented DSA PS-b-PMMA patterns. In addition, the off-diagonal Mueller elements are close to zero for all azimuths. The optical contrast between PS and PMMA patterns is less as the difference in refractive indices (n) of the PS and PMMA materials is about 0.1 and the extinction coefficient values for both the polymers are close to zero from 250 - 1000 nm as seen in figure 2.13. However, the MM elements for the completely disoriented PS-b-PMMA patterns can be distinguished from perfectly oriented patterns. There is a red shift in the optical spectra of Mueller elements for fingerprint like PS-b-PMMA patterns with respect to the optical spectra of Mueller elements for the perfectly oriented PS-b-PMMA patterns as seen in figure 4.3. The accuracy and repeatability of the MM ellipsometry obtained by the RC2 is approximately 0.003, and the redshift seen in figure 4.3 can be routinely observed. The red shift seen in the graph is observed in optical spectra of on-diagonal MM elements for data acquired from all nine spots from the macros with fingerprint-like PS-b-PMMA patterns. The fingerprint structure of PS-b-
PMMA patterns is confirmed by CD-SEM images (figure 4.11).

The generated optical response of the scatterometry model (figure 4.4) is fit to the experimentally measured optical spectra. The MSE values (Table 4.1) are used as the criteria to estimate the degree of mismatch between experimental and model-generated data. Scatterometry is able to differentiate between perfectly oriented and completely disoriented PS-\(b\)-PMMA patterns, but sensitivity to partially ordered PS-\(b\)-PMMA patterns is not observed for the un-etched samples. MSE values for both perfectly oriented and partially disordered PS-\(b\)-PMMA patterns is less than 1 and for fingerprint like patterns is greater than 1. The wafer map for un-etched DSA PS-\(b\)-PMMA with respect to the MSE obtained from scatterometry analysis is seen in figure 4.5.

![Figure 4.3 Experimental MMSE data (MM\(_{12}\), MM\(_{33}\), MM\(_{34}\)) collected at 0° azimuth from perfectly oriented and disoriented fingerprint-like PS-\(b\)-PMMA patterns.](image)

![Figure 4.4 Final profile of the scatterometry model for \(3L_o\) un-etched PS-\(b\)-PMMA patterns.](image)

### Table 4.1 MSE values for various macros of PS-\(b\)-PMMA patterns obtained after scatterometry analysis.

<table>
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<th>(0,3)</th>
<th>(1,-3)</th>
<th>(1,-3)</th>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>MSE</td>
<td>MSE</td>
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<tr>
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<tr>
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<td>0°</td>
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<tr>
<td>Azimuth</td>
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<td>Avg. MSE</td>
<td>MSE</td>
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<tr>
<td>Direction</td>
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</tr>
<tr>
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<td>Azimuth</td>
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4.2.2 Analysis for PS-\textit{b}-PMMA patterns

In contrast to SE and CDSEM, MMSE data is found to be sensitive to underlying chemical guide pitch for the etched samples. As explained earlier, the structure and CD of the underlying chemical guide pitch is essential for directed self-assembly process. The etched sample (PMMA etched) provides better optical contrast than the un-etched samples. Differences in the MM elements are seen in figure 4.6 (a), for perfectly oriented and disoriented fingerprint-like PS line-space structures. A clear blue shift is observed in MM elements with increasing disorder in the etched samples in contrast to the red shift observed for the un-etched samples. The intensity of all the off-diagonal elements MM elements for data acquired at 0° and 90° azimuth is zero. However, non-zero off-diagonal Mueller elements are obtained for etched samples measured at 45° azimuth, within the wavelength range between 245 - 450 nm for perfectly oriented PS line-space patterns as seen in figure 4.6 (b). As pattern order decreases, the off-diagonal MM elements tend towards zero with a minimum observed for completely disordered or fingerprint-like PS patterns.
line-space patterns. This trend in the off-diagonal elements is directly related to changes in the depolarization coefficient and anisotropy coefficient values that are used to measure the amount of disorder in the PS line-space patterns. The decrease in intensity of off-diagonal elements with increase in disorder can be understood by decrease in pseudo-anisotropic character of PS line space patterns, as for an isotropic sample the intensity of off-diagonal elements is zero irrespective of azimuthal angle and wavelength range used.

![Figure 4.6 (a)](image1.png) **Figure 4.6 (a)** Experimental MMSE data (MM$_{12}$, MM$_{33}$, and MM$_{34}$) collected at 0° azimuth from oriented and disoriented fingerprint-like PS line-space patterns.

![Figure 4.6 (b)](image2.png) **Figure 4.6 (b)** Experimental MMSE data (off-diagonal elements) collected at 45° azimuth from oriented, partially disoriented, and fingerprint-like PS line-space patterns.

Three-dimensional models with nominal dimensions (figure 4.7) are created using NanoDiffract® software. The optical response obtained from these multi-parameter model strategies are fit to the experimentally collected optical spectra using a regression RCWA based approach to extract profile dimensions (figure 4.8) like line-width, line-shape, height, and MSE values.

![Figure 4.7](image3.png) **Figure 4.7** Front view of model strategies for 3x$L_0$(84 nm), 4x$L_0$(112 nm), and 5x$L_0$(140 nm) guide pitch macros. Floating parameters (and the limiting values) are marked with red arrows.
For each azimuthal angle, the lowest MSE value is measured for macros containing parallel lines and increases, for macros with little structural order. For example, the MSE value for the 3xL_o macro at 0° azimuth for ordered structures is 0.46 and for fingerprint-like disordered structure is 4.01. Moreover, the standard deviation (SD) of the MSE for ordered structures is smaller than that for disordered structures. For example, the SD value for the 3xL_o macro at 0° azimuth for ordered structures is 0.01 and for fingerprint-like disordered structure is 0.42. The differences in MSE values are large enough to routinely distinguish between ordered, partially disordered and fingerprint-like patterns. The scatterometry results for the etched samples are found to correlate with the CDSEM images as seen in figure 4.9. The wafer map for etched samples with respect to the MSE values obtained after scatterometry analysis is seen in figure 4.10.

![Figure 4.8 Final profiles of the model strategies for 3xL_o(84 nm), 4xL_o(112 nm), and 5xL_o(140 nm) samples, determined using MMSE scatterometry.](image)

Figure 4.9 CDSEM images for (a) 3xL_o, (b) 4xL_o, (c) 5xL_o, and (d) 6xL_o macros.
Table 4.2 MSE values for various macros of PS line-space patterns.

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Figure 4.10 Scatterometry based wafer map for PS line-space patterns with respect to MSE obtained for data collected at 45° azimuthal angle.

4.2.3 Anisotropy coefficient measurements

Anisotropy coefficients (α, β, and γ) are calculated from non-depolarizing experimental MMSE data using equation 2.31 and equation 2.32. Calculated anisotropy
coefficient values; $\alpha \approx 0$, $\beta \approx 0$, and $\gamma \approx 1$ show that scattered light is circularly
anisotropic for wavelengths greater than 400 nm, at an azimuthal angle of 45°, and across the entire wavelength range for azimuthal angles of 0° and 90° as seen in figure 4.11.

![Figure 4.11](image)

Figure 4.11 Effective Anisotropy coefficients of the 3x$L_0$ guide pitch macro of (0,3) field at 0°, 45°, and 90° (left to right) azimuthal angles.

For experimental MMSE data collected at 45° azimuthal angle, due to non-zero off-diagonal MM elements it is observed that $\alpha \neq 0$, $\beta \neq 0$, $\gamma \neq 0$, in the wavelength range of 250-500 nm for perfectly oriented PS line space patterns, and an increase in disorientation of self-assembled PS lines are correlated with a decrease in the value of $\alpha$ and $\beta$ (to 0), while the value of $\gamma$ increased to 1 as seen in figure 4.12.

![Figure 4.12](image)

Figure 4.12 Anisotropy coefficients of the 3x$L_0$ guide pitch macro of (0,3), (-2,1), (-2,-1), and (0,-3) (with increasing disorder in PS line-space patterns) fields at 45° azimuth.

The changes in the anisotropy coefficients with respect to increasing in disorientation of PS lines could be understood by a loss of the anisotropic character of the sample.
There is no consensus understanding of the wavelength dependence of the anisotropy parameters for these structures. However, in terms of algebraic calculations, this trend of change in anisotropy coefficients can be correlated to change in intensity of off-diagonal Mueller elements with change in degree of alignment of PS line space patterns as seen in figure 4.6 (b). A full wafer map corresponding to the changes in the circular anisotropy coefficient (γ) values measured at 260 nm is seen in figure 4.13 and it is very similar to the MSE wafer map seen in figure 4.10.

![Figure 4.13 Wafer map for etched samples with respect to circular anisotropy coefficient (γ) calculated from depolarization free experimental data collected at 45° azimuth.](image)

**4.2.4 Depolarization coefficient measurement**

Ellipsometric characterization of the complete optical response collected from a sample includes determination of the amount of light depolarized. The depolarization is the decrease in the degree of polarization of totally polarized light after it has interacted with the medium. The depolarization coefficient is calculated directly from the experimental MMSE data using equation 2.30. It is observed that the depolarizing coefficient value increases, as structural order of the DSA patterns decreases. The
changes in the value of depolarization coefficient are only observed in the lower wavelength region (245 - 450 nm) as seen in figure 4.14. The increase in depolarization coefficient is due to certain non-idealities present in PS patterns, i.e. bridging defects, wiggles, or dislocations. The wafer map showing this increase in depolarization coefficient value at 260 nm wavelength of light is seen in figure 4.15. Comparing figures 4.9, 4.10, 4.13, and 4.15 it is seen that the depolarization coefficient is more sensitive to structural changes in PS line-space patterns than either the MSE or anisotropy maps as even the macros with parallel PS line-space patterns with slight imperfections are detected, which is confirmed by CDSEM imaging.

