Electromagnetic ray tracing model for line structures and characterization of advanced alignment marks in photolithography

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**ELECTROMAGNETIC RAY TRACING MODEL FOR
LINE STRUCTURES AND
CHARACTERIZATION OF ADVANCED ALIGNMENT
MARKS IN PHOTOLITHOGRAPHY**

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SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING

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To my parents...

ABSTRACT

Line structures are an essential part in integrated circuit (IC) fabrication. In photolithography, the electromagnetic scattering of line structures is one of the main factors that determine the advancement of the technology node. From the perspective of modeling, a theoretical model to physically understand the scattering phenomenon is necessary for a solid foundation in efficient characterization. When the domain of simulation that needs to be addressed is substantial, an approximate solution is ideal for resource efficient modeling. From the perspective of alignment using line structures, it must meet the stringent overlay budget for new fabrication processes. The robustness of the alignment marks is critical as accurate signal is required to precisely align a masking layer to the previous layer.

The key contribution in this research work is the establishment of a new electromagnetic scattering model for line structures based on a ray tracing approach. This electromagnetic ray tracing (ERT) model provides detailed understanding of every physical field that contributes to the scattering solution, which could not be offered by any other photolithography simulators found in the literature. The ERT model is capable of distinguishing all the geometrical optics and diffracted fields. The diffracted field is required to compensate the discontinuities caused by the geometrical optics field. Prior to the establishment of the ERT model for line structures, the diffraction coefficients for both external and internal regions of a wedge were formulated and studied extensively. The external diffraction coefficient was developed by using Maliuzhinets's impedance approach with the inclusion of higher order in the asymptotic expansion. On the other hand, a heuristic solution was derived for the internal diffraction coefficient by extracting the poles in dual Sommerfeld contour integrals. By exploiting both diffraction coefficients in the

ERT model, the electromagnetic field that causes a disturbance in the amplitude profile for the total solution was identified and explained in detail. The accuracy of the ERT model was also verified by comparing with the finite difference time domain (FDTD) solution. For a single polysilicon line structure with width of 1.66λ (λ is the wavelength) on silicon substrate, the developed ERT model was able to demonstrate amplitude correlation coefficient (ACC) of 0.978 and the maximum amplitude difference, $\Delta|E_z|$ of as low as -0.067. The subwavelength line width of 0.4λ was identified as the limit of the ERT model for the single polysilicon line structure.

The study of alignment marks focuses on their performance to meet the stringent overlay requirement for advanced technology node process. The simulation results obtained from rigorous coupled wave analysis (RCWA) demonstrated that by incorporating small periodic structure into the conventional alignment mark, the reflected diffraction efficiency was improved at the respective order. The experimental works were performed for 90 nm and 0.11 μm processes. It is demonstrated that overlay as low as 9 nm was achieved when 5th order mark was used for the 90 nm technology node front-end-of-line (FEOL) process. Narrow marks for backend-end-of-line (BEOL) process also showed compatible results with the lowest overlay of 10 nm.

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LIST OF ABBREVIATIONS

ACC	Amplitude Correlation Coefficient
AFM	Atomic Force Microscope
ATHENA	Advanced Technology using High Order of Enhancement Alignment
BARC	Bottom Anti-Reflection Coating
BEOL	Back-End-of-Line
CMOS	Complementary Metal Oxide Semiconductor
DE	Diffraction Efficiency
DUV	Deep Ultra-Violet
FDTD	Finite Difference Time Domain
FEOL	Front-End-of-Line
FEM	Finite Element Method
GOs	Geometrical Optics
GPs	Geometrical Poles
GTD	Geometrical Theory of Diffraction
IC	Integrated Circuit
ILD	Interlayer Dielectric
ISB	Incident Shadow Boundary
ITRS	International Technology Roadmap for Semiconductor
NA	Numerical Aperture
NTTL	Not-Through-The-Lens
OAI	Off-axis Illumination
OPC	Optical Proximity Correction

PCC	Phase Correlation Coefficient
PSM	Phase Shifting Mask
RETs	Resolution Enhancement Techniques
RCWA	Rigorous Coupled Wave Analysis
RSB	Reflection Shadow Boundary
SB	Shadow Boundary
SDP	Steepest Decent Path
SEM	Scanning Electron Microscope
SPESA	Signetics/Philips Enhanced SAMPLE Algorithm
SOLID	Simulation of Optical Lithography In 3 Dimensions
SPIE	Society of Photo-Optical Instrumentation Engineers
SPs	Surface Poles
STI	Shallow Trench Isolation
STORM	Simulation TOols for Resist Models
TIS	Transmission Image Sensor
TE	Transverse Electric
TM	Transverse Magnetic
TTL	Through-The-Lens
UAT	Uniform Asymptotic Theory
ULSI	Ultra Large Scale Integration
UTD	Uniform Theory of Diffraction
UV	Ultra-Violet
VLSI	Very Large Scale Integration

LIST OF FUNCTIONS AND SYMBOLS

$\Gamma(\bullet)$	Gamma function
$a(\bullet)$	Inverse of $b(\alpha)$
$b(\bullet)$	Inverse cosine function
$D(\bullet)$	Diffraction coefficient
$F(\bullet)$	Transition function
$H(\bullet)$	Heaviside function
$P_{2\pi}(\bullet)$	Unit rect function
$R(\bullet)$	Fresnel reflection coefficient
$T(\bullet)$	Fresnel transmission coefficient
$\text{gd}(\bullet)$	Gunderman function
$\text{sgn}(\bullet)$	Signum function
ϕ_o	Incident angle measured from wedge surface
ϕ'_o	Incident angle given by $\phi'_o = \bar{p}\pi - \phi_o$
ϕ	Observation angle measured from wedge surface
ϕ'	Observation angle given by $\phi' = \bar{p}\pi - \phi$
ρ	Distance from origin to observation point
ψ_{Φ_1}	Maliuzhinets function
$\bar{\eta}_{\pm}$	Normalized impedance

η_o	Vacuum tilted admittance
η	Tilted admittance
δ	Phase thickness
υ	Amplitude in geometrical optics field
φ	Phase in geometrical optics field
γ	Ratio of refractive index or wave number
ω	Radian frequency
σ	Sigma
λ	Wavelength in vacuum
ε	Permittivity
$\beta^\wedge$	Branch point in β complex plane
$\alpha^\wedge$	Branch point in α complex plane
θ	Incident angle in RCWA
μ_0	Permeability of vacuum
Φ_1	Wedge external angle
Φ_2	Wedge internal angle
τ	Variable in sub diffraction coefficients
κ	Variable in sub diffraction coefficients
j	Given by $j^2 = -1$ for complex number
k	Wave number in free space
k_λ	Wave number for the respective wavelength
k_1	Wave number in dielectric wedge

n_0	Refractive index in free space
n_1	Refractive index of the line structure or wedge
n_e	Effective refractive index
n_r	Refractive index in the ridge
n_g	Refractive index in the groove
$\bar{p}$	Wedge number given by $\bar{p}\pi = 2\Phi_1$
p'	Microstructure grating period
r	Distance between two points
E	Electric field
G	Green's function
H	Magnetic field
J	Operator in UAT
P	Grating period
R_i	Normalized electric field (TE) or magnitude field (TM) amplitude of the i th reflected wave
$S_{1,2}$	Wedge surfaces
T_i	Normalized electric field amplitude (TE) or magnitude field (TM) of the i th transmitted wave
U	Electromagnetic field
Y	Given by the ratio of B/C
Z_o	Free space impedance
$Z_{\pm}$	Impedance at different surfaces
L	Sommerfeld contour integral

$\hat{R}$	Radius for spherical wave
S	Steepest decent path
S	Surface in geometrical analysis for the ERT model
B, C	Elements for the characteristic matrix of film stack
$\mathcal{A}, \mathcal{B}, \mathcal{C}$	Surfaces in classical theory of diffraction
$ E_z $	Amplitude of electric field
$\Delta E_z $	Amplitude difference
ΔPhase	Phase difference
h_1	Observation distance
h_2	Thickness of line structures
Res	Residue
Re	Real part of complex number
Im	Imaginary part of complex number
Abs	Absolute value of complex number
m, i, q	Integers
A, B, C, D, T, Q	Points in the geometrical analysis for the ERT model

Note:

- (1) Symbols with subscripts or superscripts are referred to the specific case, unless otherwise stated.
- (2) Bold symbols and symbols with upper arrow, $\vec{\cdot}$ are referred to vectors.

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CHAPTER 1 INTRODUCTION

1.1 Background

1.1.1 Integrated Circuits

Since the invention of the first integrated circuit (IC) in 1958, the density of transistor manufacturable on the semiconductor substrate has increased drastically. From the 1970's to 1980's, the number of devices on a single chip had evolved from very large scale integration (VLSI) to ultra large scale integration (ULSI), i.e. increased from more than 100,000 to more than 1 million devices per chip. Today, the Intel Pentium chip easily achieves more than 10 million transistors. Figure 1.1 shows the number of transistors increased over the years with the advancement of chip technology [1]. The increased number of transistor matches with the

Figure 1.1 Number of transistors increased over the years [1].

Moore's Law, which predicts that the number of devices or transistors per integrated circuit on the chip would double every two years [2].

1.1.2 Projection Photolithography

The advancement of IC technology depends greatly on the evolution of lithographic technique, which is used to transfer the pattern on a mask to the silicon wafer as part of the fabrication process. Figure 1.2 shows the configuration of a typical projection photolithography system. A variety of projection strategies have evolved to suit the industrial needs. For example, exposure tool of step-and-scan projection systems has replaced step-and-repeat system in order to expand the size of exposure field. Typically, the reduction ratio of the mask to the wafer is 4 times. Increasing the reduction ratio from 1:1 allows easier fabrication of the reticle as the features on the reticle can be larger compared to the size of the final structure on the wafer.

Figure 1.2 Projection photolithography.

The continued dominance of projection photolithography in current mass production is the result of efforts of exploiting advanced optical exposure tools, and research and development of reticle and resist technology. In projection photolithography, the achievable feature sizes is relied on the imaging wavelength, numerical aperture (NA) of the exposure tool and use of other resolution enhancement techniques (RETs) such as off-axis illumination (OAI) [3], optical proximity correction (OPC) [4] and phase shifting mask (PSM) [5, 6]. Such RETs help to stretch the capability of photolithographic technique to print feature sizes below the imaging wavelength.

1.1.3 Reticle Pattern

The reticle consists of the IC pattern, which is usually designed in horizontal and vertical line structures. Figure 1.3 shows an example of the pattern on a reticle that will be transferred onto the wafer after exposure in the scanner. Illumination of the exposure light to the reticle will cause diffraction at the aperture of the line structure as illustrated in Figure 1.4. The diffraction pattern is well known to depend on the size of the aperture. When the width of line structure is small, higher orders of the diffraction components are excluded to be collected at the entrance pupil before the projection lens. This is particularly true for current sub-micron technology where even the plus and minus first order of the diffracted beam can also be excluded in conventional illumination. Theoretically, if all the diffraction orders are collected, a perfect aerial image without any degradation can be formed on the wafer. As a consequence of this, the current capability of the scanner is always termed as diffraction limited and other factor such as lens aberration has minimal impact on the illumination system.

Figure 1.3 Portion of the integrated circuits pattern on a reticle. (Picture courtesy of Chartered Semiconductor Mfg. Ltd.)

Figure 1.4 Various order of diffracted beam occurs at the aperture for line structure.

1.1.4 Alignment and Overlay

Masking layers well above twenty is very common for fabrication of a complete IC. Alignment of the pattern to the previous levels is important to ensure that the overlay is within the specifications. Overlay is the outcome of alignment, which is often expressed in terms of “ $|\text{Mean}| + 3\sigma$ ” to indicate the shift between two subsequent layers. Over the years, alignment techniques have evolved from a simple two-point alignment to a very complicated multi-term method [7]. This is unavoidable as the overlay budget becomes more stringent when the IC minimum feature size shrinks down. Alignment and overlay have continuously received great attention from the lithography community. This can be seen through that the annual SPIE Advanced Lithography conference (previously known as SPIE Microlithography before year 2007) allocates a particular session, i.e. Metrology, Inspection and Process Control for Microlithography to cover researches in alignment and overlay. The scopes of the presented papers range from the development of different alignment algorithms [8] to overlay improvement using various diffraction schemes [9].

The overlay budget compiled from International Technology Roadmap for Semiconductor (ITRS) 2005 [10] as presented in Figure 1.5 shows that a tight overlay requirement, below 10 nm is required in year 2010 when the minimum feature size reaches 45 nm. Generally, the overlay tolerance requirement has been 17% to 40% of the minimum feature size [10-12]. The overlay of the exposure field is known to affect the functional dies on the wafer. It has a significant influence on the production yield at the end of the manufacturing process. The fabrication of IC requires more than 20 masking steps with accurate patterning. Another impetus to reduce total overlay error is that if a smaller overlay error can be achieved, tighter tolerance for designing circuit patterns is realizable [13]. For example, a smaller metal pitch can be used which in turn reduced the chip size. Smaller die size allows more chips to be fabricated on a wafer and thereby reduced manufacturing cost.

Figure 1.5 Half pitch and the respective overlay [10].

(a) Alignment System

Alignment system is incorporated as part of the exposure tool regardless of the lithographic techniques. For projection photolithography, there are two types of alignment system in the

scanner, namely Through-The-Lens (TTL) [14, 15] and Not-Through-The-Lens (NTTL) [16] as shown in Figures 1.6 (a) and (b), respectively. The former requires the light from the alignment illumination source to pass through the lenses used for imaging. On the other hand, the alignment sensor in the latter is independent from the projection lens and allows each set of lens to be optimized severally. Typically, monochromatic light at wavelength 633 nm or 532 nm is used in the alignment system of the scanner. Light source alignment system is also used for other lithographic techniques such as X-ray [17, 18] and imprint lithography [19]. The research in alignment techniques using light source with Moiré or interferometric imaging is required to continuously improve the overlay of the exposed features.

Figure 1.6 (a) TTL [15] and (b) NTTL [16] alignment system.

(b) Alignment Marks

Alignment marks consist of line structures array, which is known as grating. The horizontal and vertical marks can be found in both reticle alignment and wafer alignment in the scanner. The

main task of reticle alignment is to match the position of the reticle to the wafer stage. It needs to ensure that the exposure is corrected for the magnification, rotation and translation, scan skew and scan scaling of the reticle. Reticle alignment marks are formed outside the reticle exposure field as shown in Figure 1.7 and will not be printed onto the wafer during exposures. On the other hand, wafer alignment marks are usually formed along the scribe-line on the wafer. The horizontal and vertical marks are required for alignment system to model the wafer grid. The model will compensate for wafer translation-X, translation-Y, rotation, expansion-X, expansion-

Figure 1.7 Reticle alignment marks, R1, R2, R3 and R4 comprise of vertical and horizontal line structures in Tyh and Txh gratings are located at four corners outside the image field [20].

Y and non-orthogonality errors. As a consequence of process sensitivity, wafer alignment is always the main contributor to alignment error. The wafer alignment marks are prone to distortion during different fabrication processes such as chemical mechanical polishing (CMP). This results in poor signal being collected by the alignment system and subsequently affects the alignment accuracy between two layers. The challenge of process sensitivity remains until today as the wafer alignments can be varied unpredictably not only from field to field within a wafer but also from wafer to wafer and different batches of wafer.

(c) Overlay Targets

Overlay measurement is performed by using a dedicated structure known as overlay target. The overlay target comprises of two integrated patterns with the first pattern is printed on one layer and the second pattern is printed on the consecutive layer. By using a stand-alone metrology system, the differences in the position, orientation and distortion of the two patterns are measured. The dominant measurement technique, optical microscopy is used to locate the pattern formed on the two different levels of substrates. Figure 1.8 shows the various designs of overlay targets. The most common pattern has been a square inside a square, called “box-in-box” as shown in Figure 1.8 (a) [21]. Other designs of overlay targets such as frame-in-frame and frame-in-segmented frame as shown in Figure 1.8 (b) [21] and (c), respectively have also come into use. Recently, overlay targets in periodic line structures as shown in Figure 1.8 (d) has also been introduced [22]. It is obvious that in the design of overlay targets in Figure (b), (c) and (d), line structures formed the basis of the overlay targets.

Figure 1.8 Different design of overlay targets (a) Box-in-box (b) Frame-in-frame (c) Box-in-segmented frame (Picture courtesy of Chartered Semiconductor Mfg. Ltd.) (d) Periodic structures [22].

1.1.5 Motivation of Research

Line structures inevitably become part of the photolithography process. The diffraction of such structures at the reticle is a critical consideration for the scanner illumination system to achieve smaller printable feature size. Besides this, line structures of alignment marks and overlay targets on the wafer are also important in advanced patterning processes. Theoretical understanding of the electromagnetic scattering at the line structures is necessary in conjunction with the development of hardware in the fabrication process. With a resource efficient and reliable model, the simulator can offer an efficient characterization to quantify the relationships for a new process.

In a rigorous approach, the electromagnetic scattering solution for line structures is obtained through a pure mathematical formulation. After specifying the properties of the structures and its illumination conditions in the computational domain, the output of the rigorous model provides the total electromagnetic field at the point of interest. In this context, the concept of individual physical mechanisms does not apply. There is no clear insight information about whether the geometrical aspect of the line structures can be identified independently to be responsible for a definite portion of the total electromagnetic field. If the total solution can be decomposed into their respective contributions, this will then provide a better understanding to predict the behavior of electromagnetic scattering for line structures.

When the technology node advances to the next level, the demand for rapid and accurate pattern placement is a difficult challenge. The alignment capability is an issue since the fabrication process is new and variation in the process may affect the overlay performance. Overlay is known as one of the most critical metrology elements for yield enhancement in semiconductor fabrication process. Hence, the alignment performance needs to be studied in a new process for advanced technology node to ensure that the overlay is within the budget.

1.2 Objectives

The objectives of this research are as follows:

- To explore high frequency approximation solution for electromagnetic scattering problem.
- To study the correlation between diffraction coefficient and wedge properties.

- To establish a new electromagnetic scattering model based on individual physical mechanisms for line structures in practical lithography problems.
- To study the alignment performance in 90 nm and 0.11 μm technology node processes and explore the use of different designs of alignment marks.

1.3 Scope

The first part of this work involves pure mathematical formulation for the modeling work. All the formulations and numerical analysis are coded in PC-based MATHEMATICATM [23] using the default accuracy of floating point in the software. The results in Chapters 3, 4 and 6 are generated using notebook PC with Intel Pentium IV 1.8 GHz microprocessor whereas the results in Chapter 5 are obtained using notebook PC with Intel Core 2 Duo Processor T5450 1.66 GHz. On the other hand, the capability of the alignment marks for advanced technology process is studied experimentally using ASML DUV scanner (PAS 5500/800) in Fab 6 Chartered Semiconductor Mfg. Ltd.. Images of the alignment marks and overlay targets are captured using optical microscope, scanning electron microscope (SEM) and atomic force microscope (AFM). The overlay results are obtained using an off-line measurement tool, KLA-Tencor Archer 10 by using of box-in-segmented frame overlay target.

1.4 Outline of Thesis

In Chapter 2, a critical literature review is given for the electromagnetic scattering of line structures from the perspective of modeling and its application in alignment for photolithography. The study of external diffraction of an impedance wedge is presented in

Chapter 3. This includes the development of higher order external diffraction coefficient using high frequency asymptotic solution. Subsequently, the internal diffraction of a penetrable wedge is studied in Chapter 4 using dual Sommerfeld contour integrals. By exploiting the external and internal diffraction coefficients, the electromagnetic scattering model of line structures is then established in Chapter 5. In Chapter 6, the application of line structures in photolithography is studied theoretically and experimentally for different designs of wafer alignment marks in advanced technology process. Finally, this research work is concluded in Chapter 7 together with the suggestions for future work.

CHAPTER 2 LITERATURE REVIEW

The main part of this chapter reviews the approach used to solve electromagnetic scattering problems particularly in photolithography. The discussion covers the basic theory, development, limitations and implementation issues in rigorous formulations, classical theory of diffraction and high frequency approximation method. A critical review is also given for the diffraction coefficient in the high frequency approximation method of geometrical theory of diffraction (GTD) and uniform theory of diffraction (UTD). Subsequently, the review also includes the application of line structures for alignment in photolithography. The flow of this chapter is given in Figure 2.1. A concluding summary is given at the end of this chapter.

Figure 2.1 The flow of literature review.

2.1 Rigorous Electromagnetic Scattering Formulations in Photolithography

The electric and magnetic field vectors, $\mathbf{E}(\mathbf{r}, \omega)$ and $\mathbf{H}(\mathbf{r}, \omega)$ that are used to describe the light scattering phenomenon must satisfy the Maxwell's equations [24, 25],

$$\nabla \times \mathbf{E}(\mathbf{r}, \omega) + j\omega\mu(\mathbf{r})\mathbf{H}(\mathbf{r}, \omega) = 0 \quad (2.1)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, \omega) + j\omega\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}, \omega) = 0 \quad (2.2)$$

$$\nabla \cdot [\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}, \omega)] = 0 \quad (2.3)$$

$$\nabla \cdot [\mu(\mathbf{r})\mathbf{H}(\mathbf{r}, \omega)] = 0 \quad (2.4)$$

where the spatial coordinate is denoted by $\mathbf{r}$ and the radian frequency is denoted by ω . The medium's permittivity and permeability are given as $\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r})$, respectively. A number of methods have been introduced to solve the Maxwell's equations using numerical analysis in various ways. They can be classified into two general approaches, which are differential and integral equation methods. Examples of differential equation methods are the well known finite difference method [26] and finite element method [27]. One of the key properties in differential equation methods is the existence of the discretization process as part of the formulation in the simulation domain. On the other hand, the integral equation methods include method of moment [28] and multipole method [29]. In integral equation methods, the solution is obtained by solving the kernel of the surface or volume integral after the derivation of a unique function such as the Green's function. In overall, the growth of different numerical methods to suit their application in related to electromagnetic analysis is tremendous. This part of literature review places an emphasis on rigorous electromagnetic scattering methods which are applied in photolithography. Interestingly, all these formulations are based on differential equation methods.

The general classification of the rigorous electromagnetic scattering formulations applied in photolithography is given in Figure 2.2.

Figure 2.2 Classification of rigorous electromagnetic scattering formulations applied in photolithography.

2.1.1 Finite Element Method (FEM)

The finite element method (FEM) was employed by Matsuzawa et al. [30] to simulate the behavior of light wave propagation in a photoresist system on flat and reflected stepped surface. In their work, they neglected the coherence effect below the resist surface when calculated the electric field strength derived from the Maxwell's equations. Later, Urbach and Bernard [31] presented an FEM based model to obtain the latent image on photoresist by repeatedly solving a boundary value problem for the Helmholtz equation. They included the effect of partially coherent illumination in their formulation. Urbach also proved the convergence in the FEM by choosing a domain with all the scatterers and sources were bounded within a homogeneous medium [32]. On another note, Hyun et al. [33] reformulated the boundary conditions in FEM and included the imaging model in their approach. Wei et al. used the FEM to study 3D rigorous simulation of mask induced polarization [34].

In recent years, the FEM has received less attention from the lithography community. There are limited work in FEM photolithography related papers being presented in journals and conferences. The use of FEM in photolithography is limited to resist simulator such as Signetics/Philips Enhanced SAMPLE Algorithm (SPESA) [31, 35] and Simulation TOol for Resist Model (STORM) [36]. At the reticle level, none of any other photolithography simulators have applied FEM extensively in solving the electromagnetic scattering problems. One of the factors that contributes to this is the availability of other rigorous electromagnetic solutions such as finite difference time domain (FDTD) method and waveguide model/rigorous coupled wave analysis (RCWA). The FDTD method and waveguide model/RCWA are reviewed in Sections 2.1.2 and 2.1.3, respectively.

2.1.2 Finite Difference Time Domain (FDTD) Method

Another approach, based on finite difference time domain (FDTD) method was employed by Gamelin et al. [37] to achieve rigorous algorithm in boundary conditions. By discretization of Maxwell's equations in time and space on a uniform grid of electric and magnetic field, FDTD provides the solution to the wafer topography of interest. Guerrieri et al. [38] exploited a massively parallel computer known as Connection Machine to study the discretization accuracy, convergence properties and efficiency of the boundary conditions in the developed FDTD algorithm. It was found that the convergence of the solutions was dominated by the physical scattering phenomenon, which depends on the thickness and refractive index of the materials. Subsequently, Wong et al. [39, 40] extended and applied the algorithm to study photolithographic problems with various conditions such as TE and TM polarizations, partially coherent imaging, obliquely incident waves and highly dispersive materials. The work done by

Gamelin [37], Guerrieri et al. [38] and Wong et al. [39, 40] was incorporated into an academic lithography simulator known as TEMPEST (Time-domain Electromagnetic Massively Parallel Evaluation of Scattering from Topography) [41]. Recently, another research group, i.e. Fraunhofer Institute of Integrated Systems and Devices Technology (IISB), Germany has also applied FDTD in their lithography simulator known as Dr.Litho [42, 43].

Current commercial lithography software is also capable of resolving rigorous FDTD solution for the electromagnetic scattering problem with the specified geometries and optical properties in the simulation domain. These simulators are frequently used to explore the effects of new processes in lithography and optimize the existing processes at the mask level. For example, PROLITH [44], Sentaurus Lithography [45] (formerly known as SOLID-E) or LithoCruiserTM [46] can be used to investigate the shift of process window by studying the phase shift mask using rigorous FDTD simulation. As these are commercial products, the exact details of the FDTD algorithms are not revealed unconditionally due to the constraint in proprietary information. However, one can trace the fundamental of the rigorous FDTD method applies in these simulators through papers published in different conferences such as given by references [47, 48] for Sentaurus Lithography. Another commercial lithography software, i.e. EM-SuiteTM [49] has applied the academic simulator TEMPEST as the core simulation engine for the rigorous FDTD simulation.

2.1.3 Waveguide Model/Rigorous Coupled Wave Analysis (RCWA)

The approach using waveguide model [50] was introduced by Nyysönen [51]. Nyysönen obtained the solution of Maxwell's equations in connection to the optical line width

measurement of printed photoresist in microlithography. The fields within the object, which is taken to be periodic in one direction and poses rectangular profile, were expanded in the eigenmodes of a waveguide having the same horizontal cross section as the object. Subsequently, the author extended the same model to analyze profile with arbitrary sidewall [52] and showed that the measured line width of a line object is affected by the physical shape of the edges.

Yuan and Strojwas [53] applied the same approach based on the stratified layer technique for the modeling of optical wafer alignment and line width measurement. Figure 2.3 shows the stratified layers in the waveguide model. Yuan also improved and optimized the algorithm of the waveguide model to achieve faster solution [54] and extended its application to simulate various images for microscope [55]. Based on this, Lucas [56] had developed the 3-dimensional waveguide model for applications in lithography.

Figure 2.3 The waveguide model [53].

In fact, the waveguide model is indifferent to rigorous coupled wave analysis (RCWA) [57-63]. Both approaches have been proven to be exact after solving the linear algebraic equation system

using eigenvalue and eigenvector [64]. The foundation of the formulation is based on Rayleigh expansion [65]. Rigorous coupled wave analysis was introduced by Moharam and Gaylord for the application in diffraction grating with infinite conductivity [57]. Later, RCWA was extended to dielectric and metallic gratings with arbitrary complex permittivities [58, 59]. References of RCWA for binary and arbitrary gratings profile, and improved TM polarization convergence rate can be found in [60, 61] and [62, 63], respectively. In the application of photolithography, this model has been incorporated not only in non-commercial simulators such as METROPOLE [66, 67] and Dr.Litho [43], but also in lithography related software available in the market such as PROLITH [44] and Sentaurus Lithography [45]. This provides the users an alternative option, other than the finite difference time domain (FDTD) method as discussed in Section 2.1.2, to study the electromagnetic scattering phenomenon in photolithography.

2.1.4 Properties of Rigorous Electromagnetic Scattering Formulations

There are several inherited properties in the waveguide model, FEM and FDTD method. Firstly, there are only two terms that can be identified, namely incident, U_i and scattered field, U_s . Summation of both terms as given in (2.5) provides the solution to Maxwell's equations.

$$U_T = U_i + U_s \quad (2.5)$$

There are no clues about each individual physical mechanism that contributes to the scattered field. The electromagnetic field of the physical phenomenon such as reflection and transmission is indistinguishable from the scattered field. All the effects of the obstructor are combined into the scattered field. Similarly, one cannot predict the scattered field based on the physical picture of the edge diffraction phenomena and ray tracing approach.

The accuracy of numerical analysis in the rigorous electromagnetic scattering formulations is well known to be dependent on its discrete grid or node sizes. For example, better accuracy is usually achieved in waveguide model when thinner stratified layers are used. However, the trade off is the increase in computational memory and time. The computational resources required by numerical analysis can be substantial. Furthermore, there are also convergence problems when dealing with different properties of the structures such as refractive index and thickness. The problem is particularly significant for high aspect ratio structures. Polarization of the incident light can also affect the convergence of the solution. On the other hand, it is impossible to obtain a particular scattered field in a numerical analysis without simulating the whole domain. For example, if only the near field information on top of layer 0 in Figure 2.3 is needed, this forces the simulation domain to include until layer n and the underneath material. As such, this would lead to a redundant consumption of computational resources.

2.2 Classical Theory of Diffraction

2.2.1 Background

The solution to electromagnetic field can also be obtained from the perspective of diffraction. Diffraction occurs when the wave propagation deviates from its original path caused by an obstruction. The well known postulation of Huygen states that every point on the primary wavefront is a source to generate secondary wavefront. Fresnel applied this postulation together with Young's interference concept to account for the diffraction phenomenon. With this, Kirchhoff established a diffraction mathematical model using certain integral theorem and

Helmholtz equation. In Fresnel-Kirchhoff diffraction theory, the disturbance at P_o caused by a point source at P in an enclosed surface of $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ is given by [68]:

$$U(P_o) = \frac{1}{4\pi} \iint_{\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}} \left(G \frac{\partial U}{\partial \nu} - U \frac{\partial G}{\partial \nu} \right) ds \quad (2.6)$$

where $\vec{\nu}$ is the normal vector as shown in Figure 2.4.

Figure 2.4 Diffraction at plane screen.