**Figure 4.14** Depolarization coefficient plots.

**Figure 4.15** Wafer map for etched samples with respect to depolarization coefficient values at 260 nm.
4.3 References


Chapter V

Optical CD Metrology and LER Measurements of Si Fins Fabricated Using DSA Patterning Technique

Measurement and control of line edge roughness (LER) is one of the most challenging issues facing patterning technology. As the critical dimensions of patterned structures decrease, not only does the line-width but also the line-shape and line edge roughness (LER) become more important. The term roughness usually denotes the deviation from a reference flat surface or from a reference straight line. The deviation from a reference flat surface of a thin film on a substrate is termed surface roughness. The deviation of the edges in a patterned structure from the mean straight line is termed LER, while the deviation from the mean line width is termed line width roughness (LWR). The LER/LWR (figure 5.1) behavior must be quantified as a function of the frequency and amplitude of the LER/LWR features.

The critical dimension (CD) can be used to provide a relative reference scale for the frequency of the LER/LWR features thus defining it as high frequency LER/LWR or low frequency LER/LWR.\(^1\) When the wavelength of roughness that appears along the line edge is small relative to the CD, the LER is termed as high frequency LER and conversely, when the wavelength of the roughness is large compared to the CD, the LER is characterized as low frequency LER. The International Technology Roadmap for
Semiconductors (ITRS) indicates that LER measurement and control improvements are significant industry requirements.\textsuperscript{2} LER does not scale down with the dimensions of the fabricated structures, i.e., as device dimensions go down, the magnitude of the roughness remains about the same and becomes an increasing fraction of their size which can negatively impact device performance.\textsuperscript{1} The ITRS states that LER/LWR affects dopant concentration profiles, interconnect wire resistance, gate leakage, and lowers the yield in sub-20 nm structures. Hence characterizing wafer-to-wafer LER/LWR during lithography is the critical step in improving overall yield of the process.

This work demonstrates the use of Mueller matrix spectroscopic ellipsometry (MMSE) based scatterometry for quantifying LER in directed self-assembly (DSA) patterned Si fins with the help of multi-parameter scatterometry models. Although research into DSA patterning has demonstrated a high potential as a nanoscale patterning process, there are critical challenges like LER that must be overcome before transferring DSA into high volume manufacturing. LER measurements carried out with the help of SEM show that the root mean-square (RMS) magnitude of the LER of ~2 - 4 nm in DSA patterned structures. LWR in DSA patterned structures is lower than LER because the DSA edges are correlated.\textsuperscript{3} ITRS requires less than 1.8 and 1.3 nm LER in the patterned structures for 22 and 16 nm half-pitch nodes.\textsuperscript{4} A number of publications addressed the influence of LER in patterned structures on the measured optical spectra.\textsuperscript{1,5-7} Approximate EMA (Effective medium approximation) scatterometry models have been used to characterize LER and grating imperfections. However, profile reconstruction of patterned structures in scatterometry models that incorporate line roughness has been largely neglected likely because it increases number of floating parameters and the correlation
between these parameters and computation time. The multi-parameter scatterometry models that include the surface roughness as demonstrated in this report can be used offline for predictive modeling and library-based search can be carried out as a quick and effective approach for LER measurements.

5.1 Experimental Details

The wafer used in this study is from the early stages of development of the neutral layer lift off (NLLO) chemoepitaxy process as seen in figure 1.7. Hence a variation in quality of Si fins is observed across the wafer. For example, the presence of LER/LWR in Si fins as observed in the top down scanning electron microscope (SEM) images (figure 5.2), the depths of the trenches between the Si fins vary across the sample, and a layer of un-etched SiN is present on top of Si fins as observed in the cross-section transmission electron microscope (TEM) image (figure 5.3). These patterning imperfections make the sample optimal for metrology testing but do not reflect the final process. MMSE based scatterometry is used to measure the pattern imperfections. The NLLO chemoepitaxy process used in this study does produce high quality patterns.

![Figure 5.2](image)

**Figure 5.2** Top down SEM images of 28 nm pitch Si fins acquired at four corners and center (top left, top right, center, bottom right, and bottom left) of a 2 x 2 mm macro.
Generalized ellipsometric data (all 16 Mueller elements) is collected from a 2x2 mm square macro at azimuthal angles between 0° - 360° with a step size of 5° over a spectral range from 245 - 1000 nm using a J.A. Woollam RC2® spectroscopic ellipsometer. The angle of incidence for all the measurements is fixed at 65° to allow use of focusing probes. Focusing optics and camera are used to center the incident beam spot (~200 μm) inside a 2x2 mm square macro. In order to confirm the results, MMSE data is collected at five different spots (four corners and center) of the 2 x 2 mm macro. Figure 5.4 shows optical spectra of seven different MM elements at 65° angle of incidence in the wavelength region of 250 - 1000 nm.

For an appropriate depiction of the anisotropic nature (structural) of the Si fin samples and its effect on MM optical spectra, the MM intensities are plotted in polar coordinates with wavelength and azimuthal angle as radial and angular coordinate, respectively. It can be observed that the highest peaks in the optical spectra of on-diagonal MM elements are observed at azimuthal angles of 0°, 90°, 180°, and 270° and the highest peaks in the optical spectra of off-diagonal MM elements are at azimuthal angles of 60°, 120°, 240°, and 300°, in the wavelength range of 300 - 500 nm (conical diffraction mode). However, the off-diagonal elements are zero at 0°, 90°, 180°, and 270° azimuthal angles (planar diffraction mode). Hence, 60° azimuthal angle is selected for sensitivity analysis.
Simulated MM optical responses for 28 nm pitch Si fins are generated by using Nanodiffract modeling software. Sensitivity analysis is carried out by comparing the optical responses generated for a range of grating shape parameters including pitch, side-wall angle (SWA), and CD and LER feature dimensions such as frequency and width. It is important to note that SiN layer present on top of Si fins is not incorporated in the

![Figure 5.4 Experimental MMSE data of individual MM elements at 0 - 360° azimuthal angles for 65° incident angle. MM intensities are plotted in polar coordinates with wavelength and azimuthal angle as radial and angular coordinate.](image)

### 5.2 Sensitivity analysis

Simulated MM optical responses for 28 nm pitch Si fins are generated by using Nanodiffract modeling software. Sensitivity analysis is carried out by comparing the optical responses generated for a range of grating shape parameters including pitch, side-wall angle (SWA), and CD and LER feature dimensions such as frequency and width. It is important to note that SiN layer present on top of Si fins is not incorporated in the
models that are used for sensitivity analysis. Figure 5.5 shows the change in MM optical spectra at 60° azimuth for 65° angle of incidence in the wavelength region of 250-800 nm, when LER amplitude is increased. When the model incorporates sinusoidal anti-correlated rectangular-shaped LER, the MM elements change significantly, and the higher the amplitude of the LER, the larger the impact on the MM elements. The changes in the MM elements with respect to increasing LER amplitude could be understood by an increase of the pseudo-isotropic character of the sample i.e. the MM elements approached zero as the LER amplitude is increased. The light is scattering from a sample that is increasingly becoming more like an isotropic film. For an isotropic sample the off-diagonal block elements are always zero independent of the wavelength and azimuthal angle.

![Generated optical spectra of individual MM elements at 60° azimuthal angle for 65° incident angle. LER amplitude of Si fins is increased from 0 - 4.5 nm in Si fin scatterometry model with LER spatial period fixed at 3 nm.](image)

**Figure 5.5** Generated optical spectra of individual MM elements at 60° azimuthal angle for 65° incident angle. LER amplitude of Si fins is increased from 0 - 4.5 nm in Si fin scatterometry model with LER spatial period fixed at 3 nm.
Similarly varying feature parameters like CD (top), SWA (bottom CD), and height of the Si fins (figure 5.6 (a)) also affect the optical response of MM elements. To observe the difference in response of the individual MM elements due to change in these feature parameters and LER, the simulated optical spectra for models with varying feature parameters is subtracted from the simulated optical spectra of the reference model as seen in figure 5.6 (a). These calculated difference values are defined as the sensitivity of MM elements. The individual response of all the MM elements to change in all these feature parameters and LER is different as seen in figure 5.6 (a). For example, there is a decrease in the intensity peaks of MM12 optical spectra at ~400 nm with increase in LER and top CD dimensions (observed as positive peak in the sensitivity plot). MM12 also shows a small increase in intensity of the peak with decrease in height, and a large increase in intensity of the same peak (observed as negative peak in the sensitivity plot) with decrease in bottom CD dimensions of the Si fins in the scatterometry model. Figure 5.6 (b) shows the average deviation of the simulated MM elements for models with varying feature dimensions with respect to the reference structure with no LER or LWR seen in figure 5.6 (b). The largest response is due to a change in CD of 3 nm (bottom and top). A change in height of 5 nm results in less response, while incorporating sinusoidal anti-correlated rectangular-shaped LER of 1.5 nm amplitude and 3 nm spatial period in the Si fin model has the least impact on the optical response of MM elements as seen in figure 5.6 (b). In general for data simulated at 60° azimuth, the off-diagonal elements have higher response to variation than the on-diagonal element and MM24 off-diagonal MM element has the highest sensitivity.
The above analysis characterizes sensitivity to changes in the ideal structure. However, it is important to characterize the effect of changes in feature dimensions like top and bottom CD, SWA, height, and LER.

Figure 5.6 (a) Sensitivity of individual MM elements at 60° azimuthal angle for 65° incident angle to change in feature dimensions like top and bottom CD, SWA, height, and LER.

Figure 5.6 (b) Average deviation in MM intensity calculated in the wavelength range from 250 - 800 nm at 60° azimuthal angle for 65° incident angle when only one of the feature dimensions in Si fin model is varied.

The above analysis characterizes sensitivity to changes in the ideal structure. However, it is important to characterize the effect of changes in feature dimensions like
spatial period of LER, SWA, height, optical properties, and pitch of line-space patterns to MM elements’ LER sensitivity. To observe the difference in response of the individual MM elements due to LER with changes in these feature parameters, the simulated optical spectra for various models with varying feature parameters and 3 nm LER feature amplitude is subtracted from the simulated optical spectra of the same model with no LER as seen in figure 5.7 (a) and 5.7 (b). These calculated values are defined as sensitivity of MM elements to 3 nm LER amplitude.

**Figure 5.7 (a)** Si fin scatterometry models without LER (Reference Models).

**Figure 5.7 (b)** Si fin scatterometry models with LER. Feature dimensions like spatial period of LER, SWA, height, pitch, and optical properties of the fins are varied to observe their impact on LER sensitivity.

It can be observed that MM elements’ sensitivity to amplitude of 3 nm LER features is a function of the optical properties of the material, spatial period of LER features, and pitch, height, CD, and SWA of the Si fins. For example, sensitivity of MM elements to LER decreases when the height of Si fins is reduced to 40 nm and pitch value is increased to 56 nm as seen in figure 5.8 (a). The average deviation of the MM elements in the wavelength range of 250 - 800 nm obtained for a model with 3 nm LER amplitude and
varying feature parameters with respect to the undisturbed reference structure are seen in figure 5.8 (b). It is observed that high frequency LER features (spatial period of 3 nm) has a higher impact on the calculated optical spectra of MM elements compared to low frequency LER (spatial period of 14 nm). In addition, the sensitivity to LER increases with height of the patterns and as the CD to pitch ratio increases. The sensitivity of MM elements to 3 nm LER features is least for the 28 nm pitch line-space patterns in which optical properties of PMMA (photoresist material) are used instead of optical properties of Si and is observed only in the wavelength region of 250 - 380 nm. Hence LER inspection in photoresist line-space patterns must be carried out using a light source with ultraviolet (UV) and vacuum UV (VUV) spectral range. And highest sensitivity of MM elements to LER is observed when SWA value is near 90° i.e. when Si fins are straight and not trapezoidal.

In addition it is observed that MM24 off-diagonal MM element has the highest sensitivity to LER for all the 28 nm pitch patterns, but on diagonal element MM34 is the most sensitive MM element for the Si fins with pitch 56 nm for data generated at 60° azimuthal angle. The spectral distribution of the MM elements, more sensitivity to certain feature parameters in different wavelength regions, and different optical responses of all MM elements to change in feature parameters is helpful in separating the impact of various feature parameters like CD, height, and LER on the optical spectra during the solution of inverse problem approach of scatterometry.
5.3 Inverse problem approach and scatterometry results

The generated optical response of the Si fin model without LER is fit to the experimentally measured optical spectra using regression based data analysis in order to extract feature dimensions like CD, height, side-wall angle, and line shape. The spectral and azimuthal angle dependencies of the calculated MM elements for Si fin model with no LER agree with experimental data. However, the data fits are poor as the MM intensity of characteristic peaks for optical spectra of each MM element do not match. In
scatterometry, MSE is used as the criteria to estimate the degree of mismatch between experimental and model-generated MM data and is calculated by using equation 4.1. The difference between experimental and generated data at each azimuth, average difference of MM intensities at each azimuth and MSE values obtained after the scatterometry analysis are seen in figures 5.9, 5.10 (a), and 5.10 (b), respectively. The average difference of experimental and generated MM intensities calculated for all azimuths is larger for the on-diagonal MM elements than off diagonal elements because the intensity of all off-diagonal elements is very close to zero at 0° and 90° azimuthal angle as seen in figure 5.4. Average MM intensity difference for all off-diagonal MM elements is maximum at 60° azimuthal angle and for all on-diagonal MM elements is maximum at 90° azimuthal angle. Maximum average MM intensity difference (0.091) calculated for all azimuths from 0 - 180° is obtained for on-diagonal MM33 element while the maximum intensity difference is obtained for off-diagonal element MM24 of ± 0.49 at 60° and 120° azimuthal angles. These observations are in accord with the simulated sensitivity analysis. For example, the strongest response of change in feature dimensions and LER is observed for MM24 off-diagonal element at 60° azimuthal angle.

The azimuthal dependence of the MSE value is observed for the Si fin model without LER. The MSE value is least for the 0° azimuthal angle, increases for the subsequent azimuthal angles and is maximum for the data collected at 60° azimuthal angle. MSE value decreases for data collected at 70°, 80°, and 90° azimuthal angles but their value is still larger than MSE obtained for data collected from 0 - 45° azimuthal angle as seen in figure 5.10 (b). Large differences between fit qualities at different azimuths indicate that the model does not include critical aspects of the real structure. Hence optimization of the
scatterometry model is necessary. The azimuthal angular dependence of the MSE data obtained using the Si fin model without LER is used to diagnose the presence of pattern imperfections in the line array.

**Figure 5.9** Difference between experimental and generated MMSE data obtained after regression based analysis for data collected at 0° - 180° azimuthal angles for 65° incident angle carried out with the help of Si fin scatterometry model without LER.

**Figure 5.10 (a)** Average MM intensity difference of individual MM elements at each azimuth from 0° to 90° azimuthal angles obtained for scatterometry model without LER.

**Figure 5.10 (b)** MSE values obtained after regression based analysis carried out with the help of scatterometry model without LER for data collected at azimuths from 0° - 180°.
Three different scatterometry models are used for the scatterometry analysis and evaluation of the LER in the Si fin samples: (a) Si fins with sidewalls having a layer with optical properties modeled using an effective medium approximation (EMA), and two multi-parameter Si fin models with periodic (b) triangular-shaped edges and (c) rectangular-shaped edges, as seen in figures 5.11 (a), 5.11 (b), and 5.11 (c), respectively. Each scatterometry model has its advantages and disadvantages. For example, EMA based Si fin model has the least number of floating parameters while the reconstructed profiles in multi-parameter model helps in extracting an average profile of the LER features. The multi-parameter model with rectangular-shaped edges can be reconstructed in such a way that LER features have correlated and anti-correlated edges. But due to software limitations, the reconstructed multi-parameter model with triangular-shaped edges can only have anti-correlated edges.

![Figure 5.11 (a)](image1.png) Side view and top view of the EMA based Si fin model.

![Figure 5.11 (b)](image2.png) Side view and top view of the multi-parameter Si fin model with triangular-shaped edges.

![Figure 5.11 (c)](image3.png) Side view and top view of the multi-parameter Si fin model with rectangular-shaped edges.
Table 5.1 Floating parameters, best fit parameters for all the scatterometry models and its average MSE value.

<table>
<thead>
<tr>
<th>Model</th>
<th>Si fins</th>
<th>Floating parameters (nm)</th>
<th>SiN layer</th>
<th>Average MSE value (Azimuth 0-90°) and parameters obtained after scatterometry analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si fin model without LER</td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD</td>
<td>22.32 nm</td>
</tr>
<tr>
<td></td>
<td>Bottom CD</td>
<td>50-70 nm</td>
<td>Height</td>
<td>13.5 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>5-15 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td>EMA based Si fin model</td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD</td>
<td>22.32 nm</td>
</tr>
<tr>
<td></td>
<td>Bottom CD</td>
<td>50-70 nm</td>
<td>Height</td>
<td>13.5 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>5-15 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td>Multi-parameter model (triangular shaped edges)</td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD</td>
<td>22.32 nm</td>
</tr>
<tr>
<td></td>
<td>Bottom CD</td>
<td>50-70 nm</td>
<td>Height</td>
<td>13.5 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>5-15 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td>Multi-parameter model (rectangular shaped edges)</td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD</td>
<td>22.32 nm</td>
</tr>
<tr>
<td></td>
<td>Bottom CD</td>
<td>50-70 nm</td>
<td>Height</td>
<td>13.5 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>5-15 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
<tr>
<td></td>
<td>Top CD</td>
<td>9.18 nm</td>
<td>Bottom CD coupled to Top CD of Si fins</td>
<td>15-25 nm</td>
</tr>
</tbody>
</table>

Model verification is performed by examining difference between generated and experimental spectra as well as MSE values obtained at different azimuthal angles after model fitting. The inverse problem approach is carried out in several steps using regression based data analysis. For example, the first step in fitting the multi-parameter model is to fix the best-fit parameters for the Si fin model without LER and then add LER to that optical model. Incorporating 1 nm LER with spatial period of 6 nm is incorporated in the Si fin model, decreased the MSE at 90° azimuthal angle from 10.8 to 8.65. LER amplitude is increased from 1 nm to 5 nm with small step size of 0.5 nm. The MSE value decreased from 8.65 to 6.97 when LER amplitude is increased from 1 nm to 3.5 nm. Further increasing LER amplitude increased the MSE value. Similarly LER spatial period is increased from 6 - 84 nm with step size of 6 nm. The MSE value decreased from 6.97 to 5.1 when LER spatial period dimensions are increased from 6 nm.
to 48 nm, increasing the LER spatial period value further increased the MSE value. Finally, all the parameters are allowed to float while fitting the generated data to experimental data and the least MSE is obtained for the feature parameters seen in Table 5.1.