Kirchhoff used the choice of Green's function, G as a spherical wave diverging from P_o ,

$$G = \frac{\exp(jkr_{01})}{r_{01}} \quad (2.7)$$

where k is the wave number and r_{01} is the magnitude of the vector $\vec{r}_{01}$. In this theorem, Kirchhoff

made the assumptions that the field, U and its derivative, $\frac{\partial U}{\partial \nu}$ across plane $\mathcal{A}$ is the same as if

the screen is absent. Kirchhoff also assumed that in the immediate region after the screen at

surface $\mathcal{B}$, the field, U and its derivative, $\frac{\partial U}{\partial \nu}$ vanish. Furthermore, the contribution from surface

C is neglected when considering a diverging spherical wave with $\tilde{R} \rightarrow \infty$. As a result of all these assumptions, (2.6) only needs to consider surface $\mathcal{A}$.

The idealization in Kirchhoff's boundary conditions contradicts with the theorem of potential theory. The theory states that the potential function of the entire plane must be zero if the potential function and its normal derivative along any finite curve segment on the plane is zero. This is physically unmatched with the Kirchhoff's boundary conditions where diffraction can still be observed behind the screen. For this contradiction, Rayleigh-Sommerfeld diffraction theory relaxes the boundary conditions by introducing different Green's functions,

$$G = \frac{\exp(jkr_{01})}{r_{01}} - \frac{\exp(jk\hat{r}_{01})}{\hat{r}_{01}} \quad (2.8)$$

or

$$G = \frac{\exp(jkr_{01})}{r_{01}} + \frac{\exp(jk\hat{r}_{01})}{\hat{r}_{01}} \quad (2.9)$$

By taking the distance between P and P_o is in the order of the wavelength, a summary of both diffraction theories for the field disturbance at P_o is given below [68],

$$U(P_o) = \frac{A}{j\lambda} \iint_{\mathcal{A}} \frac{\exp[jk(\hat{r}_{01} + r_{01})]}{\hat{r}_{01}r_{01}} \psi ds \quad (2.10)$$

where

$$\psi = \begin{cases} \frac{1}{2} [\cos(\vec{v}, \vec{r}_{01}) - \cos(\vec{v}, \vec{\hat{r}}_{01})] & \text{Fresnel-Kirchhoff} \\ \cos(\vec{v}, \vec{r}_{01}) & \text{Rayleigh-Sommerfeld using (2.3)} \\ -\cos(\vec{v}, \vec{\hat{r}}_{01}) & \text{Rayleigh-Sommerfeld using (2.4)} \end{cases}$$

The field expression in (2.10) can be further simplified using series expansion to give approximation to the Fresnel (near field) and Fraunhofer (far field) diffraction.

2.2.2 Application of Classical Theory of Diffraction

In optics field, a number of practical examples involve the use of classical theory of diffraction. Approximation of Fresnel diffraction is used to study the waist size of laser beam in Gaussian field profile [69]. The theory had also been used in diffraction grating to observe the near field diffraction pattern [70]. Fraunhofer diffraction had been applied in the image formation in microscope for coherent illumination using Abbe's theory [24]. When proximity printing is used in lithography, classical diffraction theory had also been used to find the total electromagnetic field at the mask aperture [71, 72]. In photolithography, the validity of Kirchhoff boundary conditions in aerial image simulation had also been studied [73]. Furthermore, the theory had also been explored in high numerical aperture Hopkins imaging [74, 75] for homogeneous thin films [76] based on plane wave decomposition approach. The pioneering aerial image simulator from Berkeley, SPLAT [41], had applied the same theory to its thin mask model when performing simulation for partial coherence imaging.

With the need to rapidly characterize the wafer printability of a full reticle IC pattern, the classical theory of diffraction has been incorporated widely in commercial photolithography software dedicated for optical proximity correction (OPC). For example, the ProgenTM lithography model used in ProteusTM [45] OPC software exploits the simplicity in classical theory of diffraction to provide full chip optical proximity correction of the IC pattern. The same

theory is also applied in other commercial OPC modeling tools such as Calibre[®] nmOPC [77] and Tachyon[™] OPC+ [46], which are developed by different companies. All these OPC software must be capable to perform computation of images for large IC pattern in a reasonable amount of time. It is impossible to implement rigorous electromagnetic formulations discussed in Section 2.1 due to the constraint in time and memory consumption. The classical theory of diffraction is a better choice for this particular application. However, there are some shortcomings which will be discussed in the next section.

2.2.3 Shortcoming of Classical Theory of Diffraction

In classical theory of diffraction, the unique boundary conditions are formed using plane screen assumption. The plane screen is assumed to be infinitely thin and perfectly conducting. This implies that the thickness of the obstructer has no impact to the diffraction pattern. There is no penetration of incident field into the obstructer. Although the classical theory of diffraction has been used widely in lithography OPC software they are all based on the assumption of thin substrate. For instance, the aerial image of reticle obtained using Kirchhoff's boundary conditions in classical theory of diffraction has ignored the diffraction effect near to the apertures because of thin substrate assumption. Fundamentally, the obstructer's properties such as thickness and refractive index are not taken into consideration. When the substrate thickness is no longer "thin", the validity of the assumption is questionable [78]. In order to solve this problem, a ray tracing approach in high frequency approximation solution is studied.

2.3 High Frequency Approximation Method

Another approach of solving Maxwell's equations is using high frequency approximation method. This method can be used when a small (large) parameter, for example wavelength (frequency) occurs in the problem, which allows an unknown parameter to be represented by a series of power (or its inverse power) terms. Generally, only the first few terms of the series are important as they yield useful information for the undetermined quantities in the problem. The following sections review a high frequency approximation method, namely Geometrical Theory of Diffraction (GTD) and its improved version, Uniform Theory of Diffraction (UTD), which enhanced the concept of electromagnetic ray tracing.

2.3.1 Geometrical Theory of Diffraction (GTD)

(a) Early Development

Apart from the diffraction wave theory presented in the previous section, diffraction can also be studied using ray tracing approach. The concept of ray tube [79] is well used in geometrical optics with the amplitude and phase needs to be determined. Geometrical optics (GOs) takes the first term ($m = 0$) in the high frequency Luneberg-Kline expansion [80],

$$u(\mathbf{x}, k) \sim \exp(jk\varphi) \sum_{m=0}^{\infty} \frac{\nu_m(\mathbf{x})}{(jk)^m} \quad (2.11)$$

to represent a solution to the incident, reflected or transmitted field. The respective phase and amplitude coefficient are given by φ and $\nu_m(\mathbf{x})$. The shortcoming in GOs lies in the

discontinuity at the shadow boundary separating the lit and shadow regions. A point is located in the lit region when there is at least one ray passes through. Otherwise, the point will be located in the shadow region. This missing term in GOs, which played an important part in the development of ray tracing method are the diffracted rays. The summation of the diffracted field, U_d and GOs, U_{GOs} field gives the total electromagnetic field, U_d at a point,

$$U_T = U_{GOs} + U_d \quad (2.12)$$

where the geometrical optics field includes the incident, reflected and transmitted field.

In 1962, Keller [81] introduced the geometrical theory of diffraction (GTD) to suggest the existence of diffracted rays as an extension to geometrical optics. A postulation was made to claim that diffracted rays are produced when incident rays hit some obstructions, such as edges, corners [82, 83], or vertices of boundary surfaces or grazes along such surfaces as illustrated in Figure 2.5. By analogy to the reflected and transmitted fields in geometrical optics, the diffracted field, which is a matrix for a field vector is obtained by multiplying the incident field with a diffraction coefficient [84],

$$\mathbf{E}^d(s) = \mathbf{E}^i(Q_e) \mathbf{D} A(\rho) \exp(-jk\rho) \quad (2.13)$$

where $\mathbf{E}^i(Q_e)$ is the incident field onto the point of diffraction, which is located along the edge. $\mathbf{D}$ is the dyadic diffraction coefficient and $A(\rho)$ is the spreading coefficient with ρ is the distance from the reference point to the field point. Other properties and the details of the mathematical foundation of GTD and the associated GOs can also be found in the reference [85, 86].

**Figure 2.5 (a) Cone diffracted rays at the edge of a thin screen.
(b) Surface diffracted ray at the rounded end of a screen [81].**

(b) Shortcoming of GTD

The diffraction coefficient is characterized by the physical properties of the medium at the point of diffraction. As a result of this, a unique diffraction coefficient is needed for each type of edge structure and surface properties. The original diffraction coefficient presented by Keller is restricted to perfectly conducting material [87] and limited structures. With the basis in GTD, the papers by Kaminetzky [88], Ludwig [89], Wolfe [90], Senior [91], and Keller [92] had been presented to solve different diffraction problems.

Nevertheless, the GTD field shows a serious shortcoming. When the point of observation is near to the shadow boundaries, the GTD field becomes infinite. The actual electromagnetic field must be bounded without giving any singularities. Figure 2.6 (a) shows a 40° perfectly conducting wedge is illuminated with plane wave at 10 GHz ($\lambda = 0.1$ nm) and incident angle, ϕ_o of 55° [84]. The GTD diffraction coefficient for both soft and hard polarizations (TE and TM polarizations in the context of optics), D_s^k and D_h^k respectively across the wedge external surrounding angle, ϕ is

given in Figure 2.6 (b). The distance of observation point, P from the wedge corner, ρ is 10λ . Apparently, the diffraction coefficients approach infinity at the incident shadow boundary (ISB) and reflection shadow boundary (RSB) of 125° and 235° , respectively.

Figure 2.6 (a) Geometry of the perfectly conducting wedge. (b) GTD gives infinity field at the shadow boundaries [84].

2.3.2 Uniform Theory of Diffraction (UTD)

In the previous section, the shortcoming of GTD is discussed. The GTD diffraction coefficient becomes infinite when the point of incidence is near to the incident or reflection shadow boundaries. In year 1974, Kouyoumjian and Pathak [93] presented a paper on Uniform Theory of Diffraction (UTD). The authors suggested another form of diffraction coefficient using uniform asymptotic method to describe the field in the shadow region. Their approach successfully compensated the discontinuities in the GOs at the shadow boundaries. Kouyoumjian and Pathak's diffraction coefficient for a perfectly conducting wedge is given as [93],

$$D_{s,h}(k, n, \phi, \phi_o) = D^{(1)} + D^{(2)} \mp D^{(3)} \mp D^{(4)} \quad (2.14)$$

where each sub diffraction coefficient, $D^{(1)}$, $D^{(2)}$, $D^{(3)}$ or $D^{(4)}$ is responsible for a particular incident or reflection shadow boundary as shown in the figures comprising in Figure 2.7.

Figure 2.7 Sub diffraction coefficients, (a) $D^{(1)}$, (b) $D^{(2)}$, (c) $D^{(3)}$ and (d) $D^{(4)}$ in UTD are responsible for the discontinuities along different incident shadow boundaries (ISB) and reflection shadow boundaries (RSB) [93]. Labeling of o and n faces is customary.

Each of the sub diffraction coefficients consists of a Fresnel integral and a cotangent term. When the field is near to the shadow boundary, the Fresnel integral compensates for the infinite field caused by the cotangent term. Some changes to the original formulation had been suggested by a few authors. Jakobsen [94] gave an alternative diffraction coefficient for a right-angled wedge, which used different arguments in the Fresnel integral. Umul [95] also suggested a simplified diffraction coefficient by replacing the Fresnel integral with another function. The time domain UTD [96] had also been formulated. Besides wedge structure, UTD have also been extended to study diffraction of other structures such as cone [97] and smooth convex surface [98] as shown in Figure 2.8.

Figure 2.8 Geometry of the (a) cone [97] and (b) convex curved surface [98].

2.3.3 Application of GTD/UTD in Photolithography

Study of image formation in photolithography using GTD has also been revealed recently. Khoh et al. [99] proposed an approach by relying on the edge diffracted rays to form the aerial image. The diffracted rays were formulated based on the assumption of perfectly conducting material, which is the idealized case for the chrome layer on the reticle. The same assumption was taken by Chua et al. [78] in the study of edge effects characterization of phase shift mask using GTD. At lithographic wavelength, chrome has finite refractive index and its effect is non-negligible [100]. In order to take the consequence of refractive index into consideration, diffraction coefficient for lossy and lossless materials is required. The next sections review the development of diffraction coefficient for this purpose.

2.4 External Diffraction Coefficient for Lossless and Lossy Wedges

The implementation of UTD has successfully solved the singularities problem in GTD. However, the original formulation in UTD is still limited to perfectly conducting materials. In a

paper presented by Keller [101], he pointed out the difficulty of obtaining the diffraction coefficient for each type of edge or vertex structure. Besides uniformity, the diffraction coefficient must also be accurate to predict the diffracted field for a variety of edge structures. Figure 2.9 shows the three main approaches for the solution of diffraction coefficient, which are limited to the external part of the lossless and lossy wedges. In the external part of the wedge, the diffracted and incident fields are in the same medium.

Figure 2.9 Different approaches for wedge external diffraction coefficient.

2.4.1 Maliuzhinets Diffraction Coefficient

Maliuzhinets obtained the solution for diffraction of the wedge using Sommerfeld integral [102] and impedance boundary conditions [103, 104]. His work involved the use of Laplace and Fourier transform to solve the functional differential equations for a spectral function in the Sommerfeld integral. Associated with this, a diffraction coefficient with a special function, known as Maliuzhinets function was introduced [105-107]. The Maliuzhinets function is dependent on the incident wavelength, wedge structures and its impedance. Based on this, a number of high frequency approximation solutions has been applied to solve for various wedge diffraction problems [108, 109]. This includes plane wave [110] and line source [111, 112]

illumination. For example, Herman and Volakis [113] extended the work to include double impedance wedge for second and triple order diffraction mechanisms as shown in Figure 2.10.

Figure 2.10 (a) Double and (b) triple diffraction mechanism on an impedance double wedge [113].

In general, the UTD Maliuzhinets diffraction coefficient is obtained by retaining only the first term in the Taylor series. The Taylor series is required to solve for the Sommerfeld integral using steepest descent method [114, 115]. When higher order up to m in the series is included, it achieves accuracy of $(k\rho)^{-m/2}$ in the solution. The inclusion of higher order in the series has not been presented and explored in UTD format so far. Osipov [116] had discussed this issues but is presented in the Uniform Asymptotic Theory of Diffraction (UAT) [117, 118] format.

2.4.2 Heuristic Diffraction Coefficient

The idea of heuristic diffraction coefficient was originated from Luebbers [119, 120]. The work proposed that the diffraction coefficient for a finite conductivity wedge is given as

$$D(k, n, \phi, \phi_o) = A_1 D^{(1)} + A_2 D^{(2)} + R_o D^{(3)} + R_n D^{(4)} \quad (2.15)$$

where R_o and R_n are the Fresnel reflection coefficient [24] for the o and n face of the wedge in Figure 2.7, respectively. As Luebbers assumed that no transmissions occurred, the factor of the first two sub diffraction coefficients, A_1 and A_2 are assumed to be unity. When the wedge is

perfectly conducting, it reduces to the form in (2.14). Heuristic diffraction coefficient had also been extended to include multiple edge diffraction [121, 122]. The improved version of heuristic diffraction coefficient had also been discussed by El-Sallabi [123, 124], Rouviere [125, 126] et al. and Holm [127].

The ease of implementation seems to be the main advantage of heuristic diffraction coefficient since it does not involve heavy mathematical formulation. The solution is not formed based on any rigorous mathematical foundation that satisfies the Maxwell's equations. As a result of this, the Maliuzhinets diffraction coefficient, as discussed in Section 2.4.1 is always been used to verify the validity of heuristic diffraction coefficient. For example, El-Sallabi [124] used the Maliuzhinets diffraction coefficient to verify his heuristic diffraction coefficient where Luebbers [128] and Holm [127] heuristic solution failed in the deep shadow region. This is illustrated in Figure 2.11.

Figure 2.11 Comparison of El-Sallabi's method with other approaches for (a) parallel and (b) perpendicular polarizations. Wedge angle = 50° , incident angle = 5° , other details can be found in [124].

2.4.3 Numerical Diffraction Coefficient

Another approach to obtain the diffraction coefficient is by using a numerical method. For this purpose, the moment method [129-131] can be applied. Moment method requires the spectral representation of diffraction as equivalent currents, which are fictitious current used for the convenience of analytical modeling. In the same analogy to GTD where diffraction is treated as local phenomenon, the current only extends to a small region. The diffraction coefficient is then computed from the windowed current through the radiated field. In order to extend the usability in a larger class of problems, moment method was applied by combining with GTD or UTD. For instance, Burnside et al. [132] used the moment method to study the diffraction near to the edge of a wedge ($0 \leq x < X_c$, $0 \leq y < Y_c$) and applied GTD when it was away from the edge ($X_c \leq x < \infty$, $Y_c \leq y < \infty$), as illustrated in Figure 2.12. Additional matching points in the GTD region at

Figure 2.12 Hybrid model using moment method and GTD [132]. The notations $\vec{H}^i$ and ψ_0 denote polarized magnetic field and incident angle measured from the X-wall, respectively.

$(0, Y_d)$ and $(X_d, 0)$ were introduced to provide sufficient linear equations to solve for the diffraction coefficients. The numerical diffraction coefficient has not been applied widely due to the availability of Maliuzhinets and heuristic diffraction coefficients.

2.5 Internal Diffraction Coefficient for Penetrable Wedge

As discussed in Section 2.4.1, Maliuzhinets used impedance boundary conditions to solve the Sommerfeld integral equation and subsequently obtained the external diffraction coefficient of a wedge. The Sommerfeld integral equation for medium with wave number, k is given as

$$U_1(k\rho, \phi) = \frac{1}{2\pi j} \int_L \exp(jk\rho \cos \alpha) f_1(\alpha + \Theta_1) d\alpha \quad (2.16)$$

where ρ is the observation distance, Θ_1 is a constant defined by the wedge external angle and L is the Sommerfeld integral path. In order to obtain the internal diffracted field of the wedge, with wave number k_1 , it is required to solve one additional Sommerfeld integral equation [133],

$$U_2(k_1\rho, \phi) = \frac{1}{2\pi j} \int_L \exp(jk_1\rho \cos \beta) f_2(\beta + \Theta_2) d\beta \quad (2.17)$$

where Θ_2 is a constant defined by the wedge internal angle. The original Maliuzhinets approach is no longer applied because two distinct wave numbers, k and k_1 are involved. Maliuzhinets assumed that the wedge is non-penetrable.

A few authors have presented their solutions to the dual Sommerfeld integral equations. Lyalinov [134] presented the solution for transparent wedge using the S -integrals to reduce the functional equations into a system of linear equations. In his approach, perturbation series was

used to compute the spectral function that appears in the Sommerfeld integrals. Nevertheless, the formulation was focused on highly contrast material.

Another approach to solve the two functional equations which was discussed by Budaev [135-137] was to separate the solution to two distinctive terms. The first term of the solution is expressed with pre-defined singularities within the specific strips and the second term is free of singularities within the same strip. It involves the use of some singular operators and gives numerical solution. The method was used to study the problems of elastic wave propagation in solid wedge-shaped structures but not in electromagnetic diffraction of a wedge. On the other hand, Demeterscu et al. [138] utilized Budaev's method to obtain the total fields in the interior and exterior regions of an arbitrarily angled resistive wedge. The exterior and interior fields of a right-angled resistive wedge are shown in Figure 2.13. In this work, both regions of the wedge were in the same medium and reduces (2.16) and (2.17) to the identical wave number using the same refractive index. The application is not well suited for a wedge with different refractive indices and wave numbers in the exterior and interior regions.

Figure 2.13 (a) Exterior and (b) interior fields for a right-angled resistive wedge. Incident angle = 5° , relative complex permittivity = $2.2 - j0.181$, observation distance = 5 wavelength [138].

Another method of solving the dielectric wedge problem with internal diffraction is using the form of physical optics approximation. The solutions were derived based on dual integral

equations in terms of inverse Fourier transform for the total internal field of the wedge [139]. It is required to identify all the geometrical optics field before solving for the diffracted field using physical optics solution. As part of the approach, the Green's function and both Sommerfeld contour integral equations given in (2.16) and (2.17) were also applied [140]. The solution unavoidably involves the use of series expansion and resulted in a numerical solution. The dielectric wedge problem using physical optics approximation is also explored by Joo et al. [141, 142] and Seo and Ra [143]. Other numerical solution for dielectric wedge problem with internal electromagnetic field was also given by Berntsen [144] but it is not straight forward to implement the numerical analysis for any practical application.

2.6 Alignment in Photolithography

The problem of electromagnetic scattering of line structures in alignment marks remains a concern in the lithography community. As projection photolithography is the most common and cost effective way of fabricating IC in the industry, the discussion of optical alignment will be based on this lithographic technique. Alignment for other lithographic technique such as imprint and x-ray lithography can be found in the references [145, 146] and [17, 18, 147], respectively. This section covers the review of process sensitivity in alignment, the location and size of the alignment marks.

2.6.1 Process Variation to Alignment Performance

Alignment signal depends on the scattered electromagnetic waves from the line structures of the marks. The signal is required to give accurate position of the marks without any deviations.

Nevertheless, this is the ideal case where in real practice, different wafer processes can cause the signal to be distorted. The alignment signal can become asymmetrical by two main causes, physical deformation of the marks and layer deposition deformation on top of the mark. These two causes are briefly discussed below.

Physical deformation is mainly due to chemical mechanical process (CMP) [148]. CMP is a planarization process of removing excessive materials from the wafer surface. However, CMP suffers from the well-known dishing and erosion problems [149], which in turn degrades the topographical conformity as shown in Figure 2.14. Besides affecting the chips electrical properties [150], it can also cause severe distortion and asymmetry to the alignment marks and its signal in the front-end and back-end processes.

Figure 2.14 Realistic case of trenches after CMP [151].

Layer deposition deformation is caused by uneven coating of thin film on top of the wafers. Layers such as polysilicon or silicon dioxide can be deposited on top of the marks. Before the exposure of wafer in the scanner, the coated resist also may not achieve a uniform profile due to the existing of topography from the underlying layers [152]. The layer can be thicker on one side of the mark than the other. As a result of these asymmetry overlying layers, the collected alignment signal is very likely to be asymmetric [153, 154].

The discussion above concerns the main causes to wafer alignment problem. In addition to that, when a new process flow is introduced for advanced technology node, it requires the study of

alignment performance. This is to ensure that overlay performance is within the allowable budget and achieves stability. Rivera et al. [155] had studied the performance of alignment marks in the tungsten CMP process of a 0.25 μm device. The overlay of the six metal interconnect layers was below 15 nm. On the other hand, the evaluation of alignment marks in a copper interconnect process using dielectric layers for 0.18 μm device had also been performed [156]. The results claimed to achieve a minimum mean overlay of 40 nm. The robustness of alignment marks in 0.18 μm and 0.13 μm device was studied by Laidler et al. [157]. All the critical layers, which include gate, contact and metal layers, gave an overlay of below 30 nm. This list does not give a complete review of alignment at every technology node. However, it provides a clear indication that when the technology node advances, especially to below 0.13 μm , study of the alignment marks performance is necessary.

2.6.2 Location and Size of Alignment Marks

During the photolithography step, an exposure layer is aligned to the existing marks on the wafer. When this layer is printed, new wafer alignment marks are created and being aligned by the subsequent layers. These wafer alignment marks are usually segmented grating [158, 159] and they are not part of the functional integrated circuits. The idea of using circuit structures as the alignment targets is impractical since complex alignment algorithms needs to be developed. Even though the complex algorithms can be created, the accuracy is not comparable with the simple algorithms from the dedicated alignment marks [160]. The properties of the wafer alignment marks such as the location and size are important factors that determine the number of fabricated chips on a wafer. These are briefly discussed below.

The way of placing alignment marks on sacrificial die or partial cell at the edges of the wafer as shown in Figure 2.15 are not cost effective and reliable. In order not to waste the precious space on the wafers, alignment marks are preferably to be placed along the scribe-line of the circuit patterns. Scribe-line defines the boundaries between different exposure fields and dies on the wafer. More importantly, scribe line does not contain any useful IC structures. After the completion of IC process, dicing is accomplished along the scribe-line to transform the wafer into individual chips. Total destruction of the wafer alignment marks is not an issue since they are no longer usable.

Figure 2.15 Possible location of wafer alignment marks [161].

A narrower scribe-line width allows the increase in number of chips on the wafer and improves the overall yield per wafer. The scribe-line width can be ranged from 10 μm to 500 μm [162, 163]. In conjunction with this, the alignment marks must be able to give a comparable overlay when they are fit into a narrower scribe-line width. The ASML scanner employs alignment

marks with dimension of $72\text{ }\mu\text{m} \times 727\text{ }\mu\text{m}$ (width $\times$ length), which can be fit into a $80\text{ }\mu\text{m}$ scribe-line. Most of the alignment studies were performed using this dimension except Warrick [156] had studied the alignment marks with shorter length but not for the width.

2.7 Concluding Summary

The following are the conclusions drawn from this literature review,

1. Both the rigorous formulations and classical theory of diffraction are commonly applied to solve for the electromagnetic scattering problems in photolithography. The rigorous electromagnetic scattering formulations are computational intensive and unfavorable for large domain of modeling although high accuracy can be achieved. On the other hand, the classical theory of diffraction ignores the consequences of aperture (obstructor) thickness, which is not realistic in practical application. Most importantly, both of the approaches do not give an in-depth understanding of how each physical field associated with the geometry of the obstructor can contribute to the electromagnetic disturbance. In order to fulfill this requirement, a high frequency electromagnetic ray tracing (ERT) model for line structures is established in this work.
2. The crux of the high frequency ERT model is the need to obtain the external and internal diffraction coefficients of a wedge to characterize the diffracted field. The Maliuzhinets impedance model for UTD can be applied to study the external diffraction of a wedge. However, there is still room for improvement and in-depth study in the formulation. Higher order in the asymptotic series, which has not been explored extensively so far, is developed in this research work.

3. There are several versions available for the internal diffraction coefficient of a wedge. However, they remain numerically dependent in solving the problems. The associated numerical schemes are rather difficult for direct implementation since they involve the use of singular integral operators and complex functional equations. As a remedy to this, a heuristic internal diffraction coefficient is proposed in this work, which could be applied for a good estimation to the exact solution.

4. Alignment in photolithography is a process dependent issue. When a new process for advanced technology node is introduced, the alignment performance is required to meet the stringent overlay budget. The alignment study is also required when implementing new advanced alignment marks such as enhanced order and narrow alignment marks to fit into a smaller scribe-line on the wafer. Arising from this conclusion, part of the research work focuses on the study of new alignment marks in 90 nm and 0.11 μm technology processes.

CHAPTER 3 HIGH FREQUENCY ASYMPTOTIC ANALYSIS OF IMPEDANCE WEDGE FOR EXTERNAL DIFFRACTION

Arising from the findings in the literature review, a high frequency ray tracing approach can be used to study the electromagnetic scattering of line structures. This could provide a detailed understanding of the physical field that contributes to the disturbance at an observation point. A wedge can be considered as part of the line structures. When the incident plane wave illuminates a wedge as shown in Figure 3.1, besides geometrical optics phenomenon such as reflection, there are two types of diffraction occurring, which correspond to the external and internal regions of the wedge. The external diffraction occurs in the same medium as the incident plane wave. On the other hand, the internal diffraction involves wave that originated from the corner of the wedge and propagates in the same medium as the wedge. The study of electromagnetic scattering for the wedge external region is addressed in this part of work.

Figure 3.1 External diffraction surrounding a wedge.

The main objective of this chapter is to obtain the electromagnetic solution for the external region of a wedge, particularly the diffracted field. The diffracted field is presented in Uniform

Theory of Diffraction (UTD) format with detailed formulation on the higher order in asymptotic series for Maliuzhinets coefficient. The study of higher order has not been explored extensively so far. Here, leading terms up to $(k\rho)^{-5/2}$ are considered (k is the wave number and ρ is the distance from the origin). The evaluation is limited to a right-angled wedge. For other angle, the formulation can be modified accordingly. The differences between Uniform Asymptotic Theory (UAT) and UTD for a diffracted field resides on the wedge surfaces are also demonstrated. The results focus on two main parts. The first part is devoted for field point on the impedance wedge surface. Subsequently, the second part presents the transverse electric (TE) and transverse magnetic (TM) polarizations diffraction results for both lossless and lossy wedges, which are modeled as isolated impedance structures. The chosen materials are commonly found in IC fabrication. A time harmonic of $\exp(j\omega t)$ is assumed and suppressed throughout. A function with roman superscripts denotes the respective order of derivative.

3.1 Formulation of the Impedance Wedge Problem

The geometry of the impedance wedge with external angle of $2\Phi_1$ is shown in Figure 3.2. The impedance at both surfaces of the wedge, i.e. $\phi = 0$ and $\phi = 2\Phi_1$, is given by Z_+ and Z_- , respectively. A linearly polarized electromagnetic wave, normally illuminating the wedge with an incident angle of ϕ_o , produces a diffracted wave at angle of ϕ . The incident field, which is normal to the plane of incidence, is given by

$$U_z = \hat{z} \exp[jk\rho \cos(\phi - \phi_o)] \quad (3.1)$$

where the wave number in the free space is denoted as k .

Figure 3.2 Geometry of the impedance wedge.

With the necessary impedance boundary conditions, the total field surrounding an isolated impedance wedge is represented using the following contour integral [164],

$$U_z(\rho, \phi) = \frac{1}{2\pi j} \int_L \exp(jk\rho \cos \alpha) s\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right) d\alpha \quad (3.2)$$

where $L = L_1 + L_2$ is the Sommerfeld integration path shown in Figure 3.3 and $\bar{p}$ is correlated to the wedge external angle using $\bar{p}\pi = 2\Phi_1$. For a right-angled impedance wedge, $\bar{p}$ is equals to 1.5.

 Figure 3.3 Deformation of Sommerfeld contour $L = L_1 + L_2$ into steepest decent paths, $-\pi$ and π .