Similar approach is used for the EMA based Si fin model and the multi-parameter model (triangular-shaped edges). Incorporating LER features with correlated edges in the multi-parameter model (rectangular-shaped edges) did not improve the MSE value and hence further analysis is only carried out for the anti-correlated edges. Out of all the three models the multi-parameter model (triangular-shaped edges) has the best average MSE value and its MSE value is not sensitive to change in azimuthal angle as seen in figure 5.12. Final profile of this model and the difference in generated and experimental data are seen in figure 5.13.

![Figure 5.12](image.png)

**Figure 5.12** MSE values obtained for different scatterometry models at azimuths from 0-90°.
In order to validate the results obtained from scatterometry analysis, PSD analysis of top down SEM images of Si fins acquired at five different positions in a 2 x 2 mm macro as seen in figure 5.2 is carried out using SuMMIT software of EUV Technology Corporation. For a measured edge deviation $\Delta(y)$, where $y$ represents the different points along the line where the edge is measured, the spatial period behavior is analyzed by examining its Fourier transform. A convenient way of describing this frequency behavior is through the power spectral density (PSD), defined as the square of the magnitude of the edge deviation Fourier transform as seen in equation:\(^\text{12}\)

$$PSD(f) = \left| \int_{-\infty}^{\infty} \Delta(y) e^{-i2\pi fy} dy \right|^2$$ \hspace{1cm} (5.1)

A simple model for roughness correlation is to assume that very close points are...
perfectly correlated, and then the degree of correlation falls off exponentially with
distance as described in equation: \(^{12}\)

\[
R(\tau) = \sigma_{LER}^2 e^{-\left(\frac{\tau}{L_c}\right)^{2\alpha}},
\]

(5.2)

where \(R(\tau)\) is correlation function, \(\tau\) is the distance between two points along the line,
PSD is the Fourier transform of the correlation function, \(\sigma_{LER}\) is the magnitude of the
LER, \(L_c\) is called the correlation length, and \(\alpha\) is called the roughness exponent.\(^{12}\) It is
important to note that correlation length is not the average spatial period value of the
LER features. The correlation length is determined from the PSD based on the effective
roughness bandwidth represented by the PSD (point at which the PSD curve goes from
straight to linear-falling off region). About 90\% of the roughness is contained in periods
that are longer than the correlation length and the exact fraction depends on the roughness
exponent value, which is essentially a measure of the slope of the linear-falling off region
of the PSD.

![Figure 5.14 (a) The averaged PSD plot (LER (3\(\sigma\)) = 4.5 nm, correlation length = 32.9 nm,
and roughness exponent = 0.67).](image1)

![Figure 5.14 (b) The averaged PSD plot (LWR (3\(\sigma\)) = 3 nm, correlation length = 21.01 nm,
and roughness exponent = 0.52).](image2)

It has been previously reported that PSDs of many line-space patterns (here, \(~20\) in
each SEM image) must be averaged to reduce random errors and all three PSD
parameters (\(\sigma\), \(L_c\), and \(\alpha\)) must be reported, as all of them are essential for understand
line-edge roughness.\(^{13,14,15}\) The advanced LER tool in SuMMIT software is used to obtain
PSD LER and LWR parameters for the averaged PSD plot of all the lines in the SEM image. The PSD LER and LWR parameters for each SEM image acquired at five different positions in a macro are seen in Table 5.2. PSD LER plot (average of all lines), and PSD LWR plot (average of all lines) for the SEM image acquired at the center of the macro, is seen in figure 5.14 (a) and 5.14 (b), respectively. The correlation plot of LER values acquired from scatterometry analysis and PSD analysis of MMSE data and SEM images, respectively acquired at five different positions (four corners and center) in a 2 x 2 mm macro, is seen in figure 5.15.

Table 5.2 LER results obtained from PSD and scatterometry analysis.

<table>
<thead>
<tr>
<th>LER PSD Parameters</th>
<th>Position (2x2 mm macro)</th>
<th>Average value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Top right</td>
<td>Top left</td>
</tr>
<tr>
<td>LER (3σ)</td>
<td>4.3 nm</td>
<td>4.7 nm</td>
</tr>
<tr>
<td>Correlation length</td>
<td>28.5 nm</td>
<td>40.4 nm</td>
</tr>
<tr>
<td>Roughness exponent</td>
<td>0.58</td>
<td>0.64</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>LWR PSD Parameters</th>
<th>Position (2x2 mm macro)</th>
<th>Average value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Top right</td>
<td>Top left</td>
</tr>
<tr>
<td>LWR (3σ)</td>
<td>3.6 nm</td>
<td>3.1 nm</td>
</tr>
<tr>
<td>Correlation length</td>
<td>15.4 nm</td>
<td>25.7 nm</td>
</tr>
<tr>
<td>Roughness exponent</td>
<td>0.53</td>
<td>0.62</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Scatterometry results</th>
<th>Position (2x2 mm macro)</th>
<th>Average value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LER amplitude</td>
<td>Top right</td>
<td>Top left</td>
</tr>
<tr>
<td></td>
<td>3.1 nm</td>
<td>3.9 nm</td>
</tr>
<tr>
<td>LER spatial period</td>
<td>46 nm</td>
<td>51 nm</td>
</tr>
</tbody>
</table>

Figure 5.15 Correlation plot of LER values at five different spots (four corners and centre) on 2 x 2 mm macro obtained from PSD and scatterometry analysis.
5.5 References


Chapter VI

Optical CD Metrology of 15 nm CD contact holes fabricated using DSA contact hole shrink process

This chapter presents a modeling and simulation study of MMSE based scatterometry for contact hole structures fabricated using a templated DSA flow as seen in figure 1.8. Optical properties of PS, PMMA, Si-ARC, and OPL materials in the DSA graphoepitaxy contact hole stack are obtained by acquiring traditional ellipsometry data over a spectral range from 150 - 1000 nm using a VUV-VASE® Woollam spectroscopic ellipsometer of the post PMMA etch DSA contact hole sample. Data is collected from their respective blanket (non-patterned) films that are processed in the same manner. These optical properties are used in the scatterometry models of different templated contact hole structures. Simulated optical responses of MM elements are obtained with different measurement configurations, such as changing angle of incidence, azimuthal angle as well as varying feature dimensions. Sensitivity analysis is carried out by comparing the optical responses generated by allowing each grating shape parameter to vary in discrete steps over a certain range. MMSE based scatterometry’s sensitivity to different DSA contact hole templates and various DSA induced defects are also investigated.

MMSE experimental data is collected from different guide CD macros of both pre-DSA and post-DSA wafer over a spectral range from 245 - 1000 nm using a J.A. Woollam RC2® spectroscopic ellipsometer. A regression-based approach is used to calculate the guide CD, DSA CD, height of the PS cylinder, thicknesses of underlying
layers and contact edge roughness (CER) of the DSA contact hole sample. The results obtained from scatterometry analysis are compared to the results obtained from imaging analysis of top down CD SEM images, which is carried out with the help of contact analysis recipe tool in SuMMIT software.

6.1 Simulation and results

6.1.1 Simulations and sensitivity analysis for circular one-hole templates

The dimensional and material information for the scatterometry model of the circular one-hole template is based on literature.\textsuperscript{1,2} The simulations are performed for incident angles from 30° to 70° and azimuthal angles from 0° to 90° in the wavelength range 150 - 1000 nm with following parameters of the stack on silicon substrate: pitch values in x and y direction; $P_x = P_y = 90$ nm, Guide pattern CD = 60 nm, DSA CD = 20 nm, Si-ARC thickness; $T_{ARC} = 20$ nm, OPL thickness; $T_{OPL} = 60$ nm, and PMMA wetting layer of 1.5 nm as seen in figure 6.1. The curves in figure 6.2 show simulated MM optical response at 22.5° azimuthal angle for selected incident angles. It is important to note that the 15 nm thick underlying layers of SiO$_2$ and TiN below the guiding template of OPL and Si-ARC present in the focus-exposure matrix (FEM) samples are not incorporated in the scatterometry models used for sensitivity analysis. Incorporating these layers in the model does not impact the
sensitivity of MMSE to DSA contact hole structures’ feature dimensions. However, correlation between the thickness of the underlying layers and other feature dimensions is high. The number of floating parameters is reduced by determining the underlying layer thicknesses utilizing transmission electron microscope (TEM) cross-section images and fixing the associated parameter in the scatterometry model.

![Generated optical spectra of individual MM elements at 22.5° azimuth for 35°, 45°, 55°, and 65° incident angles.](image)

**Figure 6.2** Generated optical spectra of individual MM elements at 22.5° azimuth for 35°, 45°, 55°, and 65° incident angles.

It is observed that the calculated optical spectra of each MM element change significantly with angle of incidence. As explained before, MM can contain up to 16 independent parameters for each measurement configuration, compared to the traditional spectroscopic ellipsometry with only 2 measured parameters. However, in the case of a
symmetrical contact hole structure, there are only seven independent MM elements in experimental or theoretically generated optical spectra. Mueller element pairs M12 and M21, M14 and M41, M24 and M42, and M33 and M44 are symmetric while Mueller element pairs M13 and M31, M23 and M32, and M34 and M43 are anti-symmetric. The symmetry-antisymmetry properties associated with MM technique provide an excellent means of measuring and understanding any asymmetry present in the structure. This is further described in section 6.1.2.

As discussed in chapter 3, due to conical diffraction the intensity of off-diagonal blocks of the MM will be non-zero for DSA contact hole structures at azimuthal angles other than 0°, 45°, and 90°. However, it is observed that the simulated off-diagonal elements for DSA contact hole structures are non-zero only in the wavelength range from 150 - 300 nm as seen in figure 6.3. The intensity of off-diagonal elements is low for contact hole structures as compared to line-space patterns due to low optical contrast in the wavelength region from 300 - 1000 nm. The extinction coefficient values of PS, PMMA and Si-ARC materials are non-zero only in the wavelength region below 300 nm, i.e. above 300 nm these materials are transparent. In addition, the difference in refractive indices of the above-mentioned materials is only about 0.1 between 300 - 1000 nm. To observe the difference in response of the individual elements to changes in azimuthal angle, the simulated optical spectra for each azimuth is subtracted from the optical spectra calculated for 0° azimuth. These calculated values are defined as sensitivities of MM elements to change in azimuthal angles for 65° incident angle as plotted in figure 6.3.
Scatterometry models with varying guide CD, DSA CD, and PMMA wetting layer width are seen in figure 6.4. The curves in figure 6.5 show the simulated MM optical spectra for DSA contact hole scatterometry models with guide CD’s of 45 nm, 60 nm, and 75 nm and corresponding DSA CD’s of 15 nm, 20 nm, and 25 nm. PMMA wetting layer width is fixed at 1.5 nm in each scatterometry model.\(^3\)

Figure 6.4 Scatterometry model for the DSA contact hole structures with varying guide CD, DSA CD, and PMMA wetting layer width.
In order to observe the individual response of change in guide CD, DSA CD, and PMMA wetting layer width on the optical spectra of each MM element, the simulated optical spectra for contact hole model in which one of the parameter is varied is subtracted from the optical spectra obtained for the reference model seen in figure 6.1. These calculated values are defined as sensitivities of MM elements to change in guide CD, DSA CD, and PMMA width values. It is observed in figure 6.6 that varying guide CD, DSA CD, and PMMA wetting layer width influence the MM elements response. Furthermore, the individual responses of the MM elements to guide CD, DSA CD, and PMMA wetting layer width variations are different. For example there is a blue shift as well as a decrease in intensity of the MM12 optical spectra peaks observed at 400 nm when either the DSA CD or guide CD values increase. In contrast, a red shift and increase in intensity of the MM12 peak is observed when PMMA wetting layer width increases. Figure 6.7 shows the average difference of the calculated MM optical spectra for individual on-diagonal elements in the wavelength region of 150 - 800 nm, with respect to the reference structure seen in figure 6.1, when either the DSA CD, guide CD,
or the PMMA wetting layer width is changed. It is observed that MM elements have higher sensitivity to guide CD deviation in comparison to DSA CD and guide CD deviations. In addition, it is observed that the impact of guide CD, DSA CD, and PMMA wetting layer width variations on the on-diagonal MM elements is approximately 10 times stronger than the off-diagonal elements.

Figure 6.6 Sensitivity of MM elements to change in guide CD, DSA CD and PMMA width values.

Figure 6.7 Average difference in MM intensity calculated in the wavelength range from 150 - 800 nm when only one of the DSA CD, guide CD or PMMA wetting layer width parameter is varied.

The scatterometry models of post-PMMA removal DSA contact hole structure with
varying DSA CD values are seen in figure 6.8 (a). Figure 6.8 (b) shows the average the MM intensity differences in the wavelength range from 150 - 800 nm for individual on-diagonal elements when the DSA CD is varied with respect to the reference structure (20 nm DSA CD). The MM elements have comparatively higher sensitivity to DSA CD for the PMMA etched vs. unetched DSA contact hole structure.  

6.1.2 Simulations of DSA induced defects in circular one-hole templates

Detection of DSA unique defects is key to reducing defect density for eventual manufacturability and production use. Scatterometry simulations are done for several types of defect structures such as hole placement inaccuracy, missing vias, and process induced defects, for example an increase in DSA CD dimensions after etching PMMA away.  

The simulated optical spectra for scatterometry models with defects are subtracted from the optical spectra calculated for scatterometry models without any defects. These calculated values are defined as sensitivities of MM elements.

The spot size of a light beam used for spectroscopic ellipsometry is typically several millimeters, leading to the low spatial resolution of the measurement. In order to improve
spatial resolution, focusing optics with appropriate optical elements can be used to
decrease the spot size of ellipsometers. Ellipsometers with spot size as low as \( \sim 15 \, \mu m \) are
now available commercially.\(^{6}\) The spot size of the laboratory RC2\(^{6}\) Woollam ellipsometer
used to characterize contact hole can be reduced to \( \sim 200 \, \mu m \times \sim 200 \, \mu m \), with the help of
the focusing optics. If the pitch of contact holes is 90 nm, then experimental data
measurements will include data from \( 8.8 \times 10^7 \) contact holes. Detecting a single missing
via from \( 8.8 \times 10^7 \) contact holes is not possible. Extending scatterometry to measure the
position of local process induced defectivity is extremely challenging but possible if
MMSE data is acquired by scanning the light probe of smaller spot-size across the wafer
and measuring the difference in the data acquired from different spots from the wafer.

![Figure 6.9](image)

**Figure 6.9** Top down view of the scatterometry model with 56 DSA contact holes with one to
five missing vias (left to right).

![Figure 6.10](image)

**Figure 6.10** Sensitivity of calculated MM elements to presence of missing via defect in
DSA contact holes.

A scatterometry model with a much larger field of view is created. It consists of 56
DSA contact holes and missing vias are incorporated in these models as seen in figure 6.9. The optical properties of the missing via are modeled using an effective medium approximation (EMA) of 70% PS and 30% PMMA. Sensitivity of MM elements to presence of missing vias in the scatterometry model with 56 DSA contact holes is seen in figure 6.10. Each curve corresponds to number of missing vias in the array of 56 contact holes and distinct differences in calculated optical spectra of each individual MM element are observed only in the wavelength region of 150 - 250 nm. For example, an increase in number of missing vias in the array leads to a red shift and a decrease in the associated MM12 spectral peaks observed near 200 nm. It is important to note that there is a trade-off between smaller spot size and amount of noise in experimental data acquired with the help of an ellipsometer. Also, the small spot size of the incident beam is not considered in these calculations.

![Figure 6.11](image)

**Figure 6.11** Scatterometry model for the DSA contact hole structures without hole placement errors (left) and with 0.5 nm hole placement errors in 80% holes in varying directions (right).

Hole placement inaccuracy in the DSA contact hole samples of around 1 - 2 nm have been reported earlier. To measure the sensitivity of MM elements to placement error, the center of the PMMA cylinders in the DSA contact hole model is shifted by 0.5 nm, 1 nm, and 1.5 nm in varying directions as seen in figure 6.11 and MM optical spectra is generated for each configuration. Differences in generated MM optical spectra with
increase in amplitude of hole placement error is seen in figure 6.12. For example, decrease in intensity of the MM12 peak observed at 400 nm with increase in amplitude of the hole placement errors from 0 nm to 1.5 nm. But the magnitude of this change in the spectra is significantly small it is estimated that the measurement accuracy has to be on the order of 0.001 for the detection of hole placement inaccuracy. The accuracy of the MM elements obtained by the laboratory ellipsometer which is used to characterize contact hole structures is ~0.003.

![Figure 6.12](image)

**Figure 6.12** Sensitivity of calculated MM elements to hole placement inaccuracy defects in DSA contact holes.

As mentioned earlier for symmetrical profile MM coefficients obey symmetry-antisymmetry relations. But for asymmetrical profiles in the case of conical diffraction symmetry-antisymmetry are generally not valid as seen in figure 6.13. Overlay errors in line space gratings are characterized with the help of the symmetry breaking term as described in equation 6.2.\(^5\) Due to the isotropic nature of contact hole structures, low intensity off-diagonal elements are obtained and consequently the value of the symmetry breaking term is small when hole placement inaccuracy is duplicated in the scatterometry model.
For symmetric profiles: 
\[ \text{MM13} + \text{MM31} = \text{MM23} + \text{MM32} = 0, \]  
\[ \text{and} \]
\[ (6.1) \]

for asymmetric profiles: 
\[ \text{MM13} + \text{MM31} = C \]  
\[ \text{and} \]
\[ \text{MM23} + \text{MM32} = D. \]
\[ (6.2) \]

**Figure 6.13** Calculated spectra of the combination of two MM elements (MM13 + MM31 and MM23 + MM32). Each curve corresponds to a different shift of holes in the +/- 1.5 nm.

### 6.1.3 Simulations and sensitivity analysis of multiple hole templates

The natural symmetry and feature size of different DSA patterns can be controlled by adjusting the shape, size, and density of guiding topographical templates with sizes comparable to the block copolymer natural pitch. A larger template could be used to guide the formation of multiple DSA holes with same CD and center-to-center distance. Five templates seen in figure 6.14 are reported as feasible templates for DSA contact hole patterning technique.\(^9\) Use of these small topographical templates to fabricate contact holes for SRAM, DRAM, and NAND circuits has been demonstrated.\(^7,10\) Scatterometry models for each of these different templates are prepared and MM optical responses for these structures are generated.
Distinct differences in the simulated optical spectra of MM elements for each template are observed. For example, the MM12 spectral peak varies from template to template. A blue shift in MM12 peak (figure 6.5) is observed when the guide CD and DSA CD values are increased but the red shift in MM12 peak as seen in figure 6.15 are related to increase...
in pitch values of the templates. The intensity of off-diagonal elements for all the feasible DSA templates is zero at 0° and 90° azimuths due to symmetry along the direction of incident light, except the diagonal two-hole template. The off diagonal intensity for the diagonal two-hole template is maximum at 0° and 90° azimuth and minimum at 45° azimuth. Also the intensity of the off-diagonal elements at 45° azimuth are non-zero for all the DSA templates except the circular one-hole template. The simulated off-diagonal elements for multiple DSA contact hole structures are non-zero only in the wavelength range from 150 - 550 nm. In addition it is seen that as the pitch value increases, the intensity of off-diagonal MM elements tend towards zero with a minimum observed for the square four-hole template.