The integration path for L_1 and L_2 starts from $-\frac{\pi}{2} + j\infty$ to $\frac{3\pi}{2} + j\infty$ and $\frac{\pi}{2} - j\infty$ to $-\frac{3\pi}{2} - j\infty$, respectively. The spectral function, $s\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right)$ in (3.2) comprises of trigonometric functions, is given by [164]

$$s\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right) = \frac{\frac{1}{n} \sin\left(\frac{\phi_o}{\bar{p}}\right)}{\cos\left(\frac{\alpha - \phi}{\bar{p}}\right) - \cos\left(\frac{\phi_o}{\bar{p}}\right)} \frac{\Psi\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)} \quad (3.3)$$

and after applying a trigonometric identity*, it is reduced to

$$s\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right) = \frac{1}{2\bar{p}} \left\{ \cot\left[\frac{\alpha - (\phi - \phi_o)}{2\bar{p}}\right] - \cot\left[\frac{\alpha - (\phi + \phi_o)}{2\bar{p}}\right] \right\} \frac{\Psi\left(\alpha + \frac{\bar{p}\pi}{2} - \phi\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)} \quad (3.4)$$

The auxiliary function $\Psi(\alpha)$ is expressed in terms of Maliuzhinets function, ψ_{Φ_1} [105] as

$$\begin{aligned} \Psi(\alpha) = & \psi_{\Phi_1}\left(\alpha + \Phi_1 + \theta_+ - \frac{\pi}{2}\right) \cdot \psi_{\Phi_1}\left(\alpha + \Phi_1 - \theta_+ + \frac{\pi}{2}\right) \\ & \cdot \psi_{\Phi_1}\left(\alpha - \Phi_1 + \theta_- - \frac{\pi}{2}\right) \cdot \psi_{\Phi_1}\left(\alpha - \Phi_1 - \theta_- + \frac{\pi}{2}\right) \end{aligned} \quad (3.5)$$

Detailed properties of ψ_{Φ_1} can be found in the Appendix B.1 and

$$\begin{aligned} \sin \theta_{\pm} &= \frac{1}{\bar{\eta}_{\pm}} & \text{TE polarization} \\ &= \bar{\eta}_{\pm} & \text{TM polarization} \end{aligned}$$

where $\bar{\eta}_{\pm} = Z_{\pm} / Z_o$ and Z_o denotes the free space impedance. The normalized impedance is also

$$*\cot\left(\frac{x+y}{2}\right) - \cot\left(\frac{x-y}{2}\right) = \frac{2\sin(y)}{\cos(x) - \cos(y)}$$

defined as the inverse of the material refractive index. When the electric field has only component in the z direction, E_z it is considered as TE polarization whereas for TM polarization, the magnetic field has only z component, H_z . As evaluation of the contour integral of (3.2) in closed form is almost impossible, high frequency asymptotic evaluation using saddle point technique is applied. With a large parameter in the integrand, the original integration path can be deformed into the steepest decent paths (SDPs), $S(\alpha_{SDP1} = -\pi)$ and $S(\alpha_{SDP2} = \pi)$ as shown in Figure 3.3.

By using Cauchy's residue theorem [165], the original contour integral in (3.2) is re-expressed as

$$U_z(\rho, \phi) = 2\pi j \sum \text{Res} + \frac{1}{4\pi j \bar{p}} \int_{S(-\pi)-S(\pi)} \exp[jk\rho \cos \alpha] \left\{ \cot\left[\frac{\alpha - (\phi - \phi_o)}{2\bar{p}}\right] - \cot\left[\frac{\alpha - (\phi + \phi_o)}{2\bar{p}}\right] \right\} \frac{\Psi\left(\frac{\bar{p}\pi}{2} + \alpha - \phi\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)} d\alpha \quad (3.6)$$

where $\sum \text{Res}$ are the residues due to the poles being captured within the original and the deformed paths. It has been noted that the contour integral in (3.6) is similar to (3.2) except for the integral path. Two types of captured poles are introduced. The first type of poles, which is termed as geometrical poles correspond to the trigonometric functions i.e. cotangent terms in (3.4). The second type of poles, which is termed as surface poles are introduced by the Maliuzhinets function. All these poles will first be used in evaluating $2\pi j \sum \text{Res}$ in (3.6), which will give rise to geometrical optics field, i.e. incident, $U_z^i(\rho, \phi)$ and reflected, $U_z^r(\rho, \phi)$ waves. The surface wave, $U_z^{sw}(\rho, \phi)$ will also be included if it is being excited. Subsequently, the poles will also be used in evaluating the deformed contour integral in (3.6), which resulted in giving

the diffracted field $U_z^d(\rho, \phi)$. A summary of the poles which are the nearest to the SDPs and the respective residues for geometrical poles and surface poles are shown in Tables 3.1 and 3.2, respectively. Note that the first and the third geometrical poles are identical for ease of formulations.

Figure 3.4 illustrates the loci of geometrical poles (GPs) and surface poles (SPs) for a right-angled wedge with constant normalized surface impedance. The wedge is illuminated by TE polarized incoming plane wave. A geometrical pole is captured when it falls in between the SDPs of $-\pi$ and π whereas a surface pole is excited when it is close enough to any of the SDPs. The poles location in Figure 3.4 is associated with the observation angle at $\phi = 0$. When the observation angle is increased, it is expected that the poles will move to the right as indicated by their respective arrow.

Table 3.1 Geometrical poles and the respective residues

Geometrical Poles, α_i	Residues (Res), Res_i
$\alpha_1 = \phi - \phi_o$	$\text{Res}_1 = \frac{1}{2\pi j} \exp[jk \rho \cos(\phi - \phi_o)]$
$\alpha_2 = \phi + \phi_o - 2\bar{p}\pi$	$\text{Res}_2 = \frac{-1}{2\pi j} \frac{\Psi\left(-\frac{3\bar{p}\pi}{2} + \phi_o\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)} \exp[jk \rho \cos(\phi + \phi_o - 2\bar{p}\pi)]$
$\alpha_3 = \phi - \phi_o$	$\text{Res}_3 = \frac{1}{2\pi j} \exp[jk \rho \cos(\phi - \phi_o)]$
$\alpha_4 = \phi + \phi_o$	$\text{Res}_4 = \frac{-1}{2\pi j} \frac{\Psi\left(\frac{\bar{p}\pi}{2} + \phi_o\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)} \exp[jk \rho \cos(\phi + \phi_o)]$

Table 3.2 Surface poles and the respective residues

Surface Poles, α_i	Residues (Res), Res_i
$\alpha_5 = \phi + \pi + \theta_+$	$\text{Res}_5 = \frac{-1}{2\pi j} \frac{\frac{2}{\bar{p}} \sin\left(\frac{\phi_o}{\bar{p}}\right) \tan(\theta_+)}{\cos\left(\frac{\pi + \theta_+}{\bar{p}}\right) - \cos\left(\frac{\phi_o}{\bar{p}}\right)} \frac{\Psi\left(\frac{\bar{p}\pi}{2} - \pi - \theta_+\right)}{\Psi\left(\frac{n\pi}{2} - \phi_o\right)}$ $\exp[-jk\rho \cos(\phi + \theta_+)]$
$\alpha_6 = \phi - (\pi + \bar{p}\pi + \theta_-)$	$\text{Res}_6 = \frac{-1}{2\pi j} \frac{\frac{2}{\bar{p}} \sin\left(\frac{\phi_o}{\bar{p}}\right) \tan(\theta_-)}{\cos\left(\frac{\pi + \theta_-}{\bar{p}}\right) + \cos\left(\frac{\phi_o}{\bar{p}}\right)} \frac{\Psi\left(-\frac{\bar{p}\pi}{2} + \pi + \theta_-\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)}$ $\exp[-jk\rho \cos(\phi - \theta_- - \bar{p}\pi)]$

Figure 3.4 Geometrical poles (GPs) and surface poles (SPs) loci for a right-angled wedge, $\bar{p} = 1.5$, TE polarization, $\phi_o = 90^\circ$, $0 < \phi < \bar{p}\pi$ and $\bar{\eta}_+ = \bar{\eta}_- = 0.254 + j0.00464$. (Geometrical pole: GP, Surface pole: SP)

Hence, the total field in (3.6) is expressed in a general form as

$$U_z(\rho, \phi) = U_z^i(\rho, \phi) + U_z^r(\rho, \phi) + U_z^{sw}(\rho, \phi) + U_z^d(\rho, \phi) \quad (3.7)$$

where

$$U_z^i(\rho, \phi) = 2\pi j \text{Res}_1 H(\pi - |\phi - \phi_o|) \quad (3.8)$$

$$U_z^r(\rho, \phi) = 2\pi j [\text{Res}_2 H(\pi - |\phi + \phi_o|) + \text{Res}_3 H(\pi - |\phi + \phi_o - 2\bar{p}\pi|)] \quad (3.9)$$

$$\begin{aligned} U_z^{sw}(\rho, \phi) = & 2\pi j \text{Res}_4 H\{-\phi - \text{Re}(\theta_+) - \text{gd}[\text{Im}(\theta_+)]\} \\ & + 2\pi j \text{Res}_5 H\{\phi - \bar{p}\pi - \text{Re}(\theta_-) - \text{gd}[\text{Im}(\theta_-)]\} \end{aligned} \quad (3.10)$$

and $\text{gd}(x)$ is the Guderman function defined as $\text{gd}(x) = \cos^{-1}[1/\cosh(x)]\text{sgn}(x)$.

Function $H(x)$ is the Heaviside step function that gives 1 when $x > 0$ and 0 when $x < 0$. It accounts for the conditions required to capture the poles within the SDPs and the Sommerfeld contour integrals. The diffracted field, $U_z^d(\rho, \phi)$ is obtained by solving the integral function in (3.6) using additive method [166] of asymptotic approach. In order to obtain a complete solution of diffracted field, the surface poles must be included although the poles are not captured within the enclosed region. The solution to the integral involves expansion of Taylor's series, is given by

$$\begin{aligned} U_z^d(k\rho) \sim & \frac{\exp[-jk\rho]}{\sqrt{k\rho}} \left\{ \sqrt{\pi} \sum_{i=1}^6 \frac{\tilde{R}_i}{\sqrt{-2j} \cos(\alpha_i/2)} \left(1 - F \left[2k\rho \cos^2 \left(\frac{\alpha_i}{2} \right) \right] \right) \right. \\ & \left. + G_s \sqrt{\pi} + \sum_i \sum_{m=1}^{\infty} \frac{A_{im} \Gamma(m+1/2)}{(k\rho)^m} \right\} \end{aligned} \quad (3.11)$$

where

$$A_{im} = \frac{G^{(2m)}(0)}{(2m)!} + \frac{\tilde{R}_i}{\left\{ \sqrt{-2j} \cos \left(\frac{\alpha_i}{2} \right) \right\}^{2m+1}}$$

$$\tilde{R}_i = \text{Res}_i \exp[jk\rho \cos(\alpha_i)]$$

and
$$G_s = \sqrt{\frac{-2}{j}} [g_1(-\pi) - g_2(-\pi) - g_3(\pi) + g_4(\pi)]$$

$$g_{1,3}(x) = \frac{1}{4\pi j\bar{p}} \cot\left[\frac{x - (\phi - \phi_o)}{2\bar{p}}\right] \frac{\Psi\left(\frac{\bar{p}\pi}{2} + x - \phi\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)}$$

$$g_{2,4}(x) = \frac{1}{4\pi j\bar{p}} \cot\left[\frac{x - (\phi + \phi_o)}{2\bar{p}}\right] \frac{\Psi\left(\frac{\bar{p}\pi}{2} + x - \phi\right)}{\Psi\left(\frac{\bar{p}\pi}{2} - \phi_o\right)}$$

The notation, G_s should not be taken as the Green's function. Higher order derivatives of $G^{(2m)}(0)$ are given in Appendix C.1. $F(x)$ is the transition function [93] defined as

$$F(x) = 2j\sqrt{x} \exp[jx] \int_{\sqrt{x}}^{\infty} \exp(-j\xi^2) d\xi \quad (3.12)$$

and the function is extended to complex number by taking the branch cut along the positive imaginary axis [167]. $\Gamma(x)$ is the gamma function [168]. More details for $F(x)$ and $\Gamma(x)$ are given in Appendix B. The poles, α_i are defined in Tables 3.1 and 3.2.

If only the first term in the solution ($m = 0$) is included, the last term in the right hand side of (3.11) yields value of zero. In this case, the diffracted field is expressed as

$$U_z^d = \frac{\exp(-jk\rho)}{\sqrt{\rho}} (D^{nu} + D^{go+sw}) \quad (3.13)$$

where
$$D^{nu} = \sqrt{\frac{\pi}{k}} G_s + f_1(m) \quad (3.14)$$

and
$$D^{go+sw} = \frac{\exp(-j\pi/4)}{2\sqrt{2k\pi}} \sum_{i=1}^6 Q_i \frac{\left\{1 - F\left[2k\rho \cos^2\left(\frac{\alpha_i}{2}\right)\right] + f_2(m)\right\}}{\cos\left(\frac{\alpha_i}{2}\right)} \quad (3.15)$$

$$\begin{aligned}
 Q_1 &= \hat{R}_1 \cdot [1 - P_{2\pi}(\alpha_1 - \pi)] & Q_2 &= \hat{R}_2 \cdot P_{2\pi}(\alpha_4 - \pi) \\
 Q_3 &= \hat{R}_3 \cdot P_{2\pi}(\alpha_1 - \pi) & Q_4 &= \hat{R}_4 \cdot P_{2\pi}(\alpha_2 - \pi) \\
 Q_5 &= \hat{R}_5 \cdot P_{2\pi}[\text{Re}(\alpha_5) - \pi] & Q_6 &= \hat{R}_6 \cdot P_{2\pi}[\text{Re}(\alpha_6) - \pi]
 \end{aligned}$$

with $\hat{R}_i = 2\pi j \tilde{R}_i$. $P_{2\pi}(x)$ is the unit rect function defined as 1 for $-\pi < x < \pi$ and 0 otherwise.

When higher order terms in the series ($m \geq 1$) are considered, additional terms of $f_1(m)$ and $f_2(m)$ are added into (3.14) and (3.15). The additional terms, $f_1(m)$ and $f_2(m)$ are given in Table 3.3. The functions involve higher order derivative of $g_{1,3}(x)$ and $g_{2,4}(x)$ which are defined earlier in (3.11) for G_s . From (3.13), one can easily identify there are four individual components, I_i that contribute to each higher order term in the diffracted field. The expressions are given in Table 3.4.

Table 3.3 Additional terms in (3.14) and (3.15)

Term	m	$f_1(m)$	$f_2(m)$	Accuracy
First	0	-	-	$(k\rho)^{-1/2}$
Second	1	$\frac{\sqrt{\pi}}{4k^{3/2}\rho} [G_1''(0) - G_2''(0) - G_3''(0) + G_4''(0)]$	$\frac{j}{2k\rho[\cos(\alpha_i) + 1]}$	$(k\rho)^{-3/2}$
Third	2	$\frac{\sqrt{\pi}}{32k^{5/2}\rho^2} [G_1^{IV}(0) - G_2^{IV}(0) - G_3^{IV}(0) + G_4^{IV}(0)]$	$\frac{-3}{4k^2\rho^2[\cos(\alpha_i) + 1]^2}$	$(k\rho)^{-5/2}$

where

$$\begin{aligned}
 G_{1,2,3,4}''(0) &= -\frac{1}{j} \sqrt{\frac{-2}{j}} \exp(-j\pi/4) \left[\frac{g_{1,2,3,4}(\alpha)}{2} + 2g_{1,2,3,4}''(\alpha) \right] \\
 G_{1,2,3,4}^{IV}(0) &= -\sqrt{\frac{-2}{j}} \left[4g_{1,2,3,4}^{IV}(\alpha) + 10g_{1,2,3,4}''(\alpha) + \frac{9}{4}g_{1,2,3,4}(\alpha) \right]
 \end{aligned}$$

with $\alpha = -\pi$ for subscript of 1, 2 and $\alpha = \pi$ for subscript of 3, 4.

Table 3.4 Individual component, I_i for each higher order term, m in the diffracted field

Term	m	Individual Component, I_i
Second	1	$\frac{\exp(-jk\rho)}{4(k\rho)^{3/2}} \left(\pm \sqrt{\pi} G_i^{II}(0) + \frac{j \exp(-j\pi/4) Q_i}{\sqrt{2} \pi [\cos(\alpha_i) + 1] \cos(\alpha_i/2)} \right)$
Third	2	$\frac{\exp(-jk\rho)}{(k\rho)^{5/2}} \left(\pm \frac{\sqrt{\pi} G_i^{IV}(0)}{32} - \frac{3 \exp(-j\pi/4) Q_i}{8\sqrt{2} \pi [\cos(\alpha_i) + 1]^2 \cos(\alpha_i/2)} \right)$

where the upper sign of $\pm$ is applied when $i = 1, 4$ and the lower sign is applied when $i = 2, 3$.

Alternatively, the diffracted field can also be decomposed into

$$U_z^d = U_z^{d-GPs} + U_z^{d-SPs} \quad (3.16)$$

where each individual term is corresponded to the respective GPs and SPs. The contribution from non-uniform diffraction coefficient has been lumped into the respective GPs diffracted field, U_z^{d-GPs} .

A summary of the steps for high frequency analysis of impedance wedge using UTD is given in Figure 3.5. The total electromagnetic field in the external region of the wedge is a combination of geometrical optics, surface and diffracted fields. These fields are contributed from the poles that are being captured in the deformed path of Sommerfeld integrals. Higher orders in the asymptotic series of the diffracted field are also given.

Figure 3.5 Flow in high frequency electromagnetic analysis of impedance wedge using UTD.

3.2 Comparison of UAT and UTD

The UAT and UTD formats are known to be identical to each other. This is provided that a complete expansion of the series is taken into consideration. The differences when a finite number of terms in the series are retained in the solution are discussed below. In UAT, the diffracted field is expressed as follows [169],

$$U_z^d = \frac{\exp(jk\rho)}{\sqrt{2\pi}} \sum_{m=0}^q \left(\frac{j}{k\rho} \right)^{m+1/2} J_m \left[s \left(\frac{\bar{p}\pi}{2} - \phi - \pi \right) - s \left(\frac{\bar{p}\pi}{2} - \phi + \pi \right) \right] \quad (3.17)$$

where q denotes positive integers and the J_m operator is given by

$$J_0 = 1$$

$$J_{m \geq 1} = \frac{(-1)^m}{2^m m!} \left[\frac{d^2}{d\phi^2} + \left(m - \frac{1}{2} \right)^2 \right]$$

and $s(\alpha)$ is the spectral function defined in (3.3). When the point of observation is located far away from the edge but near to the impedance surface, it is shown that if only the first term of the operator, J_0 is considered, the diffracted field yields value of zero. This is because (3.17) reverts to the diffracted field with non-uniform diffraction coefficient, D^{nu} as in UTD.

$$U_z^d = \frac{\exp(-jk\rho)}{\sqrt{\rho}} D^{nu} \quad (3.18)$$

At the wedge surface, be it at $\phi = 0$ or $\phi = \bar{p}\pi$, the spectral functions in (3.17) cancel out each other to give zero non-uniform diffraction coefficient, i.e. $D^{nu} = 0$. Hence, the edge diffracted field in UAT can only be determined by taking the higher order of the operator, i.e. $m \geq 1$. This implies that leading terms with at least up to $(k\rho)^{-3/2}$ is required to obtain the solution for a field point on the wedge. However, it does not apply when the edge diffracted field in UTD is obtained using additive method. As shown in (3.13), there are two main parts of diffraction coefficient, namely non-uniform diffraction coefficient, D^{nu} and diffraction coefficient, D^{go+sw} contributed from GPs and SPs. Although the D^{nu} term vanishes at the wedge surfaces, the D^{go+sw} term remains non-zero and gives rise to the diffracted terms. Apparently, the first leading term of $(k\rho)^{-1/2}$, $m = 0$ in the series is able to provide a solution to the field point along or near to the wedge surfaces. Contribution of higher order terms ($m \geq 1$) to the accuracy of solutions depends on the series convergence and the distance factor, $k\rho$.

3.3 Numerical Results and Discussion

3.3.1 Field on Wedge Surface

In this section, plane wave with amplitude of 1 arbitrary unit is considered to illuminate a right-angled impedance wedge as shown in Figure 3.2. The normalized surface impedance along $\phi = 0$ and $2\Phi_1$ is taken as 0.1 and j , respectively. These are arbitrary values but it simplifies the formulation such that no surface fields are involved. For each distance, the results obtained using asymptotic approach for different order of terms is compared with the exact solutions of the contour integral in (3.2) [116].

(a) Total Field

Figures 3.6 and 3.7 show the total field along $\phi = 2\Phi_1$ for a right-angled wedge, $\bar{p} = 1.5$ with different incident angles and observation distances from the wedge corner. In these figures, the legend of one term, two terms and three terms denote that the asymptotic solutions are obtained by including the expansion series up to the first ($m = 0$), second ($m = 1$) and third terms ($m = 2$), respectively for the diffracted field. For example, the first ($m = 0$) and second ($m = 1$) terms are included in the two terms solution. It is seen that at distance of $k\rho = 5$, matching of the one term asymptotic results with the exact solution is excellent as presented in Figure 3.6. It is also shown that inclusion of higher order terms in the series for two and three terms results does not improve accuracy of the numerical results drastically, as the solution has converged to a limit and overlapped with the results of one term solution. More results and findings of the contribution

Figure 3.6 Total field along wedge surface, $\phi = 2\Phi_1$ with $k\rho = 5$. The normalized wedge impedance is 0.1 and j at $\phi = 0$ and $2\Phi_1$, respectively.

Figure 3.7 Total field along wedge surface, $\phi = 2\Phi_1$ with $k\rho = 1$. The normalized wedge impedance is 0.1 and j at $\phi = 0$ and $2\Phi_1$, respectively.

from each higher order term, m are presented in Section 3.3.1 (d). When $k\rho$ reduces to 1, the results deviate from the exact solution as presented in Figure 3.7. On the other hand, the total fields obtained using non-uniform diffraction coefficient, D^{nu} are also shown in Figures 3.6 and

3.7. As expected, incident angle below 90° yields zero total field when the non-uniform diffraction coefficient vanishes.

(b) Individual Field

The total field presented in Figures 3.6 and 3.7 is a combination of geometrical optics and diffracted fields. Figure 3.8 shows the contribution of each individual field to the total field. As the observation point is located at $\phi = 2\Phi_1$ of the wedge surface, incident field is shown after incident angle of 90° . In this case, incident angle of 90° can be treated as the incident boundary. Below this angle, diffracted field is the only electromagnetic field that dominates the total field. In Figures 3.6, 3.7 and 3.8, the respective electromagnetic field with incident angles below 90° are denoted by Regions A[^], A['], and A, respectively. It is observed that the total field (using three terms) in Regions A[^] and A['] of Figures 3.6 and 3.7, respectively are identical to the diffracted

Figure 3.8 Distribution of fields at different $k\rho$ using three terms in the series expansion.

field in Region A of Figure 3.8 at their respective observation distance, $k\rho$, either 1 or 5. On the other hand, when the point of observation is far away from the wedge corner, it is expected that the influence of the diffracted field becomes less prominent. The total field will revert to the free space condition, which is without any disturbances. However, if the point of observation is near to the wedge corner, the influence of the diffracted field becomes more significant. It is clearly shown in Figure 3.8 that the magnitude of the diffracted field for $k\rho = 1$ is greater than $k\rho = 5$ at any incident angles. The results presented in this figure are based on three terms expansion, which include leading term up to $(k\rho)^{-5/2}$.

(c) Contribution of Poles to Diffracted Field

As noted in (3.15) and (3.16), the total diffracted field is obtained from the residue of geometrical and surface poles. Geometrical poles are caused by the trigonometric terms and surface poles are caused by the Maliuzhinets's terms in the integrand. In evaluating the diffracted field using the additive method of high frequency asymptotic approach, the surface poles must be considered even though their corresponded surface waves are not excited. The contribution of the respective poles to the diffracted field following (3.16) will now be studied. Figure 3.9 shows the magnitude of diffracted field contributed by solely the geometrical poles or surface poles at different $k\rho$ distances. Number of terms included is the same as in Figure 3.8. At $k\rho = 10$, the contribution of surface poles to the total diffracted field is relatively insignificant as compared to the geometrical poles. However, when $k\rho$ reduces to 5, the contribution of surface poles is no longer negligible and it is important to include them to give an accurate solution to the total diffracted field.

Figure 3.9 Distribution of diffracted fields at different $k\rho$ using three terms in the series expansion. (Geometrical Poles: GPs, Surface Poles: SPs)

(d) Individual Component in Higher Order Term of Diffracted Field

The total field presented in Figure 3.6 is constructed by including the expansion series up to the first ($m = 0$), second ($m = 1$) and third terms ($m = 2$) for the diffracted field. This part aims to study the contribution of each single higher order term ($m = 1, 2$) to the diffracted field. Each higher order term, m is dominated by four distinguished components, I_i ($i = 1, 2, 3, 4$). The explicit expressions are given in Table 3.4. Figure 3.10 (a) and (b) show the real and imaginary parts of all the four components that contribute to the second order, $m = 1$ in the diffracted field used to construct the total field in Figure 3.6. It is shown that the real and imaginary parts of the first and second components, I_1 and I_2 are in opposite sign when the incident angles are below 75° . The absolute values of $\text{Re } I_{1,2}$ and $\text{Im } I_{1,2}$ decrease exponentially to near zero when the incident angles are increased from 0° to near 75° . Above incident angle of 75° , the absolute

values are closed to zero as well. On the other hand, the contribution from the third and fourth components, I_3 and I_4 are negligible. The same trends are also observed for the components in the third order, $m = 2$ of the diffracted field, as presented in Figure 3.11 (a) and (b). All these individual components, I_i ($\text{Re } I_i + j \text{Im } I_i$) are added up to give the resultant amplitude of the second ($m = 1$) and third ($m = 2$) orders of the diffracted field presented in Figure 3.12. With I_1 & I_2 almost cancel out each other completely and I_3 & I_4 are negligible, the amplitudes for both orders across different incident angles are relatively low, i.e. below 0.06. This explains why the contribution from the higher order terms, $m \geq 1$ in the diffracted field is relatively insignificant and does not contribute to the accuracy improvement of the total field presented in Section 3.3.1 (a).

Figure 3.10 (a) Real part and (b) imaginary part of the components, I_i ($i = 1, 2, 3, 4$) that contribute to the second order, $m = 1$ in the diffracted field.

Figure 3.11 (a) Real part and (b) imaginary part of the components, I_i ($i = 1, 2, 3, 4$) that contribute to the third order, $m = 2$ in the diffracted field.

Figure 3.12 Amplitude of each higher order term, $m = 1$ and $m = 2$ in the diffracted field.

3.3.2 Lossless and Lossy Wedges

The following section is devoted to study the electromagnetic scattering of lossless and lossy wedges using the formulation developed in Section 3.1. Lossless wedge is characterized by a real number of refractive index, whereas the refractive index for lossy wedge is a complex number. The study of electromagnetic scattering here can be applied in wafer integrated circuits fabrication, especially in metrology. The wedge can be formed as part of the line structures on the wafer for alignment marks or overlay targets. The materials of the wedge that are being considered here are resist (lossless material) and polysilicon (lossy material). Both materials are commonly used in wafer integrated circuits fabrication. The refractive index of resist and polysilicon at wavelength, λ of 633 nm are given in Appendix A. When UTD is applied here, the wedge is modeled as an impedance wedge. Plane wave with arbitrary linear polarization at perpendicular incidence is considered and the region surrounding the wedge has a refractive index of 1. In the usual case, the observation points are located at certain elevated distance, h_1 on top of the wedge as shown in Figure 3.13. All the results presented subsequently are based on three terms expansion. All the parameters remain the same unless otherwise stated. The UTD

Figure 3.13 Geometry of the right-angled wedge.

results are also compared with FDTD solution obtained from an electromagnetic solver, EM Explorer [170]. The step size in FDTD is 0.01 μm and the value is considered as converged when the variation is less than 0.001. The two parameters, $\Delta|E_z|$ and ΔPhase (radian) defined as

$$\Delta|E_z| = |E_z|(\text{UTD}) - |E_z|(\text{FDTD}) \quad (3.19)$$

$$\Delta\text{Phase} = \text{Phase}(\text{UTD}) - \text{Phase}(\text{FDTD}) \quad (3.20)$$

are used to denote the amplitude and phase differences of the UTD and FDTD results.

(a) Transverse Electric (TE) Polarization

Figures 3.14 and 3.15 show the magnitude and phase of total electric field for an isolated resist wedge (633 nm wavelength) at $ky = 5$ ($h_1 = 0.8\lambda$) and $ky = 10$ ($h_1 = 1.6\lambda$), respectively. The incident electric field is considered to be TE polarized and has amplitude of 1. The UTD results for both magnitude and phase show an excellent match for $ky = 10$ with the results obtained from the reference FDTD solution, as presented in Figure 3.15. It is shown in Figure 3.14 that the accuracy of the results for resist wedge drops but it is not significant when the level of observation is nearer to the wedge surface, i.e. $ky = 5$. The maximum magnitude of amplitude and phase differences, $\Delta|E_z|$ and ΔPhase are increased from 0.023 and 0.029 radian for $ky = 10$ (Figure 3.15) to 0.032 and 0.033 radian for $ky = 5$ (Figure 3.14), respectively. On the other hand, Figures 3.16 and 3.17 show the magnitude and phase of electric field for an isolated polysilicon wedge (633 nm wavelength) at $ky = 5$ and $ky = 10$, respectively. The UTD results for both observation distances show a good match with the FDTD results. The maximum magnitude of amplitude difference, $\Delta|E_z|$ is reduced from 0.018 for $ky = 5$ (Figure 3.16) to 0.014 for $ky = 10$ (Figure 3.17). On the other hand, the maximum magnitude of phase difference, ΔPhase is 0.018 radian for both observation distances, $ky = 5$ and 10.

Figure 3.14 Magnitude and phase of electric field at $ky = 5$ for resist wedge.

Figure 3.15 Magnitude and phase of electric field at $ky = 10$ for resist wedge.

Figure 3.16 Magnitude and phase of electric field at $ky = 5$ for polysilicon wedge.

Figure 3.17 Magnitude and phase of electric field at $ky = 10$ for polysilicon wedge.