6.2 Experimental data and scatterometry results

The DSA process window response is first characterized by acquiring CD-SEM images at each macro in the two wafers (pre-DSA and post-DSA), fabricated with varying focus-exposure conditions. Image analysis of these top down CD SEM images is carried out with the help of the contact analysis recipe tool in SuMMIT software in order to extract profile dimensions like guide CD, DSA CD, and contact edge roughness (CER). The pre-DSA FEM wafer is a bilayer stack of guiding pattern (with varying guide CDs) of Si-ARC and OPL on the underlying 15 nm thick layers of SiO₂, TiN, and SiO₂. The post-DSA FEM wafer is a post PMMA etch sample with PS column in the bilayer stack of guiding pattern (with varying guide CDs) of Si-ARC and OPL on the underlying 15 nm thick layers of SiO₂, TiN, and SiO₂. MMSE experimental data is then collected from different guide CD macros of both pre-DSA and post-DSA wafer at 0°, 22.5°, and
45° azimuthal angles over a spectral range from 245 - 1000 nm using a J.A. Woollam RC2 spectroscopic ellipsometer for scatterometry analysis. The angle of incidence for all the measurements is fixed at 65° for focusing probe measurements. Focusing optics and camera are used to center the incident beam spot (200 μm) inside a 2x2 mm square macro. MMSE experimental data acquired at 0° azimuth for 65° incident angle and CD-SEM images collected from varying guide CD macros of pre-DSA FEM wafer are seen in figure 6.16 (a) and 6.16 (b), respectively. A clear blue shift is observed in the optical spectra of on-diagonal MM elements with increase in guide CD of the guiding patterns. For example, the peak shifts from 700 nm to 550 nm as well as a decrease in intensity of the MM12 optical spectra peaks with increase in guide CD value is observed in figure 6.16 (a).

![Graph](image.png)

**Figure 6.16 (a)** Experimental optical spectra of on diagonal MM elements acquired from varying guide CD macros of pre-DSA sample at 0° azimuth for 65° incident angle.

<table>
<thead>
<tr>
<th>Macro</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
<th>j</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exposure (mJ/cm²)</td>
<td>69</td>
<td>71</td>
<td>73</td>
<td>75</td>
<td>77</td>
<td>81</td>
<td>83</td>
<td>85</td>
<td>87</td>
<td>89</td>
</tr>
<tr>
<td>Focus (μm)</td>
<td>0.040</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Guide CD</td>
<td>50.3 nm</td>
<td>47.7 nm</td>
<td>46.8 nm</td>
<td>44.9 nm</td>
<td>42.5 nm</td>
<td>40.6 nm</td>
<td>39.5 nm</td>
<td>38 nm</td>
<td>36.9 nm</td>
<td>37.2 nm</td>
</tr>
</tbody>
</table>

**Figure 6.16 (b)** CDSEM images of different macros of pre-DSA sample for the same focus value and varying exposure values. The guide CD values are obtained from imaging analysis carried out with the help of SuMMIT software.
MMSE experimental data acquired at 0° azimuth and 65° incident angle and CD-SEM images collected from varying guide CD macros of post-DSA FEM wafer are seen in 6.17 (a) and 6.17 (b), respectively. Defects like bridging defects, missing vias, and CER are observed in some of the top down CD-SEM images of the macros in post-DSA sample. The amount of defects observed in the macros with smaller guide CD of the guiding patterns are higher than that for the macros with larger guide CD. A clear red shift is observed in the experimental optical spectra of on-diagonal MM elements acquired from macro with 44.9 nm guide CD of post-DSA wafer with respect to the
experimental optical spectra of on-diagonal MM elements acquired from the same guide CD macro of pre-DSA sample, as seen in figure 6.18. In addition, a similar blue shift is observed in the optical spectra of on-diagonal MM elements with increase in guide CD of the guiding patterns in macros of post-DSA sample. For both pre-DSA and post-DSA samples, the intensity of all the off-diagonal MM elements is very close to zero for data collected at 0°, 22.5°, and 45° azimuthal angles. As explained earlier, the influence of change in azimuthal angle on experimentally collected optical spectra of all the MM elements is small due to sample symmetry and low optical contrast in the wavelength region from 250 - 1000 nm. Both of these observations; the blue shift in optical spectra of on-diagonal MM elements with increase in guide CD of the guiding patterns and small impact of azimuthal angle on the optical spectra in the wavelength region from 250 - 1000 nm, are in accordance with the simulated sensitivity study reported in section 6.1.

![Figure 6.18 Experimental optical spectra of on-diagonal MM elements acquired from the same guide CD macro (44.9 nm) of pre-DSA and post-DSA sample at 0° azimuth for 65° incident angle.](image)

Figure 6.18 Experimental optical spectra of on-diagonal MM elements acquired from the same guide CD macro (44.9 nm) of pre-DSA and post-DSA sample at 0° azimuth for 65° incident angle.
Three-dimensional contact hole models for pre-DSA and post-DSA samples constructed with the help of NanoDiffract® software are seen in figure 6.19 (a) and 6.19 (b), respectively. Optical response obtained from these multi-parameter scatterometry model strategies are fit to the experimentally collected optical spectra using a regression-based approach to extract profile dimensions like guide CD, DSA CD, CER, thickness of the underlying layers and height of PS column. There is high correlation between all these fitting parameters and hence some of the parameters in the structure measured at an earlier step, the common values and profiles are inserted into the model of the structure at the later step in the process. This approach is used to reduce the number of floating parameters in the model. For example, thickness information of the underlying film stack is obtained from cross-sectional TEM image and hence the thickness values of the underlying stack are fixed and only the height and guide CD values of guiding patterns and width of EMA layer is floated in the model prepared for pre-DSA sample. The
sidewalls of guide columns are modeled using EMA of 50% Si-ARC and 50% void and of 50% OPL and 50% void. The EMA is used to characterize the CER in guide templates observed in the top-down CD-SEM images. The floating parameters in the model for post-DSA structure are DSA CD, height of the PS column and width of the EMA layer (50% PS and 50% void). Also, the height of the Si-ARC guiding pattern is floated in order to incorporate the etch effect.

Table 6.1 DSA contact hole parameters obtained from imaging and scatterometry analysis.

<table>
<thead>
<tr>
<th>Macro</th>
<th>Parameters obtained after CD SEM imaging analysis (SuMMIT)</th>
<th>Parameters obtained after regression-based scatterometry analysis (Nanodiffract)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Top CD</td>
<td>CER</td>
</tr>
<tr>
<td>a</td>
<td>50.3(6) nm</td>
<td>23.3 nm</td>
</tr>
<tr>
<td>b</td>
<td>47.7(4) nm</td>
<td>22.8 nm</td>
</tr>
<tr>
<td>c</td>
<td>46.8(2) nm</td>
<td>22.7 nm</td>
</tr>
<tr>
<td>d</td>
<td>44.9(3) nm</td>
<td>22.4 nm</td>
</tr>
<tr>
<td>e</td>
<td>42.5 nm</td>
<td>22.9 nm</td>
</tr>
<tr>
<td>f</td>
<td>40.6 nm</td>
<td>22.4 nm</td>
</tr>
<tr>
<td>g</td>
<td>39.4(7) nm</td>
<td>22.8 nm</td>
</tr>
<tr>
<td>h</td>
<td>38.0(5) nm</td>
<td>22.6 nm</td>
</tr>
<tr>
<td>i</td>
<td>36.9(2) nm</td>
<td>23.1 nm</td>
</tr>
<tr>
<td>j</td>
<td>37.2(8) nm</td>
<td>22.4 nm</td>
</tr>
</tbody>
</table>

Figure 6.20 Correlation plots of guide CD, guide CER, DSA CD, and DSA CER (left to right) values obtained from imaging and scatterometry analysis.

Guide CD, DSA CD, and CER values obtained from scatterometry analysis and imaging analysis are seen in Table 6.1 and the correlation plot for the same is seen in figure 21.11 CER (3σ) values are obtained using advanced contact toolbox in the SuMMIT software. A high correlation factor is obtained between extracted values of guide CD,
guide CER, DSA CD, and DSA CER obtained from scatterometry analysis and CD-SEM imaging analysis. Thus, EMA based layers can be used to calculate CER in contact hole structures. Here, scatterometry is found to be insensitive to the process induced defects like missing vias, hole-placement inaccuracy, and bridging defects. As explained in section 6.1.2, the detection of the presence of a missing contact, hole-placement inaccuracy or bridging defects using MMSE based scatterometry is challenging, requiring better focusing optics than available for the laboratory system and capability to acquire data in VUV and UV wavelength region.

6.3 References


Chapter VII

Conclusion and future directions

7.1 Optical CD Metrology of PS-b-PMMA and PS line-space patterns

MMSE scatterometry has the capability to optically characterize PS-b-PMMA patterns and PS line-patterns with CD ~14 nm. MMSE based scatterometry has the capability of measuring important feature dimensions of un-etched polymer samples and is able to differentiate between perfectly oriented and completely disoriented PS-b-PMMA patterns, but sensitivity to partially ordered PS-b-PMMA patterns is not observed for the un-etched samples due to the isotropic nature of PS-b-PMMA patterns or very similar optical properties of PS and PMMA materials in the wavelength range of 250 - 1000 nm.

Scatterometry is more effective in characterizing the line-space patterns where part of the polymer (PMMA) has been selectively etched. This is determined by comparing scatterometry wafer maps for un-etched samples, etched samples, and CDSEM wafer map. Sensitivity to structural parameters such as line-width, line-shape, and even the underlying guide pitch is observed for etched samples. Samples with different guide pattern pitches are all distinguished for fully aligned line patterns and additionally amount of disorder in patterns is measured. It is observed that lower wavelengths are more sensitive to the alignment of PS line space patterns for the 28 nm pitch PS line-space patterns. Process control for BCP DSA based patterning requires advances in CD metrology and defect detection. The spectral comparison based on optical anisotropy and depolarization is found to be sensitive to DSA pattern defectivity. Slight imperfections in the PS line-space patterns are detected by changes in depolarization values. The changes
in MSE, anisotropy, and depolarization values are used as a quick and efficient method to judge the degree of alignment of the DSA patterns across wafer without substantial CD-SEM resources.

**7.2 Optical CD Metrology and LER measurements of Si fins**

Simulations of Si fin structures show that MM ellipsometry for the conical diffraction mode is more sensitive to the feature details of Si fins than MM ellipsometry for planar diffraction or classical spectroscopic ellipsometry. Feature dimensions such as top and bottom CD, line-shape, pitch, SWA, height as well as LER influence the MM elements response. Also sensitivity of MM elements is a function of the optical properties of the material, frequency of LER/LWR features, and pitch, height, CD, and SWA of the Si fins. MM elements sensitivity to LER increases when the CD to pitch ratio of the line-space patterns increases, height of line-space patterns increases and when SWA value of the fins is near 90°, i.e. when Si fins are straight and not trapezoidal. Also the materials’ optical properties affect the sensitivity of MM elements to LER. Sensitivity to LER in photoresist line-space patterns is less than that of LER in Si fins. MM coefficients in the UV and VUV spectral ranges are more sensitive to feature dimensions of photoresist line-space patterns as shorter wavelength are more sensitive to nanoscale changes in LER and the photoresist materials start absorbing light in this wavelength range.

The Mueller spectrum taken at each individual azimuth is sufficient to reconstruct the profile by fitting data with a simple model but data acquired at different angles of incidence and azimuthal angles provide more information and build a more robust scatterometry model. For example, the intensity difference between experimental and
generated data is least at 0° azimuth for the Si fin model without LER but scatterometry analysis and MSE values obtained at different azimuthal angles showed that optimization of scatterometry models is necessary. Reconstructed scatterometry models can be used to characterize LER in Si fins as well as photoresist line space patterns. All the reconstructed scatterometry models had lower average MSE values than that obtained for Si fin model without LER. This investigation shows that the off-diagonal MM elements in conical diffraction mode provide additional non-redundant information about Si fin structures that aids in model fitting. The final profile of the reconstructed scatterometry model extracted low frequency LER of 46 nm spatial period with amplitude of 3.6 nm in Si fin samples. The inverse problem approach in this work is time consuming as it is carried out with the help of linearized regression based data analysis. LER inspection is carried out off-line after the sample is prepared. Reconstructed scatterometry models demonstrated in this work to quantify LER must be used to generate data offline and library based search should be carried out as a quick and effective approach for LER measurements in industry, where the size of the library is not a concern and the general profile is known beforehand. In addition, an algorithm can be prepared on the basis of the difference in generated data and experimental data and used in the in-line control method that could monitor and alarm when the LER appears above a certain level.

Although the MSE values obtained using multi-parameter Si fin model (triangular-shaped edges) did not change with azimuthal angle, the average MSE value of 2.81 is a little higher than expected MSE values. This is attributed to the use of periodic LER features and the models’ inability to incorporate the varying height of Si fins as seen in its TEM image. Optimizing features like correlated or anti-correlated edges, unevenness in
the height of the Si fins across the sample and using multiple spatial period edges in the multi-parameter model to get better data fits and lower MSE values can be some of the future steps in this project. Various numerical methods can be used to generate rough edges, surfaces, and volumes that follow the specific PSD parameters of sigma, roughness exponent, and correlation length obtained from PSD analysis of top down images of Si fin samples. These specific rough edges whether correlated or anti-correlated edges with different spatial periods can be incorporated in the scatterometry models with a much larger field of view.

7.3 Optical CD Metrology of DSA contact holes

MMSE based scatterometry simulations of DSA contact hole structures show that MM ellipsometry in the conical diffraction mode is more sensitive to the contact hole feature details than MM ellipsometry for planar diffraction or classical spectroscopic ellipsometry. MM coefficients in the ultraviolet and VUV spectral ranges are more sensitive to feature dimensions of DSA contact hole structure due to the shorter wavelengths compared to visible and infrared. Due to the isotropic nature of DSA contact hole structures or very similar optical properties of Si-ARC, PS, and PMMA materials in the wavelength range of 300 - 1000 nm, the intensity of the off-diagonal elements is low and they are non-zero in the wavelength range of 150 - 300 nm. Hence, the overall sensitivity of the off-diagonal elements to changes in feature dimensions is low, but more information about the sample can be obtained by acquiring data in the wavelength range of 150 - 300 nm at multiple incident and azimuthal angles. The MM elements response is influenced by various feature dimensions like guide CD, DSA CD, PMMA wetting layer,
and guide pattern pitch of DSA contact hole structures and the response to each individual parameters is different. Distinct differences in the on-diagonal and off-diagonal MM elements’ optical spectra for various multi-hole templates with different shapes and size is observed.

The regression-based approach is used to extract feature dimensions like guide CD, DSA CD, CER, height of PS column, and guiding patterns of the pre-DSA and post-DSA contact hole structures. CER in guide patterns and PS column is calculated with the help of EMA based layers. High correlation factor between values obtained from scatterometry analysis and CD-SEM imaging analysis emphasizes that MMSE based scatterometry has the capability to extract profile dimensions of DSA contact hole structures. Symmetry-antisymmetry properties of MM elements can provide some important and non-redundant information about the DSA induced defects. For example, symmetry-antisymmetry relations are not valid when hole-placement inaccuracy is present in contact hole structures. DSA specific defects such as missing vias and hole placement inaccuracy do not scatter much of the incident light and hence, are difficult to detect with conventional inspection methods. From the simulated sensitivities, it is estimated that measurement accuracy on the order of 0.001, improved focusing optics to reduce the spot size of the incident beam and capability to collect data in the UV and VUV region are required for the detection of the DSA specific defects.
APPENDIX I

The rigorous-coupled wave analysis (RCWA) method

RCWA is widely applied for diffraction analysis of periodic nano-structures of arbitrary shapes and dimensions and is based on solutions of Maxwell’s electromagnetic equations. A brief overview of the principle of the RCWA theory for transverse electric (TE) and magnetic (TM) polarization is presented here. TE waves are defined as the case when electric field vector is perpendicular to the plane of incidence, which is defined by the surface/interface normal, and incident light’s wave vector. For TM waves the electric field is parallel to the plane of incidence, i.e. the magnetic field is perpendicular to the plane of incidence.

![Diagram of diffraction](image)

**Figure A1** Schematic of diffraction of incident light by a periodic grating structure (TE wave).

Figure 1 shows the scattered (reflected) light consisting of distinct diffraction orders for incident light at an angle on the grating structure, with the plane of incidence being perpendicular to the gratings. Figure 1 consists of three regions: the incident region, the periodic gratings, and the substrate. Region 1 is free space with permittivity of $\varepsilon_b=1$. 
Region 3 is homogeneous isotropic substrate with permittivity of $\varepsilon_c$. Region 2 is the grating region, a heterogeneous medium whose permittivity is a periodic function of $x$. The permittivity or the dielectric function ($\varepsilon = (n + ik)^2$, where $n$ is the refractive index and $k$ is the extinction coefficient) in the grating stack is $\varepsilon_a$, whereas the dielectric function in the grooves $\varepsilon_b$.

For a TE wave, the normalized incident (y-component) time-harmonic electric field is given by:\textsuperscript{2,3}

$$E = \exp(i\kappa_{1x}x + i\kappa_{1z}z) \hat{y},$$  \hspace{1cm} (A.1)

where $\exp(-i\omega t)$ term has been neglected, $\hat{y}$ is the unit vector for the direction perpendicular to the plane of incidence, $\kappa_{1x}$ and $\kappa_{1z}$ are the $x$-component and $z$-component of the incident wavevector $\kappa_1$, and its magnitude in region 1 and region 3 is given by:

$$\kappa_1 = \frac{2\pi n_1}{\lambda} = \frac{2\pi}{\lambda} = \kappa, \text{ and}$$

$$\kappa_3 = \frac{2\pi n_3}{\lambda} = n_3\kappa, \hspace{1cm} (A.2)$$

where $n_1$ and $n_3$ are the refractive index of the region 1 and medium 3. The $x$-component of the diffracted wave-vectors is given by the Floquet condition as seen in the expression:\textsuperscript{4}

$$\kappa_{x,m} = \frac{2\pi}{\lambda} \left( \sin \theta + \frac{m\lambda}{P} \right),$$  \hspace{1cm} (A.3)

where $m$ is the order of the diffracted wave, $P$ is the pitch of the rectangular gratings, $\theta$ is the angle of incidence, and $\lambda$ is the wavelength of the incident light. Due to phase matching conditions (tangential components of electric and magnetic fields should be continuous across an interface), $\kappa_{x,m}$ value will be same in all the regions.\textsuperscript{2,3} However $\kappa_z$ value will vary. For the first region $\kappa_{z,m}$ can be calculated by:
\[ \kappa^2 = \kappa^2_{x,m} + \kappa^2_{z,m}, \tag{A.4} \]

where \( \kappa^2 \) is the magnitude of the incident wavevector in region 1. The value of \( \kappa_{z,m} \) for the second and third regions can be calculated similarly. And from the equation A.4 it can be observed that if the magnitude of the x-component \( (\kappa_{x,m}) \) of diffracted wave-vector is greater than the magnitude of incident wave-vector, \( (\kappa_{z,m}) \) will be imaginary number and the \( m^{th} \) order diffracted wave will decay exponentially and become an evanescent wave (i.e. for region 1 if \( \kappa_{x,m} > \kappa_1, \kappa_{1,z,m} \) is imaginary).\(^5\)