The study of the electromagnetic scattering of lossless and lossy wedges is extended to 193 nm wavelength. This is to validate the formulation developed in this chapter is applicable to other application, especially in imaging involving DUV wavelength for advanced photolithography process. The subsequent results in this part are devoted for incident wavelength of 193 nm, with the other parameters remain the same as previous. For lossless wedge, the refractive index is taken as 1.55 whereas for lossy wedge, the refractive index is taken as $3.93 - 0.0717j$. Figures 3.18 and 3.19 show the magnitude and phase of the total electric field for a lossless wedge at $ky = 5$ and 10, respectively. One can observe that the UTD results show an excellent match with the reference FDTD solution. There is no significant deviation of the UTD results from the reference solution. The maximum magnitude of amplitude and phase differences, $\Delta|E_z|$ and ΔPhase are reduced from 0.033 and 0.034 radian for $ky = 5$ (Figure 3.18) to 0.024 and 0.025 radian $ky = 10$ (Figure 3.19), respectively. On the other hand, the magnitude and phase of the total electric field for a lossy wedge at $ky = 5$ and 10 are presented in Figures 3.20 and 3.21, respectively. Similarly, there is no significant deviation of the UTD results from the reference solution. The maximum magnitude of amplitude difference, $\Delta|E_z|$ is reduced from 0.022 for $ky = 5$ (Figure 3.20) to 0.017 $ky = 10$ (Figure 3.21). However, the maximum magnitude of phase difference, $\Delta|E_z|$ shows a slight increase from 0.024 radian for $ky = 5$ (Figure 3.20) to 0.038 radian for $ky = 10$ (Figure 3.21). With all these findings, it is concluded that the UTD approach is applicable to 193nm, with no significant sacrifice in the accuracy.

Figure 3.18 Magnitude and phase of electric field at $ky = 5$ for a lossless wedge with refractive index of 1.55. The illumination wavelength is 193 nm.

Figure 3.19 Magnitude and phase of electric field at $ky = 10$ for a lossless wedge with refractive index of 1.55. The illumination wavelength is 193 nm.

Figure 3.20 Magnitude and phase of electric field at $ky = 5$ for a lossy wedge with refractive index of $3.93 - 0.0717j$. The illumination wavelength is 193 nm.

Figure 3.21 Magnitude and phase of electric field at $ky = 10$ for a lossy wedge with refractive index of $3.93 - 0.0717j$. The illumination wavelength is 193 nm.

(b) Transverse Magnetic (TM) Polarization

Figures 3.22 and 3.23 show the magnitude and phase of total magnetic field for an isolated resist and polysilicon wedge, respectively at $k_y = 5$. The incident magnetic field is considered to be TM polarized and has amplitude of 1. It is clearly shown in Figure 3.22 that the results of resist impedance wedge match with the FDTD results in the range of $k_x = -40$ to $k_x = 10$ but deviation of results is observed when k_x is 10 to 40. The results for polysilicon in Figure 3.23 shows an average error of 10 % for k_x less than 0 although a perfect match of results is obtained for k_x greater than 0. The magnitudes of the diffracted field for both resist and polysilicon wedges are presented in Figure 3.24. As predicted, a discontinuity of the magnitude exists at the origin, $k_x = 0$ to enforce continuity of total field across the shadow boundaries. For polysilicon wedge, the diffracted field decreases smoothly from $k_x = 0$ for both sides. However, the diffracted field of

Figure 3.22 Magnitude and phase of magnetic field at $k_y = 5$ for resist wedge.

Figure 3.23 Magnitude and phase of magnetic field at $k_y = 5$ for polysilicon wedge.

resist wedge decreases smoothly only for the negative part of k_x . For positive k_x , the diffracted field gives a local minimum before rising to a constant magnitude. This causes the mismatch of TM polarized total magnetic field with FDTD results for resist wedge.

Figure 3.24 Magnitude of the diffracted field at $k_y = 5$ for resist (solid line) and polysilicon (dashed line) wedges.

3.4 Concluding Summary

In this chapter, the high frequency asymptotic method has been used to study the external diffraction of an impedance wedge. The formulation presented here is based on UTD additive method and leading terms up to $(k\rho)^{-5/2}$ has been included. One of the findings shows that the UTD solution with the first leading term, $(k\rho)^{-1/2}$ is sufficient to provide accurate results for a field point at distance of $k\rho = 5$ from the wedge. Higher order of the asymptotic series, $(k\rho)^{-3/2}$ and $(k\rho)^{-5/2}$ does not contribute to the improvement of the results in a significant way. The results for total diffracted field and its contribution from geometrical and surface poles are also shown. When the field point is far away from the corner, $k\rho \approx 10$ their influence becomes less dominant. On the other hand, when the impedance model is used to study the diffraction of isolated lossless and lossy wedges, the TE polarization results show a good agreement with the FDTD solution. However, the results for TM polarization show discrepancy due to the properties of diffracted field. The model can be extended to study the diffraction of a full line structures by incorporating the impedance wedge as part of the structures. Before performing this study, analysis of the internal diffraction of a wedge will be treated in the next chapter.

CHAPTER 4 PENETRABLE WEDGE WITH INTERNAL DIFFRACTION

In Chapter 3, the impedance model has been applied to study the electromagnetic scattering of a wedge. This includes a detailed formulation for the geometrical optics, surface and diffracted fields, which are induced in accordance to the captured poles on the Sommerfeld contour complex plane. However, the given solutions are constrained to the external region. There is no information on the scattered electromagnetic field inside the wedge. For example, the internal diffraction as illustrated in Figure 4.1 was not covered in Chapter 3. The internal diffracted field must exist to compensate the amplitude discontinuities caused by the geometrical optics field inside the wedge. Hereafter, the wedge is referred as a penetrable wedge.

Figure 4.1 Internal diffraction of a penetrable wedge.

In order to obtain the internal electromagnetic field of a penetrable wedge, the dual Sommerfeld contour integrals are required in the analysis. Here, one can expect the need to solve a more subtle problem, since two distinct wave numbers are involved, i.e. k and k_1 for the external and internal mediums, respectively. The famous Snell's law is one of the key equations to correlate the electromagnetic field in two different mediums. With a multi-valued function [171, 172] in

the Snell's law, the correct branch must be selected to give a meaningful solution to the scattered electromagnetic field inside the wedge. The complexities of the problem are further exacerbated by the existence of branch cuts on the dual Sommerfeld contour integral planes. When the branch cut and poles are located near to the steepest decent path, it is difficult to obtain an explicit expression for the diffracted field based on rigorous asymptotic analysis [173]. In this work, the approaches to tackle these problems are addressed in the current chapter.

The main objective of this chapter is to obtain a solution for the internal electromagnetic scattering of a right-angled penetrable wedge, which includes both geometrical optics and diffracted fields. For a complete solution, the electromagnetic scattering solution for the external region of a penetrable wedge is also given. The flow of this chapter is as follows.

1. Firstly, the electromagnetic scattering problem for a right-angled penetrable wedge is established by the use of dual Sommerfeld contour integrals. For different quadrants of incident angles, the poles that give rise to physical field are identified and the corresponded residues are deduced.
2. Subsequently, a detailed discussion on the selection of branch cuts for multi-valued functions in the formulation is given. Understanding of the branch cut selection is important to obtain a unique solution across different complex domains.
3. By exploiting the deduced residues, all the geometrical optics and diffracted fields, for a penetrable wedge are given. The diffracted fields developed in this work are based on a proposed heuristic solution to correctly compensate the discontinuities caused by the geometrical optics field. Besides that, the existence of lateral field in the wedge is also discussed.

4. Finally, the numerical results for the internal electromagnetic field of a penetrable wedge are presented. Different illumination angles, wavelengths and refractive indices for the penetrable wedge are studied.

The formulations presented in this section focus on transverse electric (TE) polarization, which the electric field has its only component in the z -axis. A time harmonic of $\exp(j\omega t)$ is assumed and suppressed throughout the formulation.

In this chapter, the formulation for the external geometrical optics and diffracted fields of a penetrable wedge is also included. One may wonder why this is needed, since the external scattered field has been studied using impedance approach in Chapter 3. There are three main reasons. Firstly, the internal scattered field in this chapter is obtained by solving a specific boundary value problem, which is different from the impedance model approach. It requires that the external scattered field must also co-exist and consider in the formulation. Secondly, the external diffracted field presented in this chapter is based on a heuristic solution, which in turn, gives greater tolerance in the accuracy. For better accuracy, Maliuzhinets impedance solution for the external field is preferred in this case and the formulations in Chapter 3 are required. Thirdly, another point should be clear later in Section 4.3, is that even though the (external) heuristic diffraction coefficient is formulated here, it is different from the (external) heuristic diffraction coefficient found in the literature.

4.1 Formulation of the Penetrable Wedge Problem

The geometry of a penetrable wedge is presented in Figure 4.2. Cylindrical polar coordinate $\{\rho, \phi', z\}$ is used. The external region of the wedge, $|\phi'| < \Phi_1$ is exposed to vacuum, n_0 whereas

the internal region, $|\phi' - \pi| < \Phi_2$ is occupied by materials with refractive index n_1 . The external and internal angles of the penetrable wedge are given by $2\Phi_1$ and $2\Phi_2$, respectively. For a right-angled case, Φ_1 and Φ_2 are given by $\frac{3}{4}\pi$ and $\frac{1}{4}\pi$, respectively.

Figure 4.2 Geometry of a penetrable wedge.

A plane wave with unit amplitude is considered to illuminate the wedge. The incident field is given by

$$U_z^i = \hat{z} \exp[jk\rho \cos(\phi' - \phi_o')] \quad (4.1)$$

where k denotes the wave number in the external region. The Sommerfeld contour integrals used to represent the total field in the external and internal regions of the wedge are given by

$$U_z(k\rho, \phi') = \frac{1}{2\pi j} \int_{L_{\text{ext}}} \exp(jk\rho \cos \alpha) f_1(\alpha + \phi') d\alpha, \quad |\phi'| < \Phi_1 \quad (4.2)$$

$$V_z(k_1\rho, \phi') = \frac{1}{2\pi j} \int_{L_{\text{int}}} \exp(jk_1\rho \cos \beta) f_2(\beta + \phi' - \pi) d\beta \quad |\phi' - \pi| < \Phi_2 \quad (4.3)$$

where $L_{\text{ext}} = L_{\text{ext}1} + L_{\text{ext}2}$ and $L_{\text{int}} = L_{\text{int}1} + L_{\text{int}2}$ are the double loops contour of integration shown in Figures 4.3 (a) and (b), respectively. The wave number in the wedge is denoted by k_1 . The total field given in (4.2) and (4.3) satisfies the Helmholtz and Sommerfeld radiation conditions

Figure 4.3 Sommerfeld integrals for the penetrable wedge (a) external region, $f_1(\alpha)$ and (b) internal region, $f_2(\beta)$.

where the two analytic functions, $f_1(\cdot)$ and $f_2(\cdot)$ must be sought for the diffracted field. In this work, a heuristic solution for the diffracted field is proposed. This will be discussed in Section 4.3. The next step is to express this two spectral functions using boundary conditions with respect to the problem of penetrable wedge. The boundary conditions along the two surfaces, S_1 and S_2 of the wedge are given by

$$U_z = V_z \quad (\text{Dirichlet condition}) \quad (4.4)$$

$$\frac{\partial U_z}{\partial \phi'} = \nu \frac{\partial V_z}{\partial \phi'} \quad (\text{Neumann condition}) \quad (4.5)$$

and for TE polarization, ν is the permeability ratio of the two mediums, μ_0 / μ_1 . It is equal to unity for non-magnetic materials in the wedge. In order to solve the problems by equating the Sommerfeld integrals at the boundary conditions, there is a need to reduce all kernels in the integrals to a common term, either in $\exp(jk\rho \cos \alpha)$ or $\exp(jk_1\rho \cos \beta)$. An inverse cosine function, $b(\alpha)$ is introduced and defined as,

$$b(\alpha) = \cos^{-1}(\gamma \cos \alpha) \quad (4.6)$$

and its inverse,
$$a(\beta) = \cos^{-1}(\gamma^{-1} \cos \beta) \quad (4.7)$$

with $\gamma = n/n_1$. One can easily identify that (4.6) and (4.7) are the famous Snell's law [174] for refraction phenomenon and two distinct refractive indices are involved. Equations (4.6) and (4.7) are multi-valued functions and the selection of their associated branch cuts are discussed thoroughly in Section 4.2. This is important to ensure a unique mapping between two complex domains.

Following the approach made by Budaev [175, 176], the two spectral functions, $f_1(\bullet)$ and $f_2(\bullet)$ can be sought in terms of their symmetric and antisymmetric components, given as

$$f_{1,2}(\alpha) = f_{1,2}^a(\alpha) + f_{1,2}^s(\alpha) \quad (4.8)$$

where
$$f_{1,2}^s(\alpha) = \frac{1}{2} [f_{1,2}(\alpha) + f_{1,2}(-\alpha)]$$

and
$$f_{1,2}^a(\alpha) = \frac{1}{2} [f_{1,2}(\alpha) - f_{1,2}(-\alpha)]$$

By applying (4.4)-(4.8) into the Sommerfeld integrals given in (4.2) and (4.3), a set of asymmetric and symmetric functional equations are obtained. They are rearranged to a matrix form using the reflection, $R(\alpha, \gamma)$ and transmission $T(\alpha, \gamma)$ coefficients.

$$\begin{bmatrix} f_1^{a,s}(\alpha + \Phi_1) \\ f_2^{a,s}(b(\alpha) + \Phi_2) \end{bmatrix} = \begin{bmatrix} \pm R(\alpha, \gamma) & \nu T(\alpha, \gamma) \\ \nu^{-1} T(b(\alpha), \gamma^{-1}) & \pm R(b(\alpha), \gamma^{-1}) \end{bmatrix} \begin{bmatrix} f_1^{a,s}(\alpha - \Phi_1) \\ f_2^{a,s}(b(\alpha) - \Phi_2) \end{bmatrix} \quad (4.9)$$

where
$$R(\alpha, \gamma) = \frac{\gamma \sin \alpha - \sqrt{1 - \gamma^2 \cos^2 \alpha}}{\gamma \sin \alpha + \sqrt{1 - \gamma^2 \cos^2 \alpha}} \quad (4.10)$$

$$T(\alpha, \gamma) = \frac{2\gamma \sin \alpha}{\gamma \sin \alpha + \sqrt{1 - \gamma^2 \cos^2 \alpha}} \quad (4.11)$$

and $T(\alpha, \gamma) = 1 + R(\alpha, \gamma)$. The branch of the double-valued function, $\sqrt{1 - \gamma^2 \cos^2 \alpha}$ is selected such that $\sqrt{1 - \gamma^2 \cos^2 (\pi/2)} = 1$ on the top sheet, i.e. the square root is positive when the radicand is positive. The prove for $f_1^a(\alpha + \Phi_1)$ in (4.9) is given in Appendix C.2. Its companion equations, $f_1^s(\alpha + \Phi_1)$ and $f_2^{a,s}(b(\alpha) + \Phi_2)$ can be derived accordingly.

A straight forward exchange of variables in (4.9) yields

$$f_1^{a,s}(\alpha) = \pm R(\alpha - \Phi_1, \gamma) f_1^{a,s}(\alpha - 2\Phi_1) + \nu T(\alpha - \Phi_1, \gamma) f_2^{a,s}(b(\alpha - \Phi_1) - \Phi_2) \quad (4.12)$$

$$f_2^{a,s}(\alpha) = \nu^{-1} T(\alpha - \Phi_2, \gamma^{-1}) f_1^{a,s}(a(\alpha - \Phi_2) - \Phi_1) \pm R(\alpha - \Phi_2, \gamma^{-1}) f_2^{a,s}(\alpha - 2\Phi_2) \quad (4.13)$$

which can be applied recursively to provide analytic continuation of the $f_n^{a,s}(\bullet)$ functions from a specified basic strip to the entire complex plane. Most importantly, the significant of (4.12) and (4.13) is that, they are used to initiate the propagation of poles and subsequently identify their physical meaning in geometrical optics field. Any poles that are captured within the Sommerfeld contour integrals, $-\pi < \alpha < \pi$ or $-\pi < \beta < \pi$ give rise to the geometrical optics field. The identified poles are also contribute to the diffracted field. This is important for a penetrable wedge other than the right-angled because it allows the tracing of poles for multiple reflections and transmissions. Since $f_{1,2}^{a,s}(\bullet)$ is also a function of $f_{2,1}^{a,s}(\bullet)$, it is expected that the poles would also involve the use of inverse cosine functions given in (4.6) and (4.7).

4.1.1 Poles for External and Internal Regions of a Penetrable Wedge

All the poles that give rise to different electromagnetic fields for a penetrable wedge are initiated by the primary pole, $\alpha = \phi'_o$ in the basic strip, $|\operatorname{Re} \alpha| < \Phi_1$ of $f_1(\bullet)$. This primary pole is also known as zero level pole because it is used to deduce all the higher level poles, which also include the poles for the spectral function $f_2(\bullet)$. The spectral function, $f_2(\bullet)$ is regular in its basic strip, $|\operatorname{Re} \beta| < \Phi_2$. By deducing the corresponded residues for the poles, different electromagnetic fields such as reflected and transmitted fields for the external and internal regions of a penetrable wedge can be identified. It has to be noted that not all the higher level poles of $\alpha = \phi'_o$ are associated with the physical scattering phenomenon. Existence of the poles are only prominent when they are being captured in the Sommerfeld contour integrals. The following discussion about poles focus on a right-angled penetrable wedge, which facilitate the exclusion of multiple reflections inside the wedge. In this case, the incident angle in three different quadrants, Quadrants A, B and C as shown in Figure 4.2 are considered. Quadrants A and C are conceptually similar as the incident field only illuminates one side of the wedge, either S_1 or S_2 . Quadrant B involves illumination to both surfaces of the wedge. A summary of the poles, residues and type of fields in different illumination quadrants are given in Table 4.1. Whenever the symbols $\pm$ or $\mp$ are used, the upper sign is dedicated for incident angle in Quadrant A and the lower sign is dedicated for incident angle in Quadrant C.

Table 4.1 Classification of poles for Incident Angle in Quadrants A, B and C

Quadrant(s)	Poles	Residues*	Type of Field**
A (Upper sign) and C (Lower Sign)	External Region, $f_1(\alpha)$		
	➤ $\alpha = \phi'_o$	1	I
	➤ $\alpha = -\phi'_o \pm 2\Phi_1$	$R(\Phi_1 \mp \phi'_o, \gamma)$	R
	➤ $\alpha = \mp \Phi_1 +$ $a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2)$	$T(\Phi_1 \mp \phi'_o, \gamma) \cdot$ $T(2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1})$	T-T
	Internal Region, $f_2(\alpha)$		
	➤ $\alpha = b(\phi'_o \mp \Phi_1) \mp \Phi_2$	$T(\Phi_1 \mp \phi'_o, \gamma)$	T
	➤ $\alpha = \pm 3\Phi_2 + b(-\phi'_o \pm \Phi_1)$	$T(\Phi_1 \mp \phi'_o, \gamma) \cdot$ $R(\pm 2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1})$	T-R
B	External Region, $f_1(\alpha)$		
	➤ $\alpha = \phi'_o$	1	I
	➤ $\alpha = -\phi'_o + 2\Phi_1$	$R(\Phi_1 - \phi'_o, \gamma)$	R
	➤ $\alpha = -\phi'_o - 2\Phi_1$	$R(\Phi_1 + \phi'_o, \gamma)$	R
	Internal Region, $f_2(\alpha)$		
	➤ $\alpha = b(\phi'_o - \Phi_1) - \Phi_2$	$T(\Phi_1 - \phi'_o, \gamma)$	T
	➤ $\alpha = b(\phi'_o + \Phi_1) + \Phi_2$	$T(\Phi_1 + \phi'_o, \gamma)$	T

* See Appendix C.3 for the residues deduced directly from the zero-level poles.

** I - Incident, T - Transmitted, R-Reflected.

(a) Incident Angle in Quadrants A and C

For the external region of a penetrable wedge, the primary pole, $\alpha = \phi'_o$ that located in the basic strip of $|\text{Re } \alpha| < \Phi_1$ is considered as zero level pole. The corresponding residue recovers the incident field given in (4.1). Subsequently, a first level pole, $-\phi'_o \pm 2\Phi_1$ is induced by the zero level pole to give rise to the reflected field in the external region of the penetrable wedge. The residue of this pole is given by the reflection coefficient in (4.10). Another pole that can be captured for the external region is given by $\alpha = \mp\Phi_1 + a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2)$ with the residue $T(\Phi_1 \mp \phi'_o, \gamma) T(2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1})$. This particular pole gives rise to geometrical optics field that transmitted-in and subsequently transmitted-out from the penetrable wedge.

For the internal region of a penetrable wedge, all the poles are deduced from the zero level pole, $\alpha = \phi'_o$ given for the external region. Physically, one can relate this to all the scattered fields inside a penetrable wedge are induced by the incident field. The first pole that needs to be considered is given by $\alpha = b(\phi'_o \mp \Phi_1) \mp \Phi_2$, which corresponds to the transmitted field. The residue is given by the transmission coefficient in (4.11). For the geometrical optics field that transmitted in and subsequently reflected from the internal surface of the wedge, the pole is given by $\alpha = \pm 3\Phi_2 + b(-\phi'_o \pm \Phi_1)$ with the residue $T(\Phi_1 \mp \phi'_o, \gamma) R(\pm 2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1})$. Other higher level poles can be obtained in a similar recursive way using (4.12) and (4.13) but it may not be captured within the Sommerfeld contour integrals and no physical electromagnetic fields are excited. Hence, they are ignored here.

(b) Incident Angle in Quadrant B

Similarly, the primary pole, $\alpha = \phi_o$ is required to recover the incident field with residue of unity. Since the incident field illuminates both sides of the wedge, it is expected that two distinct poles are required to recover the reflection from the two surfaces, S_1 and S_2 . This is given by the poles, $\alpha = -\phi'_o + 2\Phi_1$ and $\alpha = -\phi'_o - 2\Phi_1$ with residues of $R(\Phi_1 - \phi'_o, \gamma)$ and $R(\Phi_1 + \phi'_o, \gamma)$, respectively. The geometrical optics field that transmitted-in and transmitted-out from the wedge is not present as their poles are not captured within the Sommerfeld contour integrals. On the other hand, geometrical optics field insides the wedge only involves transmiited field which is induced by the poles, $\alpha = b(\phi'_o - \Phi_1) - \Phi_2$ and $\alpha = b(\phi'_o + \Phi_1) + \Phi_2$ for the surafce, S_1 and S_2 , respectively. Their residues are represented by the transmission coefficient, $T(\Phi_1 - \phi'_o, \gamma)$ and $T(\Phi_1 + \phi'_o, \gamma)$, respectively. There are no multiple reflections inside the right-angle penetrable wedge.

4.2 Multi-Valued Functions

Since the inverse cosine functions given in (4.6) and (4.7) are multi-valued functions [171, 172], a proper branch must be selected for a unique mapping between the two complex planes, i.e. α and β . The branch selection is characterized by the coefficient, γ or $1/\gamma$. The wedge surrounding medium is taken to be vacuum. By using the definition of $\gamma = k/k_1$ or $\gamma = n_o/n_1$, it is identified that when the wedge is occupied by lossless materials with real refractive index, it will give γ values of smaller than one, i.e. $\gamma < 1$. The branch cuts and branch points of $b(\alpha)$

and $a(\beta)$ are shown in Figure 4.4. On the other hand, lossy materials with complex refractive index give complex values of γ . The immediate consequence is seen through the branch cuts and branch points in Figure 4.5, which are displaced from the real or imaginary axis to indicate the presence of the losses. When the losses of the materials are reduced to zero, by all means, their branch cuts and branch points in Figure 4.5 revert to Figure 4.4. The following discussion on $b(\alpha)$ and $a(\beta)$, together with their selection of domain focuses on γ is real and smaller than one. The same interpretation can be applied analogously to γ with complex values.

By referring to Figure 4.4 (a) for $b(\alpha)$ with γ is a real number and smaller than one, the primary cuts are found on the imaginary axis (y-axis), with the branch points, $\alpha^\wedge$ are located at $\pm i \cosh(1/\gamma)$. There are also other branch cuts and branch points located in the interval of π . On the other hand, the branch cuts for $a(\beta)$ are located along the imaginary axis as well as on the real axis (x-axis) with the branch point, $\beta^\wedge$ located at $\pm \cos(\gamma)$ as shown in Figure 4.4 (b). Other branch cuts and branch points are also found in the interval of π . The vertical branch cuts of $a(\beta)$ located along the imaginary axis are mapped onto the imaginary axis of $b(\alpha)$ for $|\alpha| > |i \cosh(1/\gamma)|$. The horizontal branch cuts in $a(\beta)$, i.e. $|\beta| < |\cos(\gamma)|$ are mapped onto the imaginary axis of $b(\alpha)$ for $|\alpha| < |i \cosh(1/\gamma)|$. The same mapping is also applied to other branch cuts in the interval of π . In this work, the principal plane of both the multi-valued functions are selected such that that it has the following properties,

$$b(0.5\pi) = 0.5\pi$$

$$b(-\alpha) = -b(\alpha)$$

$$b(\bar{\alpha}) = \overline{b(\alpha)}$$

and

$$b(\alpha + m\pi) = b(\alpha) + m\pi, m = \text{integers}$$

with the upper bar ($\bar{\cdot}$) indicates the complex conjugate in complex numbers.

Figure 4.4 Branch cuts for (a) $b(\alpha)$ and (b) $a(\beta)$ with real number of γ .

Figure 4.5 Branch cuts (a) $b(\alpha)$ and (b) $a(\beta)$ with complex number of γ .

4.3 Geometrical Optics and Diffracted Fields

The geometrical optics field presented here is for a right-angled penetrable wedge with the incident field illuminates to either one side or both sides of the wedge surfaces, S_1 and S_2 .

These geometrical optics field include reflected (U_z^r), transmitted (U_z^t), transmitted-reflected (U_z^{tr}) and transmitted-transmitted (U_z^{tt}) fields through the penetrable wedge. The amplitudes are obtained from the residues given in Table 4.1, which are the reflection and transmission coefficients or their combination. The expressions for the geometrical optics field are given in Tables 4.2 and 4.3. The Heaviside function, $H(\bullet)$ is used to confine a particular geometrical optics field to a specified region. The Guderman function, $\text{gd}(x)$ is defined as $\text{gd}(x) = \cos^{-1}[1/\cosh(x)]\text{sgn}(x)$. When the poles are captured within the Sommerfeld contour integrals, the Heaviside function gives value of unity and when the poles propagate out from the Sommerfeld contour integrals, it gives value of zero.

The diffracted field is also identified for the external and internal regions of a penetrable wedge. Physically, the diffracted field is required to compensate the discontinuities caused by the geometrical optics field at different shadow boundaries. In a rigorous approach, the diffracted field is obtained by solving the two spectral functions, $f_1(\bullet)$ and $f_2(\bullet)$ given in (4.2) and (4.3) using a series of singular integral equations, which unavoidably involves some complex numerical scheme. These mathematical techniques are rather difficult to implement. Furthermore, as mentioned in the beginning of this chapter, an explicit expression for the diffracted field is difficult to obtain when the branch cuts and poles are near to the steepest decent path [173] on the Sommerfeld contour complex planes. Hence, in this work, a proposed heuristic solution is used to obtain the external and internal diffracted fields of the penetrable wedge. The solution is in the form of Uniform Theory of Diffraction (UTD) as discussed in Chapter 3 but with asymptotic evaluation using multiplicative approach [166].

Table 4.2 Geometrical optics field for incident angle in Quadrants A and C

Quadrants	Geometrical Optics Field	Expressions
A (Upper sign) and C (Lower Sign)	Reflected, $U_z^r(k\rho, \phi')$	$R(\Phi_1 \mp \phi'_o, \gamma) \exp(jk\rho \cos(2\Phi_1 \mp \phi' \mp \phi'_o)) H(\pi - \phi' + \phi'_o \mp 2\Phi_1)$
	Transmitted, $U_z^t(k_1\rho, \bar{\phi})$	$T(\Phi_1 \mp \phi'_o, \gamma) \exp(jk_1\rho \cos(b(\phi'_o \mp \Phi_1) \mp \Phi_2 + \bar{\phi}))$ $H(\pi - \text{Re}[b(\phi'_o \mp \Phi_1)] + \text{gd}(\text{Im}[b(\phi'_o \mp \Phi_1)]) \mp \Phi_2 + \bar{\phi})$
	Transmitted-transmitted, $U_z^{tt}(k\rho, \phi')$	$T(\Phi_1 \mp \phi'_o, \gamma) T(2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1}) \exp(jk\rho \cos(\mp \Phi_1 + a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2) - \phi'))$ $H(\pi - \mp \Phi_1 + \text{Re}[a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2)] + \text{gd}(\text{Im}[a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2)]) - \phi')$
	Transmitted-reflected, $U_z^{tr}(k_1\rho, \bar{\phi})$	$T(\Phi_1 \mp \phi'_o, \gamma) R(\pm 2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1}) \exp(jk_1\rho \cos(\pm 3\Phi_2 + b(-\phi'_o \pm \Phi_1) + \bar{\phi}))$ $H(\pi - \pm 3\Phi_2 + \text{Re}[b(-\phi'_o \pm \Phi_1)] + \text{gd}(\text{Im}[b(-\phi'_o \pm \Phi_1)]) + \bar{\phi})$

Table 4.3 Geometrical optics field for incident angle in Quadrant B

Quadrant	Geometrical Optics Field	Expressions
B	Reflected, $U_z^r(k\rho, \phi')$	$R(\Phi_1 - \phi'_o, \gamma) \exp(jk\rho \cos(2\Phi_1 - \phi' - \phi'_o)) H(\pi - \phi' + \phi'_o - 2\Phi_1) +$ $R(\Phi_1 + \phi'_o, \gamma) \exp(jk\rho \cos(2\Phi_1 + \phi' + \phi'_o)) H(\pi - \phi' + \phi'_o + 2\Phi_1)$
	Transmitted, $U_z^t(k_1\rho, \bar{\phi})$	$T(\Phi_1 - \phi'_o, \gamma) \exp(jk_1\rho \cos(b(\phi'_o - \Phi_1) - \Phi_2 - \bar{\phi}))$ $H(\pi - \text{Re}[b(\phi'_o - \Phi_1)] + \text{gd}(\text{Im}[b(\phi'_o - \Phi_1)]) - \Phi_2 + \bar{\phi}) +$ $T(\Phi_1 + \phi'_o, \gamma) \exp(jk_1\rho \cos(b(\phi'_o + \Phi_1) + \Phi_2 - \bar{\phi}))$ $H(\pi - \text{Re}[b(\phi'_o + \Phi_1)] + \text{gd}(\text{Im}[b(\phi'_o + \Phi_1)]) + \Phi_2 + \bar{\phi})$

The proposed heuristic solution for external diffracted field of a penetrable wedge is given by

$$U_{z_ext}^d(\rho, \phi') = \frac{\exp(-j k \rho)}{\sqrt{\rho}} D_{ext}(\phi', \phi_o) \quad (4.14)$$

where $D_{ext}(\phi', \phi_o)$ for incident angle in Quadrants A and C is given by

$$\begin{aligned} D_{ext}(\phi', \phi_o) = & D_{ext}^{(1)} + D_{ext}^{(2)} + R(\Phi_1 - \phi_o', \gamma) D_{ext}^{(3)} + R(\Phi_1 + \phi_o', \gamma) D_{ext}^{(4)} \\ & + T(\Phi_1 - \phi_o', \gamma) T(2\Phi_2 + b(\Phi_1 - \phi_o'), \gamma^{-1}) D_{ext}^{(5)} \\ & + T(\Phi_1 + \phi_o', \gamma) T(2\Phi_2 + b(\Phi_1 + \phi_o'), \gamma^{-1}) D_{ext}^{(6)} \end{aligned} \quad (4.15)$$

and $D_{ext}(\phi', \phi_o')$ for incident angle in Quadrant B is given by

$$D_{ext}(\phi', \phi_o') = D_{ext}^{(1)} + D_{ext}^{(2)} + R(\Phi_1 - \phi_o', \gamma) D_{ext}^{(3)} + R(\Phi_1 + \phi_o', \gamma) D_{ext}^{(4)} \quad (4.16)$$

For all the quadrants, the sub-external diffraction coefficients are obtained from

$$D_{ext}^{(i)} = -\frac{\exp(-j\pi/4)}{2\sqrt{2\pi k}} \cot(\kappa_{ext}^{(i)}) F(2k\rho \cos^2(\tau_{ext}^{(i)})) \quad (4.17)$$

where the variables, τ_i and κ_i are determined from the Table 4.4. The transition function, $F(\bullet)$ is evaluated using the same expression (3.12) given in Chapter 3. The diffraction coefficient given in (4.15) consists of six sub-terms. The last two terms involve the use of transmission coefficient to compensate the discontinuities caused by the incident field that transmitted in and transmitted out from the penetrable wedge. This is not considered in the (external) heuristic diffraction coefficient given by (2.15) in Chapter 2. In (2.15), there are only four terms that contribute to the diffraction coefficient where the wedge is treated as a non-penetrable structure, i.e. no transmission occurs.