Total magnitude of electric field in region 1 is given by the superimposition of the incident and reflected waves and in region 3 is given by superimposition of all the transmitted waves as seen in the expressions:\(^2\,^3\)

\[ E_1(x,z) = \exp(i\kappa_{x,x} + i\kappa_{1z,x}) + \sum_m r_m \exp(i\kappa_{x,m} x - i\kappa_{1z,m} z), \text{ and} \]

\[ E_3(x,z) = \sum_m t_m \exp(i\kappa_{x,m} x + i\kappa_{3z,m} (z - d)) \tag{A.5} \]

where \( r_m \) is the reflection coefficient for the interface between region 1 and region 2, \( t_m \) is the transmission coefficient for the wave transmitted through region 2 into region 3, \( m \) is the order of the reflected and transmitted wave, \( d \) is the height of the rectangular gratings, and \( z \) is the position in the substrate. Due to the periodic grating structure, the electric field in the region 2 (heterogeneous medium), must be expanded in terms of its spatial harmonic components and these components must be phase matched with the diffraction orders in the first and third regions. Total magnitude of electric field in region 2 is given by:\(^2\,^3\,^4\)

\[ E_2(x,z) = \sum_m \psi_m(z) \exp(i\kappa_{x,m} x). \tag{A.6} \]

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where $\psi_m$ is the field amplitude for the m\textsuperscript{th} diffraction order. And the periodic function of permittivity with respect to pitch of the rectangular gratings (P), can be expanded in terms of a Fourier series as seen in the expression:\textsuperscript{5}

$$\varepsilon(x) = \sum_u \varepsilon_u \exp\left(\frac{i2u\pi x}{P}\right), \quad (A.7)$$

where $\varepsilon_u$ is the u\textsuperscript{th} Fourier coefficient and is given by:

$$\varepsilon_u = \frac{(\varepsilon_a - \varepsilon_b) \sin(u\phi\pi)}{u\pi}. \quad (A.8)$$

Here $\phi$ is the filling fraction of material in the rectangular gratings. The wave equation for the electric field in non-homogeneous region 2 can be obtained by solving Maxwell’s equations and is given by:\textsuperscript{3}

$$\nabla^2 E_2 + \nabla(E_2 \cdot \nabla \ln \varepsilon) + \nabla \ln \mu \times (\nabla \times E_2) + \kappa^2 \mu \varepsilon E_2 = 0, \quad (A.9)$$

where $E_2$ is along the y-direction and $\nabla \ln \varepsilon$ is non-zero only in the z-direction. So the product $(E_2, \nabla \ln \varepsilon)$ is zero. Also assuming that the medium is non-magnetic ($\mu=1$) the wave equation is now given by the expression:

$$\nabla^2 E_2(x, z) + \kappa^2 \varepsilon(x) E_2(x, z) = 0. \quad (A.10)$$

By substituting equations A.6 and A.7 in equation A.10, the final coupled wave formulation is obtained and given by the expression:\textsuperscript{3}

$$\sum_m \left(\frac{d^2 \psi_m}{dz^2} - \kappa^2 \varepsilon_{x,m} \psi_m + \kappa^2 \sum_p \varepsilon_{m-p} \psi_p\right) \exp(i\kappa_{x,m} x) = 0. \quad (A.11)$$

Equation A.11 is a set of second order coupled difference-differential equations where each space harmonic term is coupled to other terms through the harmonics of the grating.
Similarly, in the TM polarization the incident magnetic field is normal to the plane of incidence. The wave equation for the magnetic field in non-homogeneous region 2 can be obtained by solving Maxwell’s equations. Similar to equation A.6, the magnetic field in region 2 can be expressed by:

\[ H_{2,x} = \frac{i}{\omega \mu} \sum_m \kappa \gamma_m (z) \exp(i \kappa_{x,m} x), \]

and

\[ H_{2,z} = \frac{i}{\omega \mu} \sum_m \kappa \psi_m (z) \exp(i \kappa_{x,m} x), \tag{A.12} \]

where \( \mu \) is the magnetic permeability, \( \omega \) is the angular frequency of light, and \( \gamma \) and \( \psi \) are related by:

\[ \frac{d\psi_m (z)}{dz} = \kappa \gamma_m (z). \tag{A.13} \]

Another relation between \( \gamma \) and \( \psi \) is required in order to solve the above equation and is obtained by substituting equations A.12 and A.6 in the equation:

\[ \nabla \times H - \frac{\partial (\varepsilon E)}{\partial t} = 0, \tag{A.14} \]

which upon expansion yields the following relationship:

\[ \frac{\partial \gamma_m (z)}{\partial t} = \left( \frac{\kappa^2}{k} \psi_m (z) - \kappa \sum_n \varepsilon_{(m-n)} \psi_m (z) \right). \tag{A.15} \]

Solution of equations A.13 and A.15 can be expressed in matrix form as seen in the expression:

\[ \frac{\partial^2 \Psi}{\partial (\kappa z)^2} = [A][\Psi]. \tag{A.16} \]

Here \( \Psi \) is the matrix of \( \psi_m (z) \) and matrix \( A \) is defined by the equation:

\[ A = K^2_x - D, \tag{A.17} \]
where \( K_x \) is a diagonal matrix given by:

\[
K_x (a,a) = \frac{K_x (a-q-1)}{K},
\]

and \( D \) is the matrix formed by the Fourier coefficient of the dielectric function. If the diffraction orders are \( m = 0, \pm 1, \pm 2, \ldots, \pm q \), then \( N \) is the total number of diffraction orders \( (N=2q+1) \) and the size of matrices \( \Psi \), \( A \), and \( D \) are \( N \times N \). Equation A.16 is solved by applying appropriate boundary conditions and carrying out eigenvalue analysis.

The unknown amplitudes of reflection \( (r_m) \) and transmission \( (t_m) \) coefficients of the diffracted waves corresponding to \( m^{th} \) diffraction order can be determined by matching the solutions for all three regions and an exact solution of diffraction of light from the grating structure can be achieved by slicing the gratings into rectangular subdomains. Typically, the number of subdomains varies from 1 to 50 based on the number of the spatial orders, the grating structure, and its dielectric function.

The scattered or diffracted light pattern obtained from RCWA is referred to as an optical response and can be represented in the form of the reflection coefficients \( (r_{pp}, r_{ss}, r_{ps}, \text{and } r_{sp}) \), the traditional ellipsometry parameters \( (\Psi \text{ and } \Delta) \), or the MM elements. The optical response contains the scattered light information from the structure and hence can be used to characterize the details of the grating shape. Reflection coefficients can be determined using the RCWA derivation. The ratio of \( r_{pp} \) and \( r_{ss} \) can be used to determine traditional ellipsometry parameters; \( \Psi \) and \( \Delta \), using the Jones matrix formalism:

\[
\begin{bmatrix}
E_{rp} \\
E_{rs}
\end{bmatrix} =
\begin{bmatrix}
r_{pp} & 0 \\
0 & r_{ss}
\end{bmatrix}
\begin{bmatrix}
E_{ip} \\
E_{is}
\end{bmatrix}
J = r_{ss}
\begin{bmatrix}
r_{pp}/r_{ss} & 0 \\
0 & 1
\end{bmatrix},
\]

(A.19)
where the ratio: \[
\frac{r_{pp}}{r_{ss}} = \left(\frac{E_{rp}}{E_{pp}}\right) \left/ \left(\frac{E_{rs}}{E_{ss}}\right)\right. = \tan \Psi_{pp} e^{-\Delta_{pp}}. \tag{A.20}
\]

Similarly the MM elements can be calculated from reflection coefficients using the Jones-Mueller matrix expression:\textsuperscript{9,10}

\[
M = \begin{bmatrix}
(r_{ss}^* + r_{pp}^* r_{pp} + r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) / 2 & (r_{ss}^* + r_{pp}^* r_{pp} - r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) / 2 & \text{Re}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) & \text{Im}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) \\
(r_{ss}^* + r_{pp}^* r_{pp} + r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) / 2 & (r_{ss}^* + r_{pp}^* r_{pp} - r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) / 2 & \text{Re}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) & \text{Im}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) \\
\text{Re}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) & \text{Re}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) & \text{Re}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) & \text{Im}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) \\
\text{Im}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) & \text{Im}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp}) & \text{Im}(r_{pp}^* r_{pp} + r_{pp}^* r_{pp}) & \text{Re}(r_{pp}^* r_{pp} - r_{pp}^* r_{pp})
\end{bmatrix}, \tag{A.21}
\]

where \( r_{ij}^* \) is the complex conjugate of \( r_{ij} \). It is important to note that the MM elements in the equation A.21 do not contain the depolarization information obtained from experimental MM data.

References