Table 4.4 Variables in sub-external diffraction coefficients

Quadrants	i	$\tau_{ext}^{(i)}$	$\kappa_{ext}^{(i)}$
A, B, and C	1*	$\phi - \phi_o$	$\pi - \tau_{ext}^{(1)}$
	2*	$\phi - \phi_o$	$\pi + \tau_{ext}^{(2)}$
	3*	$\phi + \phi_o$	$\pi - \tau_{ext}^{(3)}$
	4*	$3\pi - (\phi + \phi_o)$	$4\pi - \tau_{ext}^{(4)}$
	5^	$\phi' - \Phi_1 + a(b(\phi'_o - \Phi_1) - 2\Phi_2)$	$\pi - \tau_{ext}^{(5)}$
	6^	$\phi' + \Phi_1 + a(b(\phi'_o + \Phi_1) + 2\Phi_2)$	$\pi + \tau_{ext}^{(6)}$

* $\phi = 1.5\pi - \phi'$ and $\phi_o = 1.5\pi - \phi'_o$.

^ For Quadrant B, $i = 5$ and 6 are not applicable.

On the other hand, the proposed heuristic solution for internal diffracted field of a penetrable wedge is given by

$$U_{z_int}^d(\rho, \bar{\phi}) = \frac{\exp(-jk_1\rho)}{\sqrt{\rho}} D_{int}(\bar{\phi}, \phi'_o) \quad (4.18)$$

where $D_{int}(\bar{\phi}, \phi'_o)$ for incident angle in Quadrants A (upper sign) and C (lower sign) is given by

$$D_{int}(\bar{\phi}, \phi'_o) = T(\Phi_1 \mp \phi'_o, \gamma) D_{int}^{(1)} + T(\Phi_1 \mp \phi'_o, \gamma) R(\pm 2\Phi_2 + b(\Phi_1 \mp \phi'_o), 1/\gamma) D_{int}^{(2)} \quad (4.19)$$

and $D_{int}(\bar{\phi}, \phi'_o)$ for incident angle in Quadrant B is given by

$$D_{int}(\bar{\phi}, \phi'_o) = T(\Phi_1 - \phi'_o, \gamma) D_{int}^{(1)} + T(\Phi_1 + \phi'_o, \gamma) D_{int}^{(2)} \quad (4.20)$$

The sub-internal diffraction coefficients are obtained from

$$D_{int}^{(i)} = -\frac{\exp(-j\pi/4)}{2\sqrt{2\pi k_1}} \cot(\kappa_{int}^{(i)}) F(2k_1\rho \cos^2(\tau_{int}^{(i)})) \quad (4.21)$$

where the variables, τ_i and κ_i are determined from the Table 4.5. Similarly, the transition function, $F(\bullet)$ is evaluated using the expression (3.12) given in Chapter 3.

Table 4.5 Variables in sub-internal diffraction coefficients

Quadrant(s)	i	$\tau_{\text{int}}^{(i)}$	$\kappa_{\text{int}}^{(i)}$
A (Upper Sign) and C (Lower Sign)	1	$b[\phi'_o \mp \Phi_1] \mp \Phi_2 - \bar{\phi}$	$\pi \pm \tau_{\text{int}}^{(1)}$
	2	$b[-\phi'_o \pm \Phi_1] \pm 3\Phi_2 - \bar{\phi}$	$\pi \mp \tau_{\text{int}}^{(2)}$
B	1	$b[\phi'_o - \Phi_1] - \Phi_2 - \bar{\phi}$	$\pi + \tau_{\text{int}}^{(1)}$
	2	$b[\phi'_o + \Phi_1] + \Phi_2 - \bar{\phi}$	$\pi - \tau_{\text{int}}^{(2)}$

4.4 Lateral Field

As shown in Figures 4.3 (a) and (b), there are branch cuts exist in the α and β complex plane for the Sommerfeld contour integrals. These branch cuts are originated from the inverse cosine functions discussed in Section 4.2. From a mathematical point of view, the integration that performed along the branch cuts gives rise to lateral field [177, 178]. Lateral field involves the propagation of waves in two different mediums. In this case, it will be the wedge external and internal mediums. However, the properties of the lateral field for the external and internal wedge are different owing to the location of their respective branch cuts. For the external spectral function, the branch cuts are not located on the real axis (real angle) as shown in Figure 4.3 (a). They are located parallel to the imaginary axis. This implies that lateral field has no contribution to the total external field and the branch cuts analysis is not required. For the internal spectral function, the branch cuts are located on the real axis (real

angle), which indicates that the lateral field in the wedge contributes to the total internal field. There are two main properties of the lateral field inside a penetrable wedge. Firstly, for a right-angled penetrable wedge, the lateral field needs not to be included when the refractive index is less than $\sqrt{2}$. This can be traced through the location of the branch points and branch cuts, which are not crossed into the steepest decent path region, $-\pi < \beta < \pi$. Secondly, for a right-angled wedge with refractive index greater than $\sqrt{2}$, the lateral field is characterized by lower order of $(k_1\rho)^{-1/2}$, which means that the amplitude of the lateral field decays faster than the diffracted field. The diffracted field is characterized by a spreading factor of $(k_1\rho)^{-1/2}$ as given in (4.18) and (4.21). This suggests that the contribution of the lateral field is always smaller than that of the diffracted field. Hence, the formulation for the internal lateral field is not included here.

4.5 Results and Discussion

The following results focus on internal electromagnetic field of a right-angled penetrable wedge. Both lossless and lossy materials for the penetrable wedge are considered. The illumination wavelength is 633 nm and TE polarization is assumed. These parameters remain the same unless otherwise stated. To give a clearer physical understanding, the total internal electromagnetic field is also decomposed into the diffracted field and their respective geometrical optics field. The geometrical optics field includes the transmitted and transmitted-reflected field from different surfaces. For ease of illustration, the x- and y-axes in Figure 4.2 are re-oriented to that shown in Figure 4.6. The incident angle is measured from the surface S_1

and denoted by ϕ_o . When the results obtained from this work are compared with the reference FDTD solution [170], the amplitude difference, $\Delta|E_z|$ is given by

$$\Delta|E_z| = |E_z|(\text{This Work}) - |E_z|(\text{FDTD}) \quad (4.22)$$

Figure 4.6 Geometry of the right-angled penetrable wedge with re-orientated x- and y-axes.

4.5.1 Lossless Penetrable Wedge

Figure 4.7 shows the amplitude of the total internal electromagnetic field for a right-angled penetrable wedge with refractive index of 2. The incident angle, ϕ_o is 60° (Quadrant A) and the observation level, ky is at -5. Both the results from this work and the reference FDTD solution are shown. At this condition, the results from this work have underestimated the amplitude if compared to the reference FDTD solution. The maximum amplitude difference, $\Delta|E_z|$ is 0.18, which is observed at $x = 0$. Nevertheless, it is still able to decompose the total internal field into their geometrical optics and diffracted fields. There are two types of geometrical optics field exist in the penetrable wedge, namely the transmitted and transmitted-reflected fields. The former is shown by (i) and the latter is given by (ii) in Figure 4.7. Both

transmitted and transmitted-reflected fields give constant amplitude. Their difference can be seen through the region of existence. The transmitted field is found everywhere inside the penetrable wedge whereas the transmitted-reflected field is limited to certain regions inside the penetrable wedge, i.e. $x > -0.12 \mu\text{m}$. For incidence field at angle 60° from the wedge surface S_1 , the transmitted-reflected field is associated with the surfaces S_1 and S_2 . The internal diffracted field as shown by (iii) in the same figure is used to compensate the discontinuity caused by the transmitted-reflected field at the shadow boundary, $x = -0.12 \mu\text{m}$. The amplitude of the internal diffracted field decays exponentially from the shadow boundary. When the discontinuity of amplitude in the diffracted field is supplemented to the discontinuity in the geometrical optics field, a smooth amplitude in the total field is obtained. One can note that only the amplitude of the total field exhibits oscillatory behavior compared to the geometrical optics and diffracted fields.

Figure 4.7 Amplitude of the total internal electromagnetic field obtained from this work and its comparison with the reference FDTD solution. The observation level, k_y is -5 and the incident angle is 60° measured from the surface S_1 . The total internal electromagnetic field is decomposed into (i) transmitted field, (ii) transmitted-reflected field and (iii) internal diffracted field.

Figure 4.8 (a) shows the amplitude of total internal field for a right-angled penetrable wedge with refractive index of 2. The incident angle, ϕ_o is at 120° (Quadrant B). At this incident angle, both surfaces of the wedge, S_1 and S_2 are illuminated. Firstly, the total internal electromagnetic field obtained from this work shows a good overall match with the reference FDTD solution although the maximum amplitude difference, $\Delta|E_z|$ is 0.15, given at x near to 0. Again, the advantage of this work is clearly seen when the solution presented in this chapter is able to decompose the total internal electromagnetic field into their individual field. For incident field that illuminates both sides of the wedge surfaces, two transmitted fields and two internal diffracted fields are obtained. By referring to Figure 4.8 (b), the (i) transmitted field and (iii) internal diffracted field are associated with the surface S_1 , whereas the (ii) transmitted field and (iv) internal diffracted field are associated with the surface S_2 . The amplitude of the transmitted field, regardless of the penetrated surface, gives constant amplitude in their region of existence. The single peak found in each diffracted field, at about $x = -0.12 \mu\text{m}$ and $x = -1.06 \mu\text{m}$ represent the transmission shadow boundaries in the penetrable wedge, for surfaces S_1 and S_2 , respectively. Here, the amplitude of each internal diffracted field decays exponentially from the respective shadow boundary. With the internal diffracted field, the discontinuities caused by the transmitted field are perfectly compensated. There are no multiple reflections inside a right-angled wedge. Figure 4.9 (a) shows the amplitude of the total internal field for observation level up to $ky = -10$ obtained in this work. Its reference FDTD results are given in Figure 4.9 (b). It is seen that the proposed solution in this work provides an excellent prediction to the oscillating amplitude of the total electromagnetic field inside the wedge.

Figure 4.8 (a) Amplitude of the total internal electromagnetic field obtained from this work and its comparison with the reference FDTD solution. The observation level, k_y is -5 and the incident angle is 120° measured from the surface S_1 . (b) Decomposition of the total internal field into (i) transmitted field through surface S_1 , (ii) transmitted field through surface S_2 , (iii) internal diffracted field associated with transmitted field through surface S_1 and (iv) internal diffracted field associated with transmitted field through surface S_2 are also shown.

Figure 4.9 (a) Amplitude for the total internal field of a penetrable wedge with refractive index of 2, obtained using the formulation developed in this chapter, and its comparison with (b) the reference FDTD solution.

4.5.2 Lossy Penetrable Wedge

The amplitude results for incident angle, ϕ_o at 120° (Quadrant B) are extended to lossy penetrable wedge. For lossy penetrable wedge, an imaginary part is present for the refractive

index. The following results are presented based on refractive index of $2 - 0.1j$. Figure 4.10 shows the amplitude of the total internal field obtained from this work and its comparison with the reference FDTD results. An excellent match is found. Besides that, there is also other geometrical optics and diffracted fields, which can be explained analogously using the findings in the previous discussion for refractive index of 2. The transmitted field through surface S_1 and its associated diffracted field are combined together and indicated by (i)+(iii) in Figure 4.10 whereas the combination of transmitted field through surface S_2 and its associated diffracted field is indicated by (ii)+(iv). It is shown that the former combination, (i)+(iii) contributes significantly to the total field for $x < -2 \mu\text{m}$ and the latter combination, (ii)+(iv) becomes prominent only when x is approaching zero. On the other hand, Figure 4.11 (a)

Figure 4.10 Amplitude of the total internal electromagnetic field obtained from this work and its comparison with the reference FDTD solution. The observation level, k_y is -5 and the incident angle is 120° measured from the surface S_1 . Decomposition of the total internal electromagnetic field into the combination of (i)+(iii) transmitted field through surface S_1 and its associated diffracted field, and (ii)+(iv) transmitted field through surface S_2 and its associated diffracted field are also shown.

Figure 4.11 (a) Amplitude of the total internal electromagnetic field of a penetrable wedge with refractive index of $2 - 0.1j$, obtained using the formulation developed in this work, and its comparison with (b) the reference FDTD solution.

presents the amplitude of the total internal electromagnetic field for observation level up to $ky = -10$ obtained in this work. Its reference FDTD results are given in Figure 4.11 (b). The prediction obtained from this work is excellent and compatible with the reference solution. On the other note, the amplitude of the total internal field for lossy penetrable wedge ‘stabilizes’ much faster if compared to lossless penetrable wedge for decreasing x distance. This is observed through the comparison between Figures 4.11 (a) and 4.9 (a).

The amplitude results for a lossy penetrable wedge are also extended to different incident wavelengths. Figures 4.12 (a), (b), (c), (d) and (e) show the amplitude of the total internal field obtained from this work for wavelength of 532 nm, 436 nm, 365 nm, 248 nm and 193 nm, respectively with incident angle, ϕ_o of 120° (Quadrant B). The reference FDTD results are also given in each figure. It is demonstrated that when the wavelength is reduced from 532 nm in Figure 4.12 (a) to 193 nm in Figure 4.12 (e), the amplitude obtained from this work is able to give comparable match with the reference FDTD solution. Figure 4.13 shows the maximum and minimum of $\Delta|E_z|$ across all the wavelengths within the x distance given in Figure 4.12. Among all the wavelengths, the maximum magnitude of amplitude difference, $\Delta|E_z|$ is 0.13, which is observed at $x = 0$ for incident wavelength of 193 nm. Besides that, one can also notice that the amplitude profile for 193 nm stabilizes to a constant value at $x = -0.75 \mu\text{m}$ compared to $x = -2 \mu\text{m}$ for 532 nm, as shown by the arrows X in Figures 4.12 (d) and (a), respectively. This suggests that the “ripples” of amplitude profile for shorter wavelength stabilize much faster than the greater wavelength for decreasing x distance.

Figure 4.12 Amplitude of the total internal electromagnetic field for wavelength (a) 532 nm (b) 436 nm (c) 365 nm (d) 248 nm (e) 193 nm. The observation level, $k_{\lambda}y$ is -5 , where k_{λ} is the wave number for the respective wavelength. The incident angle is 120° measured from the surface S_1 .

Figure 4.13 Maximum and minimum of the amplitude difference, $\Delta|E_z|$ across different wavelengths.

4.5.3 Accuracy of the Solution

In this chapter, the geometrical optics field for a penetrable wedge is determined from the poles and extraction of the corresponded residues from the spectral function, $f_2(\bullet)$. This spectral function is found in the kernel of the Sommerfeld contour integrals given in (4.3). The expression for geometrical optics field does not require the explicit solution for $f_2(\bullet)$. However, this is not the case for the diffracted field, which requires the solution of $f_2(\bullet)$ to be evaluated. By identifying the location of the respective poles, a heuristic diffracted field is formulated and applied. The heuristic solution was able to compensate the discontinuities caused by the geometrical optics poles but may not necessarily provide a perfect match of the total internal field with the FDTD solution. It is not surprising to see such a mismatch of the results particularly near to the material boundaries. This is observed in the amplitude of the total field results presented in Figures 4.7, 4.8 (a) and 4.10 when x is near to zero. As a result of this, a small discontinuity of the total field could probably exist across the boundary of two

different mediums at $x = 0 \text{ } \mu\text{m}$. The deviation is unavoidable for a heuristic solution with the gain in simplicity of the formula.

4.6 Concluding Summary

In this chapter, a solution for the internal electromagnetic field of a right-angled penetrable wedge was established. The solution was obtained by studying the Sommerfeld integrals and identifying the necessary poles in conjunction with the physical scattering phenomenon. This includes all the geometrical poles that give rise to transmitted and transmitted-reflected fields inside the penetrable wedge. Different incident angles for a right-angled penetrable wedge were studied. The internal diffracted field was obtained by using the proposed heuristic solution to correctly compensate the discontinuities at different shadow boundaries. Although the heuristic approach was applied here, the diffracted field was able to give a good estimation to the reference FDTD solution. For a lossless penetrable wedge with refractive index of 2, the amplitude results for incident angle in Quadrant B (Figure 4.8) gives a better prediction to the total internal electromagnetic field if compared to the amplitude results for incident angle in Quadrant A (Figure 4.7). The penetrable wedge with complex refractive index also demonstrated a good match of the amplitude results with the reference FDTD solution.

CHAPTER 5 ELECTROMAGNETIC RAY TRACING (ERT) MODEL FOR LINE STRUCTURES

Line structures are typical features found in the IC fabrication process. For example, the alignment marks formed on the wafer are usually line structures that represent the grating pattern. The measurement of overlay is also performed with targets designed using line structure. These alignment marks and overlay targets are necessary in the front-end process for the formation of polysilicon transistor gate or in the back-end process for multi level interconnects metallization. As these marks and targets are important to determine the robustness of the fabrication process, understanding of the electromagnetic scattering phenomenon for the line structure is essential.

This chapter aims to establish a new electromagnetic ray tracing (ERT) model in order to study the scattering phenomenon of line structures formed on substrate. The approach clarifies and enhances understanding to every single electromagnetic field that contributes to the final solution at an observation point above the line structures. It takes into account the existence of both geometrical optics and diffracted fields. Figure 5.1 shows the modelling approach in decomposing the line structure into individual components. The single line structure is modeled as an impedance double wedge to study the external surrounded field. It involves the external diffraction coefficient developed in Chapter 3, which facilitates the analysis of different types of diffracted fields induced in accordance to the geometry of the line structures. When the diffraction coefficient is extracted from (3.11) in Chapter 3, the first term ($m = 0$) solution is applied. As part of the total solution, an analysis of the internal diffracted field of the line

structures using the formulation presented in Chapter 4 is also included. On the other hand, the film stack matrix is used to extract an effective refractive index for the line structures and underneath substrate. This effective refractive index is needed particularly for the analysis of external diffraction.

Figure 5.1 Decomposition of a line structure formed on substrate into their individual model, i.e. an impedance double wedge and single layer film.

The flow of this chapter is as follows:

1. Firstly, the approach to study the electromagnetic scattering of an impedance double wedge is presented. This forms the fundamental of the line structure in Figure 5.1. At this point, the impedance double wedge is treated as an isolated structure and the underneath substrate of the line structures is excluded. The numerical results for resist and silicon impedance double wedges at different line widths are also shown.
2. Secondly, the new ERT model for line structure is established by extending the impedance double wedge to form on substrate. Besides geometrical optics field for incidence and reflection, it also involves the formulation for different types of diffracted fields, namely direct external diffracted, external diffracted-reflected and internal diffracted-reflected-transmitted fields. The film stack approach used to extract an effective refractive index for the impedance double wedge is also discussed. The numerical results focus on the combination of resist-silicon dioxide and polysilicon-silicon for line structure-substrate at

different line widths. The decomposition of the total solution into their individual field, which is an important advantage of the ray tracing approach is also presented.

3. Lastly, the accuracy of the ERT model for line structures formed on substrate is analysed and compared with the reference FDTD solution. Various conditions such as single, two-line structures, different wavelengths and refractive indices are studied. The advantages of the ERT model in terms of computational time and memory used are then demonstrated.

The formulation and numerical results presented in this chapter are devoted for transverse electric (TE) polarization. A time harmonic of $\exp(j\omega t)$ is assumed and suppressed throughout.

5.1 Impedance Double Wedge

An isolated impedance double wedge is decomposed into two impedance wedges as shown in Figure 5.2. The total solution for the impedance double wedge is obtained by combining all the fields that are contributed from the two impedance wedges. This section aims to study the electromagnetic scattering of an isolated impedance wedge by identifying all the associated geometrical optics and diffracted fields. The electromagnetic field that propagates into the internal part of the wedges is not considered. Only the external field is included in the analysis.

Figure 5.2 Decomposition of an isolated impedance double wedge into two impedance wedges. The notation, $\bar{\eta}$ denotes the normalized surface impedance for the wedges.

5.1.1 Single Impedance Wedge

For a single impedance wedge which is illuminated by an incident wave to its top surface, S_T the surrounding medium is separated into three regions. These three regions are separated by the incident shadow boundary (ISB) and reflection shadow boundary (RSB), as shown in Figure 5.3. The notations, P and ρ denote the observation point and its distance from the origin, respectively. The total internal angle of the wedge is given by $(2 - \bar{p})\pi$. A summary of the field that contributes to each region is given below.

- Region I $U_{total} = U_{incident} + U_{reflected} + U_{diffracted}$
- Region II $U_{total} = U_{incident} + U_{diffracted}$
- Region III $U_{total} = U_{diffracted}$

Figure 5.3 Geometry of a single impedance wedge with plane wave incidence.

In Region I, the total field is a combination of the incident, reflected and diffracted fields. The reflected field is excluded from Region II as it is beyond the reflection shadow boundary. In Region III, the diffracted field is the only field that exists. It is shown that diffracted field exists

in every region to ensure continuity of the total field across different shadow boundaries. The geometrical optics field gives abrupt changes of the total field across the shadow boundaries.

5.1.2 Incident Field

For uniform incident plane wave at an angle of ϕ_o , the field at point $P(\rho, \phi)$ in Figure 5.3 is represented by

$$U_z^i = \exp(jk\rho \cos[\phi - \phi_o]) \quad (5.1)$$

with all the angles, ϕ are measured from the top surface, S_T and the origin is located at the wedge corner. The wavenumber in the vacuum and distance from the origin to the field point are denoted by k and ρ , respectively.

5.1.3 Reflected Field

The incident field that reaches the top surface, S_T at point $Q_{r1}(x_{r1}, 0)$ as shown in Figure 5.4 will be subsequently reflected and the amplitude will be attenuated. At a distance of ρ from the origin as illustrated in Figure 5.4, the field at observation point $P_I(\rho, \phi)$ caused by the reflection from point $Q_{r1}(x_{r1}, 0)$ is represented as

$$\begin{aligned} U_z^{r1}(\rho, \phi) &= R_{TE, S_T} U_z^i(Q_{r1}) \exp(-jk\rho^{r1}) \\ &= R_{TE, S_T} \exp(jk\rho \cos[\phi + \phi_o]) \end{aligned} \quad (5.2)$$

A particular observation point corresponds to a unique reflection point on the wedge surface. The location of this reflection point is obtained using direct geometrical derivation. The reflection coefficient, R_{TE, S_T} for TE polarization is given by

$$R_{TE, S_T} = \frac{\sin(\phi) - \sqrt{n_1^2 - \cos^2(\phi)}}{\sin(\phi) + \sqrt{n_1^2 - \cos^2(\phi)}} \quad (5.3)$$

where n_1 is the refractive index of the wedge, which is the inverse of its normalized surface impedance, $\bar{\eta}$.

Figure 5.4 Reflection from the top surface, S_T of a single impedance wedge.

5.1.4 External Diffracted Field

When the incident field illuminates the wedge as shown in Figure 5.3, the diffracted field in any of the regions can be expressed as

$$U_z^d = U^i(Q_E) D_{TE}(\phi, \phi_o) \frac{\exp(-jk\rho)}{\sqrt{\rho}} \quad (5.4)$$

where $U^i(Q_E)$ is the phase reference point to the origin. When the phase reference point and the origin are coincided at the edge of the wedge, the expression is simplified to

$$U_z^d = D_{TE}(\phi, \phi_o) \frac{\exp(-jk\rho)}{\sqrt{\rho}} \quad (5.5)$$

where $D_{TE}(\phi, \phi_o)$ is the diffraction coefficient for TE polarization. The external diffraction coefficient is obtained from (3.11) in Chapter 3. The spreading factor of $\frac{1}{\sqrt{\rho}}$ suggests that the diffracted field is emanating in the cylindrical wave form from the edge, which is acting as a line source.

5.1.5 Combination of Two Impedance Wedges

The expressions for incident, reflected and diffracted fields given in (5.1), (5.2) and (5.5), respectively are based on the origin located at the edge of an impedance wedge. When two impedance wedges are merged to form an impedance double wedge, there is a need to identify a common origin so that the phase reference point is synchronized. The phase reference point has been selected to coincide with the new origin in the coordinate shown in Figure 5.5. For an observation plane which is normal to the diffracted field on top of the impedance double wedge as shown in the same figure, the resultant diffracted field is given by

$$U_z^d = D_{TE}(\phi_R, \phi_{oR}) \frac{\exp(-jk\rho_R)}{\sqrt{\rho_R + \frac{l}{2}jk \sin \theta_R}} \exp\left(-\frac{l}{2}jk \cos \phi_{oR}\right) \exp\left(\frac{l}{2}jk \sin \theta_R\right) +$$

$$D_{TE}(\phi_L, \phi_{oL}) \frac{\exp(-jk\rho_L)}{\sqrt{\rho_L + \frac{l}{2}jk \sin \theta_L}} \exp\left(-\frac{l}{2}jk \cos \phi_{oL}\right) \exp\left(\frac{l}{2}jk \sin \theta_L\right) \quad (5.6)$$

and

$$\theta_R = \phi_R - \frac{\pi}{2}$$

$$\theta_L = \frac{\pi}{2} - \phi_L$$

where ϕ_{oR} , ϕ_{oL} and ϕ_R , ϕ_L denote the incident and observation angles which are all measured from the top surface of the impedance double wedge, S_T . The terms, $\exp\left(-\frac{l}{2}jk \cos \phi_{oR}\right)$ and $\exp\left(-\frac{l}{2}jk \cos \phi_{oL}\right)$ in (5.6) is used to account for the phase shift of incident plane wave due to the shifting of origin. If the plane wave is at normal incidence ($\phi_{oL}, \phi_{oR} = 90^\circ$), this term is reduced to unity. On the other hand, the terms, $\exp\left(\frac{l}{2}jk \sin \theta_R\right)$ and $\exp\left(\frac{l}{2}jk \sin \theta_L\right)$ in (5.6) are used to correct the phase shift of emanating diffracted wave when the origin is moved from each corner to the center of the impedance double wedge. These phase factors are also applicable to incident and reflected fields when two impedance wedges are combined.

Figure 5.5 Observation plane is normal to the diffracted fields emanating from both edges.

When the observation plane is on top of the impedance double wedge, with distance of $y = h_1$ as shown in Figure 5.6, the resultant diffracted field is given by

$$U_z^d = D_{TE}(\phi_R, \phi_{oR}) \frac{\exp(-jk\rho)}{\sqrt{\rho}} \exp\left(-\frac{l}{2}jk \cos \phi_{oR}\right) + \quad (5.7)$$

$$D_{TE}(\phi_L, \phi_{oL}) \frac{\exp(-jk\rho)}{\sqrt{\rho}} \exp\left(-\frac{l}{2}jk \cos \phi_{oL}\right)$$

Figure 5.6 Observation plane is on top of the impedance double wedge, with distance of $y = h1$.

5.1.6 Surface Field for Impedance Double Wedge

When the incident field illuminates an impedance double wedge as shown in Figure 5.7, the primary diffracted field is induced at the edge of point A. There is also primary diffracted field induced at the edge of point B, which the discussion here is applied similarly. The primary diffracted field is identical to the external diffracted field discussed in Section 5.1.4. Besides that, another type of electromagnetic field that may induce at the edge of point A is the surface field, which propagates along the surfaces of the impedance double wedge. The surface field is given by (3.10) in Chapter 3 and its existence is dependent on the Heaviside function, which is a function of the normalized surface impedance of the wedge. If the propagated surface field reaches another edge, such as point B in Figure 5.7, the secondary diffracted field is induced.

The amplitude of the secondary diffracted field is characterized by the surface field and diffraction coefficient corresponds to the wedge properties at point B. The resultant amplitude is relatively small in terms of magnitude if compared to the primary diffracted field at point A. Hence, the contribution of secondary diffracted field to the final electromagnetic solution is relatively insignificant and is ignored in the analysis.

Figure 5.7 Surface field propagates along the surface of an impedance double wedge.

5.2 Results and Discussion for Impedance Double Wedge

The results presented in this section for the electromagnetic scattering of an isolated single line structure without underneath substrates are based on the impedance double wedge model discussed in Section 5.1. Here, the impedance double wedge model is also known as the electromagnetic ray tracing (ERT) model since all the required geometrical optics and diffracted fields are distinguishable. Normal illumination of plane wave to the resist and polysilicon isolated impedance double wedges is considered. The illumination wavelength, λ is 633 nm with transverse electric (TE) polarization is assumed and has unit amplitude for the incident electric field. The refractive index of resist and polysilicon at wavelength 633 nm are given in Appendix A. The coordinate and nomenclature are referred in Figure 5.6. Figures 5.8 (a), (b) and (c) show

the amplitude and phase of total electric field for an isolated resist double wedge with width, l of $4\text{ }\mu\text{m}$ (6.3λ), $2\text{ }\mu\text{m}$ (3.2λ) and $1\text{ }\mu\text{m}$ (1.6λ), respectively obtained using the ERT model. The reference FDTD solutions are also given in each figure and the observation level is taken at elevated distance of $h_1 = 0.8\lambda$ ($ky = 5$). On the other hand, Figures 5.9 (a), (b) and (c) show the amplitude and phase of total electric field for an isolated polysilicon double wedge with width, l of $4\text{ }\mu\text{m}$ (6.3λ), $2\text{ }\mu\text{m}$ (3.2λ) and $1\text{ }\mu\text{m}$ (1.6λ), respectively obtained using the ERT model. Similarly, the reference FDTD results are also shown and the observation level is at elevated distance of $h_1 = 0.8\lambda$ ($ky = 5$). The selection of elevated distance, $ky = 5$ is arbitrary, which is well-above the lower limit found in the literature [116] for deriving the diffraction coefficient using high frequency asymptotic method.

The results for both resist and polysilicon double wedges show a good agreement with the reference FDTD results [170]. The FDTD results are generated using step size of $0.01\text{ }\mu\text{m}$ and the values are considered as converged when the variation is less than 0.001. It is shown clearly in the results that there are no discontinuities of amplitudes and phases across the shadow boundaries at $x = \pm l/2$, which are indicated by all the dotted lines in Figures 5.8 and 5.9. For normal incidence ($\phi_{oL}, \phi_{oR} = 90^\circ$ in Figure 5.5), the incident shadow boundaries coincide with the reflection shadow boundaries. The discontinuity caused by geometrical field has been compensated fully by the diffracted field. Furthermore, the ignorance of secondary diffracted field caused by the surface field as discussed in Section 5.1.6, if they exist, has not affected accuracy of the impedance double wedge solution since the results obtained from this work are closely match with the reference FDTD results. This implies that the secondary diffracted field is

Figure 5.8 (a)-(c) Amplitude and phase for an isolated resist impedance double wedge with line width, l of $4 \mu\text{m}$, $2 \mu\text{m}$ and $1 \mu\text{m}$ respectively obtained using the ERT model. The reference FDTD solutions are also given.

Figure 5.9 (a)-(c) Amplitude and phase for an isolated polysilicon impedance double wedge with line width, l of 4 μm , 2 μm and 1 μm respectively obtained using the ERT model. The reference FDTD solutions are also given.

relatively insignificant and can be ignored in the total solution. In other words, the dominated electromagnetic fields at the observation points are geometrical optics (incident and reflected field) and diffracted fields.

5.3 Line Structures on Substrate

With the formulations and results presented for the isolated impedance double wedge, this section aims to extend the study with the inclusion of the underneath substrate for the line structures. The electromagnetic solution becomes more complex when the line structures are formed on substrate. It requires a detailed analysis of electromagnetic waves that propagates inside and outside the line structures. These electromagnetic waves include the incident field and different combinations of reflected and diffracted fields. The incident field is identical to Section 5.1.2, which requires no further description of the formulation. The detailed analysis of the reflected and diffracted fields is presented in Sections 5.3.1 and 5.3.2, respectively. All the discussion are based on one side of a single line structure, i.e. using single edge for the wedge, with inclusion of the underneath substrate. This forms the basis to obtain the solution for a single line structure, and it is extendable for the case of two-line structures. Furthermore, only the primary components of the geometrical optical fields are considered and any multiple reflections and transmissions in the substrate or line structures are ignored. For ease of illustration, the real line structures formed on substrate, with their associated refractive indices are shown in the figures presented in this section, instead of using the impedance wedge model.

5.3.1 Reflected Field

Figures 5.10 (a)-(c) shows a right-angled wedge (part of a line structure) formed on substrate with refractive index, n_2 . The wedge refractive index is given as n_1 . For the material boundary, n_0-n_1 , the two surfaces, S_T and S_V correspond to the top and vertical surfaces of the wedge, respectively. On the other hand, the surfaces, S_I and S_B are the material boundaries for n_1-n_2 and n_0-n_2 , respectively. When the incident wave at angle of $\phi_o \leq \frac{\pi}{2}$ illuminates the wedge, there are five types of reflected field that need to be considered for an observation level at $y = h_1$. Each of them contributes to the total solution at points B_1 , T_1 , and T_2 in Figure 5.10 (a), T_3 in Figure 5.10

Figure 5.10 (a)-(c) Existence of different reflected fields for a wedge (part of a line structure) formed on substrate.

(b), and T_4 in Figure 5.10 (c). They are discussed below. The analysis here assumes that the substrate layer, n_2 has infinite thickness and only the reflection at the surfaces S_I and S_B are included.

By referring to Figure 5.11, the direct reflected field from the substrate, n_2 at surface S_B contributes to the total field at point B_1 . At this point, the reflected field caused by reflection from the point Q_r is represented using

$$\begin{aligned} U_z^{r2}(\rho, \phi) &= R_{TE, S_T} U_z^i(Q_r) \exp(-jk\rho_r) \\ &= R_{TE, S_T} \exp(jk\rho_{Q_r} \cos[\phi_{Q_r} + \phi_o]) \exp(-jk\rho_r) \end{aligned} \quad (5.8)$$

where ρ_{Q_r} is the distance measured from the origin to the point Q_r , and ϕ_{Q_r} is the angle measured from the top surface, S_T as shown in Figure 5.11. The reflection coefficient for TE polarization, R_{TE, S_T} is similar to (5.3), except that the used refractive index is different. Here, the refractive index of the substrate, n_2 is applied. The term $\exp(-jk\rho_r)$ is used to correct the phase shift due to the movement of origin from the edge of the wedge to the point Q_r .

Figure 5.11 Plane wave reflection from the bottom surface, S_B .

As shown in Figure 5.10 (a), when the incident wave reaches the top surface of the wedge, S_T at point T_{1-1} , part of the wave will be reflected directly and reach point T_1 . The expression for the reflected field at point T_1 as shown in Figure 5.10 (a) is obtained from (5.2). In this ERT model, an effective refractive index, n_e is applied for its reflection coefficient given in (5.3), instead of using the exact refractive index of the wedge, n_1 . By doing so, it allows the exclusion of the reflected field that contributes to the total field at point T_2 , which follows the ray path of transmission (n_0-n_1) at point T_{1-1} , reflection (n_1-n_2) at point T_{2-1} , and transmission (n_1-n_0) at point T_{2-2} . More details about the derivation of effective refractive index, n_e are given in Section 5.4. On the other hand, Figures 5.10 (b) and (c) show the field points at T_3 and T_4 both involve the transmitted field (n_1-n_0) along the side wall of the wedge at surface, S_V . In Figure 5.10 (b), the field point at T_3 follows the ray path of transmission (n_0-n_1) at point T_{3-1} , reflection (n_1-n_2) at point T_{3-2} , and transmission (n_1-n_0) at point T_{3-3} . In Figure 5.10 (c), the field point at T_4 follows the ray path of transmission (n_0-n_1) at point T_{4-1} , transmission (n_1-n_0) at point T_{4-2} , and reflection (n_1-n_2) at point T_{4-3} . Their expressions for the electromagnetic field do not present any difficulties with the aid of reflection and transmission coefficients. If the incident field is illuminating at normal angle to the top surface, S_T , i.e. $\phi_o = \frac{\pi}{2}$, the points T_1 - T_2 and T_3 - T_4 are merged together. In this situation, the single point of T_3 - T_4 is located along the material boundary at $x = 0$.

5.3.2 Diffracted Field

The diffracted field needs to be considered to avoid any discontinuities at the shadow boundaries induced by the geometrical optics field. Similar to Section 5.3.1, a single wedge (part of a line

structure) formed on substrate is considered here. In general, there are three types of diffracted field that will contribute to the total electromagnetic field at an observation level of h_1 on top of the wedge surface as shown in Figure 5.12. They are the direct external, external diffracted-reflected and internal diffracted-reflected-transmitted fields correspond to the points A, B and C, respectively. The first two types are caused by the external diffraction of the wedge and the remaining is induced by the internal diffraction of the wedge. A more detailed description of their properties and formulations are discussed below.

Figure 5.12 Three types of diffracted rays emanating as cylindrical wave from the edge of a wedge.

(a) Point A: Direct External Diffracted Field

The direct external diffracted field contributes to the total solution at the point A as shown in Figure 5.12. The diffracted field emanates from the edge of the wedge and reaches the observation point directly. There is no alteration to the ray path. Hence, the diffracted field at the point A is identical to the study of diffraction in Section 5.1.4 and expression in (5.5) can be applied directly. Similarly, its diffraction coefficient is obtained from (3.11) in Chapter 3 without any further considerations needed.

(b) Point B: External Diffracted-Reflected Field

In Figure 5.12, the total field at point B involves reflection of the diffracted field from the substrate, n_2 at surface S_B . A more detailed illustration of these rays is given in Figure 5.13. The reflected rays are treated to emanate from an image source at point O'. Similar to the diffracted rays, these reflected rays from the bottom surface are characterized by a spreading factor of $\sqrt{\rho^i + \rho^r}$, where ρ^i is the distance from the wedge origin to the point of reflection at the substrate surface, S_B and ρ^r is the distance from the point of reflection to the point of observation. Existence of these rays ensures continuity across Regions I & II and Regions II & III. If it is neglected, the amplitude of the total field can show a significant disruption across different boundaries. Study of the geometrical optics field in different regions is similar to Section 5.1.1. With this, the external diffracted-reflected field at observation point, $B_{II} (x_{BII}, y_{BII})$ is expressed as

$$U_z^{rd} = R_{TE, S_B} D_{TE}(\phi, \phi_o) \frac{\exp(-jk(\rho^i + \rho^r))}{\sqrt{\rho^i + \rho^r}} \quad (5.9)$$

The diffraction coefficient $D_{TE}(\phi, \phi_o)$ is extracted from (3.11) in Chapter 3. On the other hand, the reflected point, $Q_r (x_{r1}, y_{r1})$ for a particular diffracted ray is required to determine the change of the phase and its attenuated amplitude. For an observation point at $B_{II} (x_{BII}, y_{BII})$, the location of the reflected point, x_{r1} is obtained by solving the following quadratic equation,

$$(y_{BII}^2 + 2 y_{BII} h_2) x_{r1}^2 + 2 h_2^2 x_{BII} x_{r1} - h_2^2 x_{BII}^2 = 0 \quad (5.10)$$

The detailed derivation of (5.10) is given in Appendix C.4. The reflection coefficient for the surface, S_B , R_{TE, S_B} is obtained from (5.3) but with the use of exact refractive index, n_2 for the substrate.

$$\begin{aligned}
 &4(1-\gamma^2)x_{t2}^4 - 4x_{cII}(1-\gamma^2)x_{t2}^3 + (x_{cII}^2 + h_1^2 - \gamma^2x_{cII}^2 - 4\gamma^2h_2^2)x_{t2}^2 \\
 &+ 4\gamma^2x_{cII}h_2^2x_{t2} - \gamma^2h_2^2x_{cII}^2 = 0
 \end{aligned} \tag{5.11}$$

where $\gamma = \frac{n_0}{n_1}$. The detailed derivation of (5.11) is given in Appendix C.5. This internal-diffracted-reflected-transmitted field is only included for the numerical results presented in Sections 5.5.1 (a) and 5.5.2 (a), which are devoted for the electromagnetic scattering analysis of resist line structures on silicon dioxide substrate.

Figure 5.14 Internal diffracted field of the wedge experiences reflection and transmission along the surfaces, S_I and S_T , respectively.

5.3.3 Cut Off Points for Diffracted Field

One of the unique properties of electromagnetic ray tracing (ERT) model developed in this work is that the total solution is obtained from the summation of all the induced electromagnetic fields. An induced electromagnetic field can be ignored when its amplitude is relatively small compared to the total field. This is also applied to the diffracted field. In this work, some parts of the diffracted field are cut off at certain points to avoid further complication of the formulation, particularly when more than a single line structure is studied. In this ERT model, there are two

cut off points being determined, which correspond to the external diffracted-reflected and internal diffracted-reflected-transmitted fields. By referring to the edge at point B in Figure 5.15, the emanating external diffracted-reflected field is cut off at point C_I . This implies that the external diffracted-reflected field emanated from point B is only considered from $x = -l_s$ to $x = C_I$ for $y = h_1$. The selection of cut off point C_I is based on the point C'_I , which is located exactly below the origin. Here, the external diffracted-reflected field is constrained by the adjacent structure. On the other hand, the internal diffracted-reflected-transmitted field is cut off at point C_{II} as shown in Figure 5.15. The cut off point, C_I is located exactly on top of the edge at point A, which is aligned with another corner of the same line structure. That is to say that the internal diffracted-reflected (S_I)-transmitted (S_{VA}) and internal diffracted-transmitted (S_{VA})-reflected (S_B) ray that reach points C_{U1} and C_{U2} , respectively are not considered. By truncating the diffracted fields, it assumes that the weightage of their amplitudes to the total field is relatively small and it can be ignored. If it is non negligible, it should show a clear discontinuity at the cut off points. Similarly, the same approach is applied to the above mentioned diffracted field emanating from the edges at points A, C and D.

Figure 5.15 Cut off points for different diffracted fields emanating from the edge at point B.

5.3.4 Surface Field for Line Structures Formed on Substrate

When the incident field illuminates the edge of a line structure, the external direct diffracted field is induced, as discussed in Section 5.3.2 (a). This diffracted field is the primary electromagnetic field. The contribution of its amplitude to the total solution cannot be ignored. Besides that, there is also surface field being induced, if the refractive index for the impedance wedge sustains its propagation along the surfaces S_T and S_v , as shown in Figure 5.16. The expression for the surface field is given in (3.10) in Chapter 3. When the surface field reaches another edge, for example the edge between surfaces S_v and S_B shown in the figure, the secondary diffracted field is induced. As the magnitude of this secondary diffracted field is relatively small, their contribution to the total solution is insignificant. Thus, it can be ignored.

Figure 5.16 Surface field propagates along the structure surface, S_T and produces secondary diffracted field.

5.4 Film Stack Approach for Effective Refractive Index

An effective refractive index, n_e is extracted for the line structures (n_1) and the substrate (n_2). By applying the effective refractive index, only the reflected field from the top surface, S_T of the

line structure is considered. This reflected field corresponds to the point T_1 in Figure 5.10 (a). It implies that the formulation for the reflected field which follows the path T_{1-1} , T_{2-1} and T_2 in Figure 5.10 (a) is not required. Associated with this is the use of effective refractive index for the impedance wedge when considering different diffracted fields. The exact refractive index is also used when the effective refractive index is inapplicable. A summary of the field type and its associated refractive index used in the ERT model is given in Table 5.1.

Table 5.1 Type of field and its associated refractive index used in the ERT model

Type of Field	Refractive Index
Incident	Exact
Reflected field from top surface, S_T	Effective
Reflected field from substrate surface, S_B	Exact
Direct external diffracted field	Effective
External diffracted-reflected field	Effective for diffracted field
	Exact for reflected field
Internal diffracted-reflected-transmitted field	Exact for all the fields

The effective refractive index is obtained from the amplitude of the film stack reflection coefficient, ρ using [179]

$$\rho = \frac{\eta_o - Y}{\eta_o + Y} \quad (5.12)$$

where η_o is the vacuum tilted admittance. It should be noted that ρ here is not referred to spreading factor for geometrical and diffracted field although the same symbols are employed. The optical admittance of the multilayer, Y which is given by the ratio, C/B is deduced from the film stack characteristic matrix,

$$\begin{bmatrix} \mathbf{B} \\ \mathbf{C} \end{bmatrix} = \begin{bmatrix} \cos \delta_1 & (j \sin \delta_1) / \eta_1 \\ j \eta_1 \sin \delta_1 & \cos \delta_1 \end{bmatrix} \begin{bmatrix} 1 \\ \eta_2 \end{bmatrix} \quad (5.13)$$

where δ_1 and $\eta_{1,2}$ are the phase thickness and the tilted admittance for the respective layer.

Figure 5.17 Simplification of two layers of film to a single layer film with an effective refractive index.

5.5 Results and Discussion for Line Structures Formed on Substrates

In this section, the study is focused on electromagnetic scattering of line structures formed on substrates. The numerical results are obtained using the ERT model developed in this work. The line structures are illuminated by plane wave with unit amplitude at normal incidence ($\phi_o = 90^\circ$ in Figure 5.3). Figure 5.18 shows the geometry of the single line structure with width of l . Due to the practical application in photolithography, the refractive indices for the line structures, n_1 and underneath substrate, n_2 are referred to two combinations, i.e. resist-silicon dioxide and polysilicon-silicon. The former combination is lossless dielectric with only real number for the refractive index and the later combination is absorbing medium with complex number for the refractive index. All the required refractive indices are given in Appendix A. The considered wavelength, λ is 633 nm. Similar to the numerical results presented in Section 5.2 for impedance double wedge, the results presented here focused on observation level at elevated distance, ky of 5. The height of the line structures is 5000 Å (0.5 μm). It is important to note that the external and internal diffraction coefficients associated with the wedge in the structures as discussed in Section 5.3.2 (a), (b) and (c) are extracted from Chapters 3 and 4, respectively. A

hybrid model with impedance wedge (Chapter 3) and penetrable wedge (Chapter 4) is applied to the resist-silicon dioxide combination. The penetrable wedge condition for internal diffraction is excluded for polysilicon-silicon combination. The reasons are given in Section 5.5.1 (b). The film stack approach discussed in Section 5.4 is used to extract the effective refractive index for the line structures and substrate, as discussed in Section 5.4.

Figure 5.18 Single line structure formed on substrate.

5.5.1 Individual Electromagnetic Field

By applying the ERT model developed in this work, the individual electromagnetic field that contributes to the total solution is identified. The results presented in this section emphasize on electromagnetic scattering of a single line structure formed on substrate. Two combinations of materials are studied, namely resist-silicon dioxide and polysilicon-silicon. The advantages of the ERT model are also discussed.

(a) Resist (Single Line Structure) – Silicon Dioxide (Substrate)

Figures 5.19 (a), (b), and (c) show each individual field that contributes to the electromagnetic scattering of a single resist line structure formed on silicon dioxide substrate. The selection of

line width, $x = 2 \mu\text{m}$ is arbitrary and mainly for elaboration purpose. The observation level is at elevated distance, ky of 5. Figure 5.19 (a) shows all the geometrical optics fields that contribute to the total solution. This includes the (i) incident field which has unit amplitude, (ii) reflected field from the top surface, S_T of the line structure and (iii) reflected field from the substrate surface, S_B . The reflected field from the top surface, S_T exists in the region of $|x| < 1 \mu\text{m}$ whereas the reflected field from the substrate surface, S_B exists in the region of $|x| > 1 \mu\text{m}$. The

Figure 5.19 Individual field that contributes to the total solution for the electromagnetic scattering of a single resist line structure. (a) Geometrical optics field (i) incident field (ii) reflected field from the top surface of the single line structure, S_T (iii) reflected field from the substrate surface, S_B (b) Diffracted field (i) direct external diffracted field (ii) external diffracted-reflected field (c) internal diffracted-reflected-transmitted field.

amplitude of both reflected fields show a clear discontinuity at the shadow boundaries, i.e. $x = \pm 1 \mu\text{m}$. These discontinuities are expected to be compensated by the direct external diffracted and external diffracted-reflected fields shown in Figure 5.19 (b), and internal diffracted-reflected-transmitted field shown Figure 5.10 (c). As shown in Figure 5.19 (b), the (i) direct external diffracted field exists across all the x distance. Its amplitude decays exponentially along the increasing direction of $|x| > 1 \mu\text{m}$. In the region of $|x| < 1 \mu\text{m}$, its amplitude gives a “ripple” trend. This can be explained by considering the direct external diffracted field is constructed based on the concurrent diffraction from two edges of the single line structure at $x = \pm 1 \mu\text{m}$ and interaction of these fields can occur. On the other hand, the (ii) external diffracted-reflected field shown in Figure 5.19 (b) only exist in the region $|x| > 1 \mu\text{m}$, with the amplitude decay exponentially from the increasing $|x| > 1 \mu\text{m}$ distance. The internal diffracted-reflected-transmitted field as shown in Figure 5.19 (c) is characterized by a very small amplitude, which is almost negligible compared to other geometrical optics or diffracted fields.

A step by step combination of all the geometrical optics and diffracted fields for a single resist line structure formed on silicon dioxide substrate is given here. In Figure 5.20 (a), the amplitude of the total geometrical optics field is shown. It is the combination of all the geometrical optics fields given in Figure 5.19 (a). The total geometrical optics field shows a step jump from 0.9 to 1.2 at the shadow boundaries, $x = \pm 1 \mu\text{m}$. By adding in the direct external diffracted field, the constant amplitude no longer exists. The amplitude is decaying smoothly in the direction of increasing $|x|$ distance from $x = \pm 1 \mu\text{m}$, as shown in Figure 5.20 (b). However, there are still discontinuities at the shadow boundaries, $x = \pm 1 \mu\text{m}$, which implies that some fields are still missing. The remedy to this discontinuity is by adding in the external diffracted-reflected field and internal diffracted-reflected-transmitted field. The final and total amplitude is given in

Figure 5.20 (c). It is observed that the amplitude across the shadow boundaries at $x = \pm 1 \mu\text{m}$ is smooth without any discontinuity. This concludes that all the prominent fields have been taken into consideration.

Figure 5.20 (a) Total geometrical optics field (b) Combination of geometrical optics and direct external diffracted fields (c) Total solution for the electromagnetic scattering of a single resist line structure formed on silicon dioxide substrate obtained using the ERT model.

(b) Polysilicon (Single Line Structure) – Silicon (Substrate)

The next part of results focused on the electromagnetic scattering of a single polysilicon line structure formed on silicon substrate. All the geometrical optics and diffracted fields discussed in the electromagnetic scattering of a single resists line structure are considered, except the internal diffracted-reflected-transmitted field. The refractive indices of polysilicon and silicon ($|n| \approx 3.9$ at 633 nm wavelength) are relatively high in comparison with that of resists and silicon dioxide. For this reason, it is expected that the amplitude of internal diffracted-reflected-transmitted field for polysilicon line structure is even smaller than the amplitude of internal diffracted-reflected-transmitted field for resist line structure. Hence, this particular field is ignored here. Figure 5.21 shows each individual field that contributes to the total field for the electromagnetic scattering of a single polysilicon line structure formed on silicon substrate. The width of the line structure is 2 μm and the observation level is taken at elevated distance, k_y of 5. All the geometrical optics fields are presented in Figure 5.21 (a), which includes the (i) incident field with unit amplitude, (ii) reflected field from the top surface, S_T of the polysilicon line structures and (iii) reflected field from the silicon substrate at surface, S_B . The reflected field from the top surface of the polysilicon line structures exists in the region of $|x| < 1 \mu\text{m}$ whereas the reflected field from the silicon substrate is found in the region of $|x| > 1 \mu\text{m}$. All the geometrical optics fields show a constant amplitude in their region of existence. There are two types of diffracted field presented in Figure 5.21 (b), namely the (i) direct external diffracted field and (ii) external diffracted-reflected field. The former exists across the entire x distance and the latter is confined in the region of $|x| > 1 \mu\text{m}$. The direct external diffracted field shows a ripple in the region of $|x| > 1 \mu\text{m}$

due to the interaction of external diffracted field emanating from the two edges of the single line structure.

Figure 5.21 Individual field that contributes to the total solution for the electromagnetic scattering of a single polysilicon line structure. (a) Geometrical optics field (i) incident field (ii) reflected field from the top surface of the single line structure, S_T (iii) reflected field from the substrate surface, S_B (b) Diffracted field (i) direct external diffracted field (ii) external diffracted-reflected field.

A step by step combination of all the geometrical optics and diffracted fields is also presented here. Figure 5.22 (a) shows the amplitude of the combination of all the individual geometrical optics field presented in Figure 5.21 (a). It gives a step jump, from 0.8 to 1.5 at the shadow boundaries of $x = \pm 1 \mu\text{m}$. Subsequently, the external diffracted field is added into the total geometrical optics field and the amplitude profile is presented in Figure 5.22 (b). An obvious discontinuity is still found at the shadow boundaries at $x = \pm 1 \mu\text{m}$. In order to solve this discontinuity, the external diffracted-reflected field is added into the solution. The amplitude profile for the final and total solution is presented in Figure 5.22 (c). The main difference in the approach in obtaining the total solution for Figure 5.22 (c) and Figure 5.20 (c) is that, the former

has excluded the internal diffracted-reflected-transmitted field. By judging from the smooth amplitude across the shadow boundaries at $x = \pm 1 \mu\text{m}$, it concludes that the amplitude of the internal diffracted-reflected-transmitted field is relatively small and the negligence has not caused any problem.

Figure 5.22 (a) Total geometrical optics field (b) Combination of geometrical optics and direct external diffracted fields (c) Total solution for the electromagnetic scattering of a single polysilicon line structure formed on silicon substrate obtained using the ERT model.

(c) Advantages of the Electromagnetic Ray Tracing (ERT) Model

There are two unique features in the ERT model for line structures developed in this work. They are discussed below.

Firstly, in the ERT model, the total solution is obtained by constructing all the geometrical optics and diffracted fields. This is one of the key advantages of ERT model for line structures, which allows the causes to an electromagnetic disturbance to be explained. For example, there is a disturbance of the amplitude at point X in both Figures 5.20 (c) and 5.22 (c) for the respective total field of the single line structure. Throughout all the step by step constructions of the solution, it is identified that the disturbance is caused by the existence of external diffracted-reflected field. On the other hand, a rigorous electromagnetic approach such as the FDTD method does not provide this explanation offered by the ERT model. In the FDTD method, only the final of the total electromagnetic solution is obtained. The users have no clue on how the geometry of the obstracter or its refractive index could have impact on the final solution. A vivid example is the discussed electromagnetic disturbance at point X in Figures 5.20 (c) and 5.22 (c). The ERT model for line structure developed in this work provides the answer to this question.

Secondly, in the ERT model, an explicit expression is derived for each electromagnetic field, be it the geometrical optics or the diffracted field. These expressions are characterized by the reflection, transmission and diffraction coefficients as discussed earlier in Sections 5.1 and 5.3. It can be applied independently to obtain a particular electromagnetic field at any points of interest, as long as the assumption of asymptotic expansion used to formulate the expressions are obeyed. In other words, this avoids the need to simulate the whole domain, which must include the entire

geometry of the structures. This is the usual case in the FDTD method where the electromagnetic field at points, which are not of interest is also generated. The ERT model developed in this work avoids a potentially large computational resource and time such as this, and only the required electromagnetic solutions are obtained. The advantages of the ERT model in terms of CPU computational time and memory used are demonstrated in Section 5.5.3. Prior to that, the accuracy of the ERT model is studied in Section 5.5.2.

5.5.2 Accuracy of the Electromagnetic Ray Tracing (ERT) Model

The aim of this section is to verify the accuracy of the ERT model. The amplitude and phase results of the total electromagnetic field obtained using the ERT model are compared with the reference FDTD solution [170]. If they match, this indicates that the decomposition of the total field into their individual electromagnetic field, particularly all the diffracted fields is valid. The study here includes the electromagnetic scattering for single and two-line structures, line structures with wavelength comparable width and variation of refractive index in the line structures. The parameters used in the study are $\Delta|E_z|$, ΔPhase , amplitude correlation coefficient (ACC) and phase correlation coefficient (PCC). The notations $\Delta|E_z|$ and ΔPhase (in radian unit) denote the difference of the amplitude and phase results. They are defined as,

$$\Delta|E_z| = |E_z|(\text{ERT}) - |E_z|(\text{FDTD}) \quad (5.14)$$

$$\Delta\text{Phase} = \text{Phase}(\text{ERT}) - \text{Phase}(\text{FDTD}) \quad (5.15)$$

On the other hand, the ACC and PCC results give an indication of the degree of matching of the ERT results to FDTD solution. The closer the ACC and PCC values to one, the better the matching of the ERT results with the reference FDTD solution. A perfect match gives value of one for both ACC and PCC. For a particular line structure, the ACC and PCC are defined as,

$$ACC = \frac{\sum_{i=1}^m ACC_i}{m} \quad (5.16)$$

$$PCC = \frac{\sum_{i=1}^m PCC_i}{m} \quad (5.17)$$

where m denotes number of points within the domain of x distance. The ACC and PCC at the point, i are defined as

$$ACC_i = \begin{cases} \frac{|E_z|_i(\text{ERT})}{|E_z|_i(\text{FDTD})} & \text{for } |E_z|_i(\text{ERT}) < |E_z|_i(\text{FDTD}) \\ \frac{|E_z|_i(\text{FDTD})}{|E_z|_i(\text{ERT})} & \text{for } |E_z|_i(\text{ERT}) > |E_z|_i(\text{FDTD}) \end{cases}$$
$$PCC_i = \begin{cases} \frac{\text{Phase}_i(\text{ERT})}{\text{Phase}_i(\text{FDTD})} & \text{for } \text{Phase}_i(\text{ERT}) < \text{Phase}_i(\text{FDTD}) \\ \frac{\text{Phase}_i(\text{FDTD})}{\text{Phase}_i(\text{ERT})} & \text{for } \text{Phase}_i(\text{ERT}) > \text{Phase}_i(\text{FDTD}) \end{cases}$$

(a) Single Line Structure

The amplitude and phase of the total field for a single resist line structure with width l of $8 \mu\text{m}$ (12.6λ), $4 \mu\text{m}$ (6.3λ), $2 \mu\text{m}$ (3.2λ) and $1 \mu\text{m}$ (1.6λ) formed on silicon dioxide substrate are shown in Figures 5.23 (a), (b), (c) and (d), respectively. The ERT results are compared with the FDTD solution. The observation level is taken at elevated distance, ky of 5. As presented in Figure 5.23 (a), the difference of amplitude, $\Delta|E_z|$ is well kept below 0.05 for line width of $8 \mu\text{m}$ (12.6λ). Here, the amplitude profile obtained using the ERT model shows a good match with the reference FDTD solution. For the same line width, the maximum difference in phase, ΔPhase is - 0.061 radian. However, when the line width is reduced to $1 \mu\text{m}$ (1.6λ), the maximum difference

Figure 5.23 Amplitude and phase of the total field for a single resist line structure with width of (a) $8 \mu\text{m}$, (b) $4 \mu\text{m}$, (c) $2 \mu\text{m}$ and (d) $1 \mu\text{m}$ obtained using the ERT model (this work) and its comparison with the FDTD solution.

of amplitude, $\Delta|E_z|$ increases to 0.07 and the mismatch of the solution is relatively significant especially outside the line width region, $|x| = 0.5 \mu\text{m}$. This is illustrated in Figure 5.23 (d). The findings of deteriorating accuracy of the ERT model with reducing resist line width is also traceable from the ACC and PCC results as presented in Figure 5.24. Both results decrease linearly from about 0.985 to 0.967 when the line width is reduced from $8 \mu\text{m}$ (12.6λ) to $1 \mu\text{m}$ (1.6λ). The discrepancy could probably be explained by considering the ignorance of certain diffracted fields in the analysis. By referring to Figure 5.15, the internal diffracted-reflected (S_I)-transmitted (S_{VA}) and internal diffracted-transmitted (S_{VA})-reflected (S_B) rays are not taken into consideration in the present ray tracing model. These rays contribute to the total solution at points C_{U1} and C_{U2} in the same figure. When the line width is as wide as $8 \mu\text{m}$ (12.6λ), their contribution can be neglected. For the case of $1 \mu\text{m}$ (1.6λ) line width, it is suspected that the absence of these rays contribute to the degradation of the accuracy, although there is no obvious discontinuities shown at the shadow boundaries.

Figure 5.24 The ACC and PCC results for a single resist line structure formed on silicon dioxide substrate. The dashed linear trendline is referred to ACC whereas the thin solid linear trendline is referred to PCC.

The ACC and PCC results for a single resist line structure on silicon dioxide substrate with subwavelength line width ranging from $0.5 \mu\text{m}$ (0.8λ) to $0.125 \mu\text{m}$ (0.2λ) are also included in

Figure 5.24. One can easily identify that the ACC and PCC values for $0.25\ \mu\text{m}$ ($0.4\ \lambda$) subwavelength resist line width are relatively high compared to $0.5\ \mu\text{m}$ ($0.8\ \lambda$) and $0.125\ \mu\text{m}$ ($0.2\ \lambda$) line width. In conjunction with this, the amplitude and phase results of the $0.25\ \mu\text{m}$ ($0.4\ \lambda$) single resist line structure obtained using the ERT model shows a good match with the reference FDTD solution as presented in Figure 5.25 (a). The $\Delta|E_z|$ and ΔPhase are bounded within 0.05 and 0.1 radian, respectively. When the line width is further reduced to $0.125\ \mu\text{m}$ ($0.2\ \lambda$), the ACC and PCC results drop simultaneously to about 0.955 as given in Figure 5.24. Figure 5.25 (b) shows the respective amplitude and phase results of the $0.125\ \mu\text{m}$ ($0.2\ \lambda$) single line structure obtained using the ERT model and its comparison with the reference FDTD solution. The $\Delta|E_z|$ is bounded within 0.1. However, the phase results show relatively poor accuracy with ΔPhase exceeds 0.1 radian as indicated by the arrows X in Figure 5.25 (b). For all the line widths stated in Figure 5.24, the respective maximum ΔPhase are less than 0.1 radian. This can be traced through Figures 5.23 (a), (b), (c), (d) and 5.25 (a). If ΔPhase is required to be bounded within 0.1 radian, the line width of $0.25\ \mu\text{m}$ ($0.4\ \lambda$) is then considered as the limit of the ERT model for a single resist line structure on silicon dioxide substrate.

On the other hand, Figures 5.26 (a), (b), (c) and (d) present the amplitude and phase of the total electric field for a single polysilicon line structure with width, l of $8\ \mu\text{m}$ ($12.6\ \lambda$), $4\ \mu\text{m}$ ($6.3\ \lambda$), $2\ \mu\text{m}$ ($3.2\ \lambda$) and $1\ \mu\text{m}$ ($1.6\ \lambda$), respectively formed on silicon substrate. The ERT results are compared with the reference FDTD results. The observation level is taken at elevated distance, k_y of 5. It is shown that the amplitude results for single polysilicon line structure obtained using the ERT model give a better match with the FDTD results if compared with the results for single resist line structure presented in the earlier part of this section. This implies that line structures

Figure 5.25 Amplitude and phase of the total field for a single resist line structure with subwavelength width of (a) $0.25 \mu\text{m}$ and (b) $0.125 \mu\text{m}$ obtained using the ERT model (this work) and its comparison with the FDTD solution.

Figure 5.26 Amplitude and phase of the total field for a single polysilicon line structure with width of (a) 8 μm , (b) 4 μm , (c) 2 μm and (d) 1 μm obtained using the ERT model (this work) and its comparison with the FDTD solution.

with absorbing medium achieves better accuracy in this ray tracing model. A similar finding is also found for the line width dependent error. At line width of $8\text{ }\mu\text{m}$ (12.6λ), the results show a maximum amplitude difference, $\Delta|E_z|$ of -0.045 and when the line width reduces to $1\text{ }\mu\text{m}$ (1.6λ), the maximum amplitude difference, $\Delta|E_z|$ increases to -0.067 . The results of ACC presented in Figure 5.27 are also consistent with this finding for line width dependent error. The ACC reduces from 0.988 to 0.978 when the polysilicon line width is reduced from $8\text{ }\mu\text{m}$ to $1\text{ }\mu\text{m}$. Nevertheless, the reduction is insignificant as ACC of as high as 0.978 is still achieved for $1\text{ }\mu\text{m}$ single polysilicon line structure on silicon substrate. On the other hand, the phase results show relatively significant discrepancy near to their respective shadow boundaries, $x = \pm l/2\text{ }\mu\text{m}$ for all the line widths shown in Figures 5.26 (a), (b), (c) and (d). The maximum phase difference, ΔPhase is 0.14 radian found at line width of $1\text{ }\mu\text{m}$ (1.6λ). As a result of this, the PCC results given in Figure 5.27 are relatively low compared to the ACC results.

Figure 5.27 The ACC and PCC results for a single polysilicon line structure on silicon substrate. The dashed linear trendline is referred to ACC whereas the thin solid linear trendline is referred to PCC.

The ACC and PCC results for a single polysilicon line structure on silicon substrate with subwavelength line width ranging from $0.5\text{ }\mu\text{m}$ (0.8λ) to $0.125\text{ }\mu\text{m}$ (0.2λ) are also included in Figure 5.27. Associated with this, Figure 5.28 (a) presents the amplitude and phase results of the

Figure 5.28 Amplitude and phase of the total field for a single polysilicon line structure with subwavelength width of (a) 0.25 μm and (b) 0.125 μm obtained using the ERT model (this work) and its comparison with the FDTD solution.

0.25 μm (0.4λ) single line structure obtained using the ERT model and its comparison with the reference FDTD solution. It is shown that a good match between the two solutions is still established, particularly for the amplitude results. The phase results obtained from the ERT model shows discrepancy with the reference FDTD solution only in the vicinity of $x = \pm 0.125 \mu\text{m}$ (indicated by the dotted lines). When the line width is further reduced to 0.125 μm (0.2λ), the ACC and PCC results drop to 0.961 and 0.926, respectively as given in Figure 5.27. Figure 5.28 (b) illustrates that the poor PCC results are due to the prominent discrepancy of the phase results in the vicinity of $x = \pm 0.0625 \mu\text{m}$ (indicated by the dotted lines). Furthermore, the mismatch of the phase results is also significant in the regions indicated by the arrows X in Figure 5.28 (b). This concludes that the line width of 0.125 μm (0.2λ) gives relatively poor accuracy. In this case, the line width of 0.25 μm (0.4λ) is considered as the limit of the ERT model for a single polysilicon line structure on silicon substrate.

(b) Two-Line Structures

The section aims to study the accuracy of the ERT model for electromagnetic scattering of two-line structures. Previously in a single line structure, the diffracted field is emanating from the two edges of the same double wedge. When two-line structures are considered, the interaction of the diffracted field emanating from the adjacent double wedge occurs. Their impact to the accuracy of the ERT model is examined in this section. The amplitude and phase results presented in Figures 5.29 (a), (b), (c) and (d) are based on the combination of polysilicon-silicon (line structure-substrate) with variation in the spacing from 8 μm to 1 μm between two identical line structures. Each single line structure has a width of 2 μm (3.2λ). It is shown that the amplitude results obtained from the ERT model are comparable with the FDTD results although they do not

Figure 5.29 Amplitude and phase of the total field for two identical 2 μm polysilicon line structures on silicon substrate with spacing of (a) 8 μm , (b) 4 μm , (c) 2 μm and (d) 1 μm obtained using the ERT model (this work) and its comparison with the FDTD solution.

perfectly match. It is observed that the prominent discrepancy is always located near to the shadow boundaries, which are denoted by the dashed lines in the figures. When the spacing between the lines structure is $1\text{ }\mu\text{m}$, it gives the greatest difference in amplitude, $\Delta|E_z|$ and phase, ΔPhase i.e. 0.166 and 0.2 radian, respectively as shown in Figure 5.29 (d). The results improved when the spacing in between the lines is increased to $8\text{ }\mu\text{m}$ (12.6λ), with the absolute difference in amplitude and phase is bounded within 0.1 and 0.1 radian, respectively as shown in Figure 5.29 (a). In general, the ACC and PCC results are also increased when the spacing of the two lines structures are increased, as presented in Figure 5.30. In Figure 5.30, it should be noted the spacing of the lines is increased from right to left along the x-axis. These findings conclude that accuracy of the ERT model is improved when there is less interaction of the diffracted field emanated from the adjacent structures.

Figure 5.30 The ACC and PCC results for two-line structures of polysilicon on silicon substrate. The spacing in between the $2\text{ }\mu\text{m}$ lines is varied from $8\text{ }\mu\text{m}$ to $1\text{ }\mu\text{m}$. A subwavelength space width of $0.5\text{ }\mu\text{m}$ is also included. The dashed linear trendline is referred to ACC whereas the thin solid linear trendline is referred to PCC.

When the spacing in between the $2\text{ }\mu\text{m}$ line structures is reduced to a subwavelength width, $0.5\text{ }\mu\text{m}$ (0.8λ), the ACC and PCC results are further reduced to 0.943 and 0.927, respectively as shown in Figure 5.30. Associated with this, the amplitude and phase results obtained from the

ERT model give a relatively poor match with the reference FDTD solution as presented in Figure 5.31. There are significant mismatch of both the amplitude and phase results, particularly in the x distance of $\pm 0.25 \mu\text{m}$. The maximum amplitude difference, $\Delta|E_z|$ and phase difference, ΔPhase are 0.172 and -0.399 radian, respectively. It is concluded that the ERT model gives relatively poor accuracy for the two-line structures with subwavelength spacing of $0.5 \mu\text{m}$ (0.8λ). In this case, the smallest allowable spacing between the two identical $2 \mu\text{m}$ (3.2λ) polysilicon line structures is identified as $1 \mu\text{m}$ (1.6λ).

Figure 5.31 Amplitude and phase of the total field for two identical $2 \mu\text{m}$ polysilicon line structures on silicon substrate with spacing of $0.5 \mu\text{m}$ obtained using the ERT model (this work) and its comparison with the reference FDTD solution.

(c) Line Structures with Subwavelength Width and Space

The two-line structures discussed in Section 5.5.2 (b) are based on line width of 3.2λ . This section studies the accuracy of the ERT model for two-line structures with subwavelength line width and space. The amplitude and phase of the total field for two-line structures with width of $0.5 \mu\text{m}$ (0.8λ) formed on silicon substrate are shown in Figure 5.32. The spacing in between the line structures is also $0.5 \mu\text{m}$ (0.8λ) and the observation level, k_y is at 5. Such a narrow line width and space has a great impact on the accuracy of the model. As shown in Figure 5.32. The amplitude results obtained from the ERT model are facing discontinuities problem. There are

Figure 5.32 Amplitude and phase of two identical $0.5 \mu\text{m}$ (0.8λ) polysilicon line structures with equal spacing obtained using the ERT model (this work) and its comparison with the FDTD solution.

obvious discontinuities in amplitude found at $x = \pm 0.5 \mu\text{m}$. The discussion here focuses on amplitude discontinuity at $x = 0.5 \mu\text{m}$. By referring to Figure 5.15, the amplitude discontinuity at $x = 0.5 \mu\text{m}$ in Figure 5.32 corresponds to the cut off point at C_1 for the diffracted-reflected field. This diffracted-reflected field emanates from the edge B. In this analysis, a secondary diffracted field emanates from the edge C (Figure 5.15) induced by the diffracted-reflected field, which follows the ray path $B-C'_1-C$ is ignored. If this field and the corresponded geometrical optics field are taken into consideration, it is expected that the amplitude discontinuity at $x = 0.5 \mu\text{m}$ can be solved. The same finding is applied to the amplitude discontinuity found at $x = -0.5 \mu\text{m}$ in Figure 5.32 but with different cut off points.

(d) Variation of Wavelength

All the results presented prior to this are based on 633 nm wavelength. This section aims to extend the accuracy study of the ERT model across different wavelengths. The selected wavelengths are meant for practical photolithography applications either in metrology and alignment purposes (633 nm and 532 nm), or exposure light source in the stepper/scanner (436 nm, 365 nm, 248 nm and 193 nm). Refractive indices of $3.93 - j0.0717$ and $3.88 - j0.01933$ are applied for the line structures and underneath substrate, respectively. The observation distance, ky is 5. Figure 5.33 (a) shows the ACC and PCC results across different wavelengths for a single line structure with width of 0.4λ . It is observed that both the ACC and PCC results are bounded within 0.961 to 0.987. There is no significant drop in the ACC and PCC results when the wavelength is reduced. On the other hand, Figure 5.33 (b) shows the ACC and PCC results across different wavelengths for two identical line structures with width of 3.2λ . The spacing in between the line structures is taken as 1.6λ . The linear trendline does not show a steep decrease

in ACC and PCC values when the wavelength is reduced. Although the results at 193 nm wavelength are the lowest across all the wavelengths, the ACC and PCC values are still as high as 0.952 and 0.941, respectively. From the results presented in this section, it is concluded that the ERT model is applicable to a wide range of wavelengths for practical applications in photolithography. This shows that the ERT model is extendable to other applications, for example in the image formation for illumination in photolithography at 193 nm wavelength.

Figure 5.33 The ACC and PCC results for (a) single line and (b) two-line structures at different wavelengths. The dashed linear trendline is referred to ACC whereas the thin solid linear trendline is referred to PCC.

(e) Variation of Refractive Index

In this section, the accuracy of the ERT model for line structures with variation in the refractive index is studied. This is to ensure that the ERT model is applicable to a wide range of materials. Lossless and lossy materials are covered in this study. For the refractive index, the former is characterized by a pure real number whereas the later is characterized by a complex number with negative imaginary part. Both the line structures and underneath have identical refractive index, i.e. $n_1 = n_2$. The ACC and PCC results for single and two-line structures across different real refractive indices are shown in Figures 5.34 (a) and (b), respectively. The imaginary part of the refractive index for lossy line structure is taken as $-0.1j$. The results are obtained based on the total solution at observation distance, k_y of 5 and all the line structures and spacings have a width of $1\ \mu\text{m}$. In Figure 5.34 (a), the ACC results for single line structure of both lossy and lossless materials show a consistent value across the real refractive index. This can be observed through the linear trendline which are almost flat at ACC of 0.98. Its companion PCC results as shown in Figure 5.34 (a) are also bounded in the range of 0.98 to 0.96. In contrast, the ACC for two-line structures of both lossy and lossless materials exhibit a relatively steep decrease in value when the real part of the refractive index increases. This is illustrated in Figure 5.34 (b). The same finding is also applied to the PCC results presented in Figure 5.34 (b). In other words, the ACC and PCC results are improved when the real part of the refractive index reduces (from right to left in the figures). For two-line structures, it is also observed that the ACC and PCC results for lossy material are higher than the lossless material. This indicates that the ERT model achieves better accuracy for lossy line structures.

Figure 5.34 (a) Amplitude correlation coefficient (ACC) and (b) Phase correlation coefficient (PCC) for single and two-line (equal spacing) structures across different real refractive indices. Each single line has width of $1\ \mu\text{m}$ and the observation distance, k_y is 5. For lossless line structures, the imaginary part of the refractive index is zero whereas for lossy line structures, the imaginary part of the refractive index is taken as $-0.1j$.

5.5.3 CPU Computational Time and Memory Used

In the FDTD method, the electromagnetic field is computed everywhere in the specified domain. The domain must be sufficiently large to include the entire geometry of the structures. This is the usual case in the FDTD method where the electromagnetic field at points which are not of interest is also generated. Furthermore, a converged FDTD solution is also required. As a result of these properties, the extensive consumption of the CPU computational time and memory is unavoidable. In this work, the amplitude and phase results of the reference FDTD solution presented in Section 5.5.2 for each condition of line structures required CPU computational time of more than one hour using a notebook PC with Intel Core 2 Duo Processor T5450 (1.66 GHz). The memory used exceeded 100 MB. In contrast to this, the ERT model gives the advantage of relatively low CPU computational time and memory used. To demonstrate this, Figure 5.35 (a) shows the CPU computational time of the ERT amplitude results presented in Figures 5.26 (a), (b), (c), (d) and 5.29 (a), (b), (c), (d) using the same CPU for the respective polysilicon line structures on silicon substrate. The CPU computational time taken for all the single and two-line structures with width or space of at least $1\text{ }\mu\text{m}$ (1.6λ) is well below 120 s. Associated with this is the relatively low consumption of memory, which is below 10 MB as presented in Figure 5.35 (b). Such a relatively low CPU computational time and memory used is due to the flexibility of the ERT model that computes only the required electromagnetic field. The solution is based on direct computation using the explicit expressions derived for each electromagnetic field, be it the geometrical optics or the diffracted fields, as discussed in Sections 5.1 and 5.3.

Figure 5.35 The (a) CPU computational time and (b) memory used for the amplitude results obtained from the ERT model for single and two-line polysilicon structures on silicon substrate.

5.6 Concluding Summary

In this chapter, a new electromagnetic scattering model for line structures was established based on the ray tracing approach. This electromagnetic ray tracing (ERT) model is able to identify individual electromagnetic field that contributes to the total solution. This includes the geometrical optics field for incidence, reflection and transmission phenomenon. Associated with this is the existence of diffracted field. The diffraction coefficients developed in Chapter 3 and 4 were applied accordingly for the direct external-diffracted, external diffracted-reflected, and

external diffracted-reflected-transmitted fields associated with the line structures. By applying this model, a vivid example was given where the causes to an electromagnetic disturbance at a particular region were identified and explained explicitly. This is one of the key advantages of ERT model developed in this work. The accuracy of the model was verified through the comparison with the reference FDTD solution. Different conditions such as line width and refractive index were also studied. For a single 1.6λ (width) polysilicon line structure on silicon substrate, the ERT model was able to demonstrate ACC of 0.978 with the maximum amplitude difference, $\Delta|E_z|$ of as low as -0.067. The subwavelength line width of 0.4λ was identified as the limit of the ERT model for the single polysilicon line structure. On the other hand, it was found that the smallest allowable spacing between two identical 3.2λ polysilicon line structures on silicon substrate was 1.6λ . A linear trend of improving ACC and PCC results with reducing the real part of the refractive index was also observed for two-line structures. This applied to both lossless and lossy materials for the line structures. Finally, the advantages of the ERT model in terms of CPU computational time and memory used were also demonstrated.

CHAPTER 6 ADVANCED WAFER ALIGNMENT MARKS FOR SUB-MICRON PROCESS TECHNOLOGY

In photolithography, line structures in wafer alignment marks are used to align the current masking layer to the previous layer. The alignment step is very sensitive to process variation especially when a new process flow is introduced. The change of process sequence and material being used can adversely affect the alignment performance. Hence, the objective of this chapter is to study the alignment capability of enhanced order marks and narrow marks for advanced technology node. The approach is as follows:

1. Firstly, a theoretical model based on Rigorous Coupled Wave Analysis (RCWA) is adopted to analyze different periodic structures of step grating alignment marks.
2. Secondly, the alignment experimental work is performed for both front-end-of-line (FEOL) and back-end-of-line (BEOL) processes in 90 nm and 0.11 μm technology nodes. Study of narrow enhanced order marks is also included.

By adopting the RCWA, the higher order reflected diffraction efficiency is studied for enhanced order marks in Section 6.2.2 (b). The rationale of adopting RCWA rather than the ERT model (given in Chapter 5) is two-fold. Firstly, the developed ERT model is based on geometrical optics and diffracted fields. All the expressions are derived using the first term in the Luneberg-Kline asymptotic expression [80]. None of the higher orders terms are included. In contrast, the approach of Fourier expansion in RCWA allows an explicit expression to be derived for each higher order of the reflected diffraction efficiency. These expressions can be conveniently applied to demonstrate the advantages of enhanced order marks. Secondly, the RCWA is better

suited for well-defined periodic structures in alignment marks when understanding of the physical field is not required. The RCWA is applied to explore consequences of different periodic structures in improving the reflected diffraction efficiency. Although the ERT model could also provide the electromagnetic scattering solution, an extensive ray tracing of the electromagnetic field is unnecessary for the study of alignment mark. In fact, this chapter emphasizes on the application of line structures in alignment for photolithography. The study of line structures aims to ensure that the alignment is capable to meet the stringent overlay for advanced technology node in real process environment. In this case, the simulation results help to provide an understanding of the selection of different dimensions for the line structures in the enhanced order marks. Based on the two reasons mentioned above, the RCWA is adopted here.

6.1 Theory of Rigorous Coupled Wave Analysis (RCWA)

Modeling of the alignment marks can be treated similarly as diffraction grating. Alignment marks have the effect of producing periodic alterations in either the phase, amplitude or both in the emergent wave. When electromagnetic wave is incident on its surface, part of the wave will be reflected and the remaining is transmitted into the marks. The marks are usually covered by a series of layers, known as film stack. In this work, RCWA is used to determine the reflected diffraction efficiency at each particular order of enhanced order marks. Diffraction efficiency is a physical quantity that characterizes how the incident power is distributed between different orders.

The geometry of the rectangular groove diffraction grating and film stack problem treated in this analysis is shown in Figure 6.1. A linearly polarized electromagnetic wave, obliquely incident

upon the geometry with an incident angle of θ , produces both backward and forward diffracted waves. The backward diffracted waves will be used in the alignment model whereas the forward diffracted waves are not involved in alignment. Planar diffraction is considered here, where all the forward and backward diffracted orders lie in the same plane, i.e. plane of incidence. All the diffracted orders have the same polarization. The grating has a period P , with alternating refractive indices, n_r (ridge) and n_g (groove) in the grating region. The film stack and the grating are treated to be bounded by two different mediums with refractive indices n_I , for Region I and n_{II} for Region II. The modulus of the wave vector of the incident wave in vacuum is denoted by k . A temporal dependence in $\exp(j\omega t)$ of the wave is assumed.

Figure 6.1 Geometry of the diffraction problem in wafer alignment marks.

For TE polarization, the normalized electric field of incident wave, which is perpendicular to the plane of incidence, is given by

$$E_{incy} = \exp[-jk n_I (x \sin \theta + y \cos \theta)] \quad (6.1)$$

and the normalized solutions with respect to the incident wave in Region I is given by

$$E_{Iy} = E_{incy} + \sum_i R_i \exp[-j(k_{xi}x - k_{Izi}y)] \quad (6.2)$$

For TM polarization, the normalized magnetic field of incident wave, which is perpendicular to the plane of incidence, is given by

$$H_{incy} = \exp[-jk n_l (x \sin \theta + y \cos \theta)] \quad (6.3)$$

and the normalized solutions with respect to the incident wave in Region I is given by

$$H_{Iy} = H_{incy} + \sum_i R_i \exp[-j(k_{xi}x - k_{Izi}y)] \quad (6.4)$$

R_i in (6.2) and (6.4) denotes the normalized i -th backward diffracted (reflected) electric (for TE polarization) and magnetic (for TM polarization) field amplitude respectively. By combining the electric and magnetic field in the film stack and grating region with Maxwell's equations, second order partial derivative equations are formed. R_i is obtained by solving the second order partial derivative equations and the required boundary conditions are applied. Wave number, k with subscript of x or z denotes the respective direction. The $\sum_i$ sign is used to indicate the summation range of $-i$ to i .

For both cases of polarization, the reflected diffraction efficiency are defined as

$$DE_{ri} = R_i R_i^* \operatorname{Re} \left(\frac{k_{Izi}}{k n_l \cos \theta} \right) \quad (6.5)$$

The asterisk denotes complex conjugate. All the formulations for TE and TM polarizations are based on references [60-63].

6.2 Simulation of Alignment Marks

6.2.1 Details of Simulation

In this section, plane wave with arbitrary linear polarization at normal incidence ($\theta = 0$) is considered. In this case, the incident electric field (for TE polarization) or magnetic field (for TM polarization) is considered to be polarized along z-axis and has an amplitude of 1. In conventional alignment applications, usually the lowest orders are of most interest. With perpendicular incidence of the incidence wave, the plus and minus ($\pm$) diffraction orders are distributed symmetrically at 0th order. Reflected diffraction efficiency is used to determine the strength of alignment signal. The higher the reflected diffraction efficiency, the stronger the strength of alignment signal. The reflected diffraction efficiency can reach a minimum of near to zero, depending on factors such as the grating depth and refractive index.

The simulation work in this part focuses on the FEOL alignment, with the mark following the depth of trenches in the Shallow Trench Isolation (STI) [180] layer. Currently, the 90 nm process requires STI depth of about 4000 Å. When the technology node advances, it is expected to achieve a deeper STI depth. In order to fit this purpose, a series of depth, from 3800 Å to 5200 Å will be used for the following RCWA simulation. A perfect planar surface is assumed after the chemical mechanical polishing (CMP) process. It is well known that CMP process can introduce damage to the marks in an unpredictable trend.

The FEOL marks are deposited or coated with a series of layers. In other words, film stack analysis needs to be incorporated into the alignment problem. The layers include polysilicon,

bottom anti-reflection coating (BARC) [181] and photoresist. Figure 6.2 shows the geometry of the FEOL alignment problem with inclusion of film stack. With this, the region above the film stack has a refractive index of 1. Table 6.1 gives the default thickness or depth for a specified layer. A constant layer thickness is assumed. These parameters are remained throughout all the conditions unless otherwise stated. The simulation results are based on alignment wavelength of 633 nm. The refractive index of the materials at 633 nm wavelength used in the simulation can be found in Appendix A.

Figure 6.2 Geometry of the diffraction problem in wafer alignment marks.

Table 6.1 Default thickness or depth for every layer

Layer (<i>l</i>)	Materials	Thickness/ Depth ($\text{\AA}^*$)
I	Vacuum	-
1	Resist	4300
2	Bottom Anti-Reflective Coating (BARC)	600
3	Polysilicon	1600
G	<i>Ridge</i> : Silicon <i>Groove</i> : Silicon dioxide	4000
II	Silicon	-

* $1 \text{ \AA} = 1 \times 10^{-10} \text{ m}$

The strength of the reflected beam will vary in a sinusoidal manner when the thickness of any layer in the film stacks changes. The analysis here has ignored the existence of a very thin silicon dioxide layer in between the polysilicon layer and silicon wafer. This relatively thin layer is used to form the gate dioxide, with a physical thickness of no more than 20 Å for advanced technology node. Furthermore, silicon oxide with real refractive index is considered to be dielectric material, which does not absorb energy from the light [182]. Hence, their impact in the film stack is neglected.

The results of the reflected diffraction efficiency are focused on both TE and TM polarizations. The complex amplitudes of the reflected orders are obtained by solving the second order partial derivative equations in the RCWA using a commercial software, MATHEMATICA™ [23]. The second order partial derivative equations in RCWA are treated as eigenproblems, which involves solution as eigenvectors and eigenvalues of the matrix.

6.2.2 Results and Discussion

(a) Normal Marks

In this section, the influence of grating depth to normal mark TE and TM reflected diffraction efficiencies is studied. The thickness of the layers in the film stack follows the default values in Table 6.1. Figure 6.3 (a) shows the plane view of normal mark with 16 µm period and its duty cycle is 0.5 with identical width of lines and spaces. The trenches of the silicon substrates are filled up with silicon dioxide as shown in Figure 6.3 (b).

Figure 6.3 (a) Plane view of normal marks with equal line and space of 8 μm. (b) Trenches of the gratings on silicon substrate are filled up with silicon dioxide.

With reference to Figure 6.4, it is observed that 0th order reflected diffraction efficiency is relatively high while the negative and positive first orders are relatively low. Beyond negative and positive first order, the reflected diffraction efficiency drops significantly to nearly zero. In this case, 0th order does not contain any information about the gratings. It is desirable to achieve low 0th order reflected diffraction efficiency and high reflected diffraction efficiency for other order. On the other hand, it is also observed that both polarizations achieved good agreement between each other. Since only plane waves with normal incidence are considered here, the reflected diffraction efficiency is symmetrical at 0th order.

Figure 6.4 Reflected DE for TE and TM polarizations using 633 nm wavelength.

Figure 6.5 shows the reflected diffraction efficiency for TE and TM polarizations across various grating depths. The results show that a minimum 1st order reflected diffraction efficiency at grating depth of 4400 Å corresponds to relatively high 1st order reflected diffraction efficiency. When the 1st order reflected diffraction efficiency increases to a maximum at grating depth of

Figure 6.5 Reflected diffraction efficiency of normal mark for TE and TM polarizations across various grating depths using 633 nm wavelength.

5200 Å, the 0th order reflected diffraction efficiency drops to almost zero. The results follow the trend that increasing 0th order diffraction efficiency is associated with decreasing 1st order reflected diffraction efficiency. The magnitude of 0th order reflected diffraction efficiency is in the order of 1st order reflected diffraction efficiency, especially in the interval of 3800 Å to 4600 Å.

The discussion so far focuses on the first order of the reflected beam from the normal marks. When the technology node advances to the sub-micron regime, the use of first order reflected beam is no longer adequate to define the properties of the marks. In order to solve this problem, higher orders of the reflected beams are collected and it is able to achieve higher frequency signal to define edges of the structures accurately as illustrated in Figure 6.6. By doing so, the position of the marks can be located more precisely. The theory behind is similar to the illumination system in projection photolithography. One of the factors that determine the resolution of printed pattern is the ability of the optical system to collect higher order diffraction

Figure 6.6 Higher frequency signal is achieved when higher order reflected beams are collected.

beam from the mask. Nevertheless, for alignment marks, the strength of reflected beams reduces and eventually diminishes to nearly zero until it is inadequate to be analyzed as the alignment signal when the diffraction order increases. The next section describes enhanced order marks to overcome this problem.

(b) Enhanced Order Marks

The discussion in the previous section covers gratings with a period of 16 μm and variation in the grating depths. The results show that 0th diffraction order always consumes a large portion of the reflected energy. The reflected diffraction efficiency decreases gradually as the diffraction order increases. This is undesirable since higher order beam is preferable to obtain a reliable alignment signals. Enhanced order marks, which give improved reflected diffraction efficiency at higher order, are discussed in this section. Only a particular reflected beam at high order is used as the alignment signal.

For enhanced order marks, gratings with smaller pitch, p' are incorporated into the 16 μm gratings. The intensities and phases of the P -periodic reflected orders are modified when small p' periodic grating are introduced. Gratings with fine periodic structure have only a few propagating orders. With a duty ratio of 0.5 for both gratings, it is expected that a given reflected order as a whole for $P = 16 \mu\text{m}$ gratings is relatively strong when its reflected direction is close to the reflected direction of the small p' periodic gratings. For normal incidence of light as in the case being considered here, the grating equation is given by $\sin \theta_m = \frac{m\lambda}{P}$, where θ_m is the angle corresponding to m reflected orders and λ is the incidence alignment wavelength. This

equation is applied to both gratings with P and p' period. When the angle of $m_{p'}$ th reflected order is close to that of m_P th reflected order, the intensity is being enhanced, i.e. at $\frac{m_P}{P} = \frac{m_{p'}}{p'}$.

Table 6.2 shows the dimension of p' periodic gratings where the first reflected order of p' gratings is used to enhance the respective reflected order of P gratings, i.e. 3rd, 5th and 7th. For example, 1st reflected order of $p' = 3.2 \mu\text{m}$ grating enhances the 5th reflected order of $P = 16 \mu\text{m}$ grating. For uniformity, such type of mark will be named as 5th order mark instead of 5th order enhanced mark. A similar naming convention is applied to 3rd and 7th order marks. The structure of enhanced order mark is depicted in Figure 6.7. In the following section, except for 0th order, whenever an order of reflected diffraction efficiency is presented, it corresponds to the respective order of the mark. For example, 3rd order reflected diffraction efficiency is understood for 3rd order mark. The type of mark for 0th order reflected diffraction efficiency will be specified.

Table 6.2 Dimensions of small p' periodic gratings to enhance the respective reflected order of P -periodic gratings

Enhanced Order	P gratings	p' gratings	Line/space of p' gratings
3rd	$16 \mu\text{m}$	$16/3 (5.33) \mu\text{m}$	$8/3 (2.67) \mu\text{m}$
5th	$16 \mu\text{m}$	$16/5 (3.20) \mu\text{m}$	$8/5 (1.60) \mu\text{m}$
7th	$16 \mu\text{m}$	$16/7 (2.29) \mu\text{m}$	$8/7 (1.14) \mu\text{m}$

(a) 3rd Order Mark

(b) 5th Order Mark

(c) 7th Order Mark

Figure 6.7 Marks with (a) 3rd, (b) 5th and (c) 7th enhanced order. The difference lies in the dimensions of small periodic gratings. Film stack on top of the marks is not shown.

Figure 6.8 shows the reflected diffraction efficiency at grating depth of 4000 Å for 3rd, 5th and 7th order marks with the film stack properties specified in Table 6.1. The TE and TM reflected diffraction efficiencies are being enhanced at the respective order. In other words, stronger signals are obtained at higher reflected orders. For example, first local peak is found at 3rd order for 3rd order mark. There are also local peaks found at order number of 6, 9, 12 and 15. This is

Figure 6.8 Reflected diffraction efficiency at grating depth of 4000 Å for (a) TE and (b) TM polarizations. The first local peak is found at order number of 3 for 3rd order mark. For 5th and 7th order marks, the first local peak is found at order number of 5 and 7, respectively.

consistent with the enhancement from higher diffracted order of the small periodic gratings, p' to P -periodic gratings. Nevertheless, the primary enhancement order received the highest reflected diffraction efficiency, i.e. peak at 3rd order is higher than the remaining peaks, even higher than the 1st order. Similar findings are also concluded from the 5th and 7th order marks. For the 5th order mark, other local peaks are also found at order number of 10 and 15 whereas for 7th order mark, the next local peak is found to be at order number of 14. Whenever the reflected diffraction efficiency is not being enhanced, it drops significantly to almost zero. It is noted that diffraction efficiency shown is dedicated for positive order only.

Figure 6.9 shows the 0th order and 3rd, 5th, 7th order reflected diffraction efficiencies across various depths, using a 633 nm wavelength for (a) TE and (b) TM polarizations, respectively. Regardless of the type of marks, 0th order reflected diffraction efficiency is relatively large as compared to that of other orders. The remaining light energy is transmitted into the silicon region. The results show that minimum 0th and the respective enhance order reflected diffraction efficiency are located at 5000 Å and 4400 Å, respectively in the range of grating depth from 3800 Å to 5200 Å. For 633 nm alignment using higher diffraction order, grating depth of 4400 Å is considered as a forbidden mark depth as the diffraction efficiency reduces to nearly zero. The curves follow a sinusoidal trend and minimum point is also expected in other range for grating depth. In general, the diffraction efficiency for 3rd order at a specified grating depth is higher than 5th and 7th orders. Both TE and TM polarizations exhibit the same properties.

Figure 6.9 Reflected diffraction efficiency of (a) TE and (b) TM polarizations for different order marks using 633 nm wavelength. The legends, 0th (3rd) and 3rd (3rd) denote 0th and 3rd diffraction orders, respectively for 3rd order mark. The same interpretation is applied to other legends for 5th and 7th order marks.

6.3 Experimental Details

The experimental works consist of two parts, which covered the alignment in front-end-of line (FEOL) and back-end-of-line (BEOL) processes. The FEOL alignment experiment is aimed to

validate the use of 5th order mark in the 90 nm and 0.11 μm technology processes whereas the BEOL alignment experiment extended the study to include 5th and 7th order narrow alignment marks. The same number of alignment marks and overlay measurements are used in both experiments. Figure 6.10 shows the flow of experiments for both FEOL and BEOL alignment marks.

Figure 6.10 Flow of experiments.

6.3.1 Alignment in FEOL Process

The smallest dimensions in IC are found in polysilicon layer where the transistors are fabricated. Hence, the polysilicon layer requires the most stringent overlay tolerance if compared to any other layers. The FEOL experimental works focuses on polysilicon layer, which was aligned to

the marks at STI layer. In order to ensure the robustness of alignment marks to process variations, two lots of wafer based on 90 nm (Lot A) and 0.11 μm (Lot B) technology nodes were used. Each lot consists of 24 wafers. Fifth order mark was used throughout the FEOL alignment experiment. Figure 6.11 shows the dimension of 5th order alignment marks, where the length and width of the marks were given as 727 μm and 72 μm . In both technology node processes, the depth of the marks followed the depth of the STI. The required overlay for 90 nm and 0.11 μm technology node were 30 nm and 40 nm, respectively. A summary of the thickness of the layers deposited or coated layers on top of the marks are given in Table 6.3.

Figure 6.11 Fifth order mark.

Table 6.3 Summary of Lots A and B

	Lot A	Lot B
Technology Node	90 nm	0.11 μm
Overlay Tolerance ($ \text{Mean} + 3\sigma$)	30 nm	40 nm
Mark at STI	Depth = 4000 Å	Depth = 4000 Å
Poly-Silicon	Thickness = 1600 Å	Thickness = 1600 Å
BARC	Thickness = 770 Å	Thickness = 600 Å
Resist	Thickness = 3375 Å	Thickness = 4250 Å

6.3.2 Alignment in BEOL Process

The aim of the experiment in the BEOL process is to study the performance of narrow alignment marks. Narrow alignment mark has smaller width, 50 μm if compared to 72 μm in the conventional mark. The study of narrow alignment marks in BEOL process will be performed using short loop wafers. The process was based on 90 nm via first copper dual damascene with silicon dioxide (SiO_2) as the inter layer dielectric (ILD). The fabrication sequence of these backend wafers start from Metal 1 until Metal 4. The first layer, Metal 1 was aligned to the wafer notch since no alignment marks are available. Layer-to-layer alignment strategy was adopted for the remaining layers. Alignment marks printed in the metal layers will be used for the alignment in subsequent via and metal layers. For example, Via 1 and Metal 2 were aligned to Metal 1.

Two different lots were used for the experiment. The first lot was used to study the performance of alignment in Via 1 (V1) and Metal 2 (M2), whereas the second lot was used to study the alignment performance in Via 2 (V2), Metal 3 (M3), Via 3 (V3) and Metal 4 (M4). Table 6.4 shows the split (8 wafers per split in the first lot and 7 wafers per split in the second lot) that is associated with a mark type and alignment recipe in a particular layer. The first split, 5th order marks were used as a reference to compare the results in the second split, narrow 5th order mark and third split, narrow 7th order mark. Figures 6.12 and 6.13 show the dimension of narrow marks with width of 50 μm . An overlay ($|\text{mean}| + 3\sigma$) of 35 nm was required for all the BEOL layers. It was less stringent compared to the FEOL process for polysilicon and STI layers.

Table 6.4 Splits in BEOL alignment experiment

Layer	Aligned To	Split 1	Split 2	Split 3
Via 1 (V1)	Metal 1	5th order mark	Narrow 5th order mark	Narrow 7th order mark
Metal 2 (M2)				
Via 2 (V2)	Metal 2	5th order mark	Narrow 5th order mark	Narrow 7th order mark
Metal 3 (M3)				
Via 3 (V3)	Metal 3	5th order mark	Narrow 5th order mark	Narrow 7th order mark
Metal 4 (M4)

Figure 6.12 Narrow 5th order mark. **Figure 6.13 Narrow 7th order mark.**

6.3.3 Alignment Details

In the experiments, 12 alignment marks (6 marks each in both X and Y directions) are specified on the wafer. The location of the marks were in the exposure field of (3, 3), (3, 0), (3, -3), (-3, 3), (-3, 0) and (-3, -3) with each field of layer consisting of 2 unidirectional marks. This is shown in Figure 6.14. The selected fields were within 60-80 % of a 200 mm wafer. One of the reasons that marks near the edge of the wafer are not selected is that these marks are more prone to process damage. Although 6 unidirectional marks were specified, only 4 marks which have maximal distance from each other are chosen to perform wafer alignment. In this case, priority was given to marks in the exposure field of (3, 3), (3, -3), (-3, 3) and (-3, -3). If any of these marks fails, the alignment system will then proceed to align marks in the exposure field of (3, 0) or (-3, 3). The alignment system compensates for error in wafer translation along X and Y axes, wafer rotation and expansion prior to exposure.

Figure 6.14 Location of the selected and back up marks.

6.3.4 Alignment System

All the evaluations were performed using ASML DUV 248 nm scanner (PAS 5500/800). The scanner is equipped with Advanced Technology Using High Order Enhancement Alignment (ATHENA) [16, 20] alignment system. ATHENA alignment system needs to perform both wafer and reticle alignments prior to exposure. The alignment sequence is shown in Figure 6.15. The position of the reticle is linked to the wafer by means of fiducial marks, which are located on the wafer stage. Off-axis alignment module is used to align the wafer on the wafer stage as shown in Figure 6.15 (a) and this step is known as wafer alignment. After that, the fiducial marks on the wafer stage are aligned to the off-axis alignment module as illustrated in Figure 6.15 (b). Lastly, the alignment system will perform reticle alignment using exposure light through Transmission Image Sensor (TIS) to determine the position of the reticle. This is shown in Figure 6.15 (c). It has to be noted that reticle alignment does not involve the use of off-axis alignment module. With wafer and reticle alignments, it allows the system to compensate for all the corresponding errors before exposures are performed. Wafer alignment compensates for wafer rotation and

Figure 6.15 (a)-(c) Alignment sequence in ATHENA alignment system [20].

wafer expansion whereas reticle alignment compensates for reticle rotation, reticle magnification, scan skew and scan scaling.

6.3.5 Overlay Measurements

After all the wafers were successfully aligned and exposed in the scanner, offline overlay measurements were then performed. Overlay indicates how accurate a layer is being aligned to the previous layer. In the experiments, KLA-Tencor Archer 10, offline overlay measurement tool was used to verify the alignment capability. Figure 6.16 shows the overlay target design, box-in-double segmented frame. The double segmented frame is printed on the previous layer and the box is printed on the resist layer. There were 4 overlay targets located at each corner of a field and 9 fields were selected to perform the overlay measurement. The selected fields were (0, 0), (-2, 2), (2, 2), (2, -2), (-2,-2), (-4,0), (0, 4), (4, 0), (0, -4) which were distributed evenly across the wafer as shown in Figure 6.17.

Figure 6.16 Box-in-segmented frame overlay target.

Figure 6.17 Distribution of overlay targets on the wafer.

6.4 Experimental Results

6.4.1 Alignment in FEOL Process

In FEOL alignment, the polysilicon layer was aligned to the marks that were formed during the formation of the STI layer. Figure 6.18 shows the trenches at the grating that were filled up with silicon dioxide as part of the alignment marks. The mark shown was without any layers deposited or coated on top of the gratings. Figure 6.19 shows the minimum, maximum and average shift in terms of translation between polysilicon and STI layers for X and Y directions. The data shown in each wafer were average measured values of 36 overlay targets. All the shifts are bounded within ± 20 nm. Variations of translation across wafers within one lot were found to be insignificant. The overlay results of Lots A and B, which is expressed in $|\text{mean}| + 3\sigma$ were well below 30 nm as presented in Figure 6.20. Most importantly, overlay as low as 9 nm was achieved for Lot A. From this, it shows that satisfactory overlay results were obtained using 5th order enhanced marks for 90 nm and 0.11 μm technology processes. Robustness of the alignment marks to process variations was also validated.

Figure 6.18 Trenches in the FEOL marks were filled up with silicon dioxide. The figure shown is without film stack on top of the mark.

Figure 6.19 Maximum, minimum and average translation shift in (a) X and (b) Y directions across different wafers.

Figure 6.20 Overlay of polysilicon layer across all the wafers in Lots A and B.

6.4.2 Alignment in BEOL Process

Figure 6.21 shows the images of 5th order and 7th order alignment structures in Metal 1 using atomic force microscope (AFM). The trenches in the silicon dioxide substrate were filled with copper using the dual damascene process. The images were taken with silicon dioxide deposited on top of the mark structures.

Figure 6.21 BEOL alignment marks in Metal 1 layer, (a) 5th order mark and (b) 7th order mark. The trenches in the silicon dioxide substrate were filled up with copper.

Figures 6.22 (a) and (b) show the minimum, maximum and average translation shift for different metal and via layers in the X and Y directions, respectively. Similarly, the data shown in each layer were average measured values of the wafers in each split, with 36 overlay targets in each wafer. Although the average translation in X and Y directions was consistent, the magnitude of maximum and minimum translation were relatively high particularly in metal 3 and metal 4

layers. Metal 3 and metal 4 layers were aligned to the previous metal layer. There is a via layer in between the metal layers which could contribute to the degradation of the alignment signal with additional noise or lower strength. In every layer of X and Y directions, the average translation in Split 1 did not show significant improvement if compared to Split 2. This implied that the performance of narrow 5th order mark in Split 2 was comparable to 5th order mark in Split 1. Furthermore, not much advantage was gained from using narrow 7th order mark in Split 3, as their translation results did not improve significantly compared to narrow 5th order mark in Split 2. The results were further represented in terms of overlay, which is expressed in $|\text{mean}| + 3\sigma$ as presented in Figure 6.23. Narrow marks in Split 2 and 3 shows that overlay below 35 nm were achieved. The lowest overlay was 10 nm . These results demonstrate the feasibility of using narrow alignment marks in the back-end process.

Figure 6.22 Maximum, minimum and average translation shift in (a) X and (b) Y directions for different backend layers across Split 1 (S1), Split 2 (S2) and Split 3 (S3).

Figure 6.23 Overlay of different BEOL layers in (a) X and (b) Y directions across all the splits.

6.5 Concluding Summary

This chapter demonstrates the performance of advanced alignment marks in photolithography for sub-micron technology node process. The RCWA theoretical results show that the reflected diffraction efficiency of normal mark reduces as the order increases. In order to achieve higher reflected diffraction efficiency at higher order, enhanced order marks were studied. By incorporating small periodic gratings of $5.33\ \mu\text{m}$, $3.20\ \mu\text{m}$ and $2.29\ \mu\text{m}$ into the $16\ \mu\text{m}$ periodic grating, the reflected diffraction efficiency were improved at 3rd, 5th and 7th order, respectively.

In general, 3rd order diffraction efficiency is higher than 5th and 7th order diffraction efficiency for the respective enhanced order marks. A forbidden depth of grating, 4400 Å was found for the specified properties of film stack. The experimental results demonstrated that overlay as low as 9 nm was achieved when 5th order mark was used for 90 nm technology node FEOL process. Narrow marks for BEOL process also showed compatible results with the lowest overlay of 10 nm. Advantages of 7th order narrow marks were not significant in terms of overlay compared to 5th order narrow marks although they are expected to give higher reflected diffraction efficiency as observed in the RCWA simulation results.

CHAPTER 7 CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

An electromagnetic scattering model for line structures was established based on a high frequency approximation solution – ray tracing approach. The electromagnetic ray tracing (ERT) model has provided an in-depth understanding to the electromagnetic disturbance by identifying individual physical mechanism that contributes to the total solution, namely geometrical optics and diffracted fields. Their correlations to the properties of the line structures are revealed through the detailed formulations. This is the key advantage of the ERT model developed in this research work, which could not be offered by any other electromagnetic scattering solutions such as the FDTD method. The formation of the ERT model requires the use of both external and internal diffraction coefficients for the wedge, which were developed and analyzed explicitly.

The external diffraction coefficient of a wedge was obtained by solving the single loop Sommerfeld contour integral, which is presented in the UTD format. Impedance boundary conditions were imposed and higher order in the high frequency asymptotic series was included. The formulation also distinguished all the geometrical and surface poles arising from the problem. It is shown that first leading term, $(k\rho)^{-1/2}$ in the diffraction coefficient is sufficient to provide accurate results for a field point on the wedge surface at distance of $k\rho = 5$ from the origin. On the other hand, when the impedance model is used to study the diffraction of isolated lossless and lossy wedges, the results show a good agreement with the FDTD solution for TE polarization.

In contrast to the external diffraction coefficient, the internal diffraction coefficient of a penetrable wedge was obtained using a proposed heuristic solution. The developed internal diffraction coefficient was able to compensate the discontinuities at different shadow boundaries caused by the geometrical optics fields that are induced in the penetrable wedge. Besides the geometrical optics and diffracted fields, the existence of lateral field induced by the branch cuts in the Sommerfeld contour integrals was also discussed. By applying the model to study dependence of the internal electromagnetic field to incident angles, it was found that the amplitude profile for incident angle at 120° has provided a better match with the FDTD solution if compared to the incident angle at 60° .

With the developed diffraction coefficients, the electromagnetic scattering of line structures was studied by using ray tracing approach. The ERT model was established based on the physical understanding of the geometrical optics field and its associated diffracted field to compensate the discontinuities at different shadow boundaries. The diffracted field includes external direct diffracted, external diffracted-reflected and internal diffracted-reflected-transmitted fields. A single line structure was treated as an impedance double wedge with an effective refractive index obtained using the film stack matrix approach. The ERT model is capable to explain and identify a particular electromagnetic field that responsible to a disturbance in the amplitude for total solution. This was demonstrated through a step by step analysis on how the total electromagnetic solution for a single line structure was obtained. On the other hand, the accuracy of the ERT model was also verified for various conditions, which includes different line widths for single line and two-line structures, and line structures with wavelength comparable width. The factor of refractive index was also studied. The accuracy results were promising. For a single 1.6λ (width) polysilicon line structure on silicon substrate, the ERT model was able to demonstrate

ACC of 0.978 with the maximum amplitude difference, $\Delta|E_z|$ of as low as -0.067. The subwavelength line width of 0.4λ was identified as the limit of the ERT model for the single polysilicon line structure. A linear trend of improving ACC and PCC results with reducing real part of the refractive index was observed for the accuracy of the ERT model for two-line structures.

As for the application of line structures in photolithography, the study focuses on wafer alignment marks. The enhanced order mark was studied using RCWA. The results show that the respective diffraction efficiency is improved when small periodic structures are incorporated into the normal alignment marks. A forbidden depth of alignment mark, 4400 Å (0.44 μm) was identified for a specified property of film stack. Here, the diffraction efficiency at the respective order dropped drastically to zero. The alignment experiment was able to demonstrate the robustness of new design alignment marks in 90 nm and 0.11 μm technology nodes FEOL and BEOL processes. Overlay of as low as 9 nm was achieved in the study.

7.2 Future Work

In the present work, the diffraction coefficients of a wedge were developed for plane wave normal incidence where the incident and diffracted fields are restricted to the same plane. The study can be extended to include skew (oblique) incidence. The solution could provide information of the internal and external diffracted fields in 3-dimensional domain. Subsequently, the solution for corner diffraction could also be deduced. Corner diffraction is the special case when two diffracted fields are merged together caused by the abrupt termination of the edges. As far as geometrical optics fields are concerned, corner diffraction is required to offset the

discontinuities along the shadow boundaries. The formulation involves certain complications as one additional dimension is involved. The current research for skew incidence and corner diffracted field is always limited to impedance boundary conditions and perfectly conducting wedge, which gives no clues about the 3D internal diffracted field.

The diffraction coefficient for impedance and penetrable wedges developed in this work has unlimited capability for different applications. It is possible to extend its application to study the electromagnetic scattering of line structures at reticle level in photolithography. Here, the predicted diffraction pattern can provide substantial understanding to relate the reticle properties to the imaging behavior. The existing imaging methodology requires the construction of total electromagnetic solution and a series of Fourier transform of the fictitious point source. In contrast to this, the development of an approximate but sufficiently accurate imaging model can be explored based on the construction of edge response on the mask through the diffracted field. The diffraction coefficients developed in this work has paved the way to this study.

The alignment experiments presented here is based on 90 nm and 0.11 μm technology nodes. Undoubtedly, study of the alignment marks capability needs to be performed when the technology nodes advances to 65 nm and further down to 45 nm. This is a challenge for a more stringent overlay budget. In addition to the enhanced order marks performed in the present study, other design of marks can also be studied. For example, blazed alignment mark, which has the properties of concentrating all the diffraction order in one particular direction, up to diffraction efficiency of about 41 % [183]. Although the main enhanced order is only in the positive or negative first order, their advantages over conventional alignment marks in lithography can be studied through the overlay performance. For symmetrical consideration, two blazed alignment

marks in opposite direction are required. Optimization of the blazed marks can be performed by varying the duty cycle of the grating to enhance the alignment signal strength in photolithography process environment.

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Appendix A Refractive Indices

Table A.1 Refractive indices of materials at 633 nm wavelength

Material	Refractive Index
Vacuum	1
Resist	1.55
Bottom Anti-Reflective Coating (BARC)	$1.57 - j\ 0.00036$
Polysilicon	$3.93 - j\ 0.0717$
Silicon dioxide	1.46
Silicon	$3.88 - j\ 0.01933$

Appendix B Special Functions

B.1 Maliuzhinets Function, $\psi_{\Phi_1}(\alpha)$

The Maliuzhinets function, $\psi_{\Phi_1}(\alpha)$ is given by

$$\psi_{\Phi_1}(\alpha) = \exp \left\{ \frac{j}{8\Phi_1} \int_0^\infty \frac{\cosh(\alpha t) - 1}{t \cosh\left(\frac{\pi t}{2}\right) \sinh(2\Phi_1 t)} dt \right\} \quad (\text{B.1})$$

Some additional properties of the function are,

$$\psi_{\Phi_1}(-z) = \psi_{\Phi_1}(z) \quad (\text{B.2})$$

$$\psi_{\Phi_1}(z^*) = \psi_{\Phi_1}^*(z) \quad \text{where } z^* \text{ denotes complex conjugate of } z. \quad (\text{B.3})$$

$$\psi_{\Phi_1}(\alpha + 2\Phi_1) = \cot \left[\frac{1}{2} \left(\alpha + \frac{\pi}{2} \right) \right] \psi_{\Phi_1}(\alpha - 2\Phi_1) \quad (\text{B.4})$$

$$\psi_{\Phi_1} \left(\alpha \pm 2\Phi_1 \pm \frac{3\pi}{2} \right) = \pm \frac{\sin \left[\frac{\pi}{4\Phi_1} (\pi \pm \alpha) \right]}{\sin \left(\frac{\pi\alpha}{4\Phi_1} \right)} \psi_{\Phi_1} \left(\alpha \pm 2\Phi_1 \mp \frac{\pi}{2} \right) \quad (\text{B.5})$$

$$\psi_{\Phi_1} \left(\alpha + \frac{\pi}{2} \right) \cdot \psi_{\Phi_1} \left(\alpha - \frac{\pi}{2} \right) = \left\{ \psi_{\Phi_1} \left(\frac{\pi}{2} \right) \right\}^2 \cos \left[\frac{\pi\alpha}{4\Phi_1} \right] \quad (\text{B.6})$$

From (B.5), the nearest poles and zeros to the origin are located at $\alpha = \pm(3\pi/2 + 2\Phi_1)$ and

$\alpha = \pm(\pi/2 + 2\Phi_1)$, respectively. For the interior $\left(\Phi_1 = \frac{3\pi}{4} \right)$ and exterior $\left(\Phi_1 = \frac{\pi}{4} \right)$ right angled

wedges, the solutions can be obtained in closed form as follows,

$$\psi_{\frac{\pi}{4}}(\alpha) = \cos\left(\frac{\alpha}{2}\right) \quad (\text{B.7})$$

$$\psi_{\frac{3\pi}{4}}(\alpha) = \frac{4}{3} \frac{\cos\left[\frac{\alpha - \pi}{6}\right] \cos\left[\frac{\alpha + \pi}{6}\right]}{\cos[\alpha]} \quad (\text{B.8})$$

For other cases of Φ_1 , approximate numerical analytical expression for the function is used.

When $\text{Im}(\alpha) < 11$, the Maliuzhinets function can be evaluated as

$$\psi_{\Phi_1}(\alpha) \approx \exp \left[-0.15 \sum_{n=1}^5 \frac{\cosh(\alpha t_n - 1)}{t_n \cosh\left(\frac{\pi t_n}{2}\right) \sinh(2\Phi_1 t_n)} \right] \quad (\text{B.9})$$

where $t_n = 0.3n - 0.15$.

When $\text{Im}(\alpha) > 11$, the large argument function can be used,

$$\psi_{\Phi_1}(\alpha) \approx \sqrt{\cos\left(\frac{\pi\alpha}{4\Phi_1}\right)} \exp\left(-\frac{\gamma}{\pi}\right) \quad (\text{B.10})$$

where $\gamma = 2.556343\Phi_1 - 3.259678\Phi_1^2 + 1.9306\Phi_1^3 - 0.3883548\Phi_1^4 + 0.03473964\Phi_1^5$

Maliuzhinets function is only valid in the strip $0 \leq \text{Re}(\alpha) \leq \pi/2$ as shown in Figure B.1. The function is extended to the entire complex plane using (B.6).

For example, if $\text{Re}(\alpha) \geq \pi/2$, assign $\alpha = \alpha' - \frac{\pi}{2}$ and substitute into (B.6). Reassign α' back to α , and the following equation is obtained

Figure B.1 Validity of Maliuzhinets function in the complex plane.

$$\psi_{\Phi_1}(\alpha) = \frac{C1}{\psi_{\Phi_1}(\alpha - \pi)} \quad (\text{B.11})$$

$$\text{where } C1 = \left\{ \psi_{\Phi_1} \left(\frac{\pi}{2} \right) \right\}^2 \cos \left[\frac{\pi}{4\Phi_1} \left(\alpha - \frac{\pi}{2} \right) \right]$$

$\psi_{\Phi_1}(\alpha)$ in the right hand side of (B.11) can be evaluated using analytical expression of the function. If α is still placed outside the strip, assign $\alpha = \alpha' - \pi$ and substitute into (B.11). Again, reassign α' back to α and the following equation is obtained,

$$\psi_{\Phi_1}(\alpha - \pi) = \frac{C2}{\psi_{\Phi_1}(\alpha - 2\pi)} \quad (\text{B.12})$$

$$\text{where } C2 = \left\{ \psi_{\Phi_1} \left(\frac{\pi}{2} \right) \right\}^2 \cos \left[\frac{\pi}{4\Phi_1} \left((\alpha - \pi) - \frac{\pi}{2} \right) \right]$$

(B.12) is substitute back to (B.11) to give

$$\psi_{\Phi_1}(\alpha) = \frac{C1}{C2} \psi_{\Phi_1}(\alpha - 2\pi)$$

The procedures are repeated to place α within the strip, $0 \leq \text{Re}(\alpha) \leq \pi/2$ before evaluating the function.

B.2 Transition Functions, $F(z^2)$ and $F_C(z)$

The modified Frenel integral introduced by Kouyoumjian and Pathak is defined as

$$F(z^2) = \pm 2jzF_C(\pm z)$$

where the lower (negative) sign is used when $\frac{\pi}{4} < \arg(z) < \frac{5\pi}{4}$. The Clemmow transition function, $F_C(\pm z)$ is given by

$$F_C(z) = \frac{1}{2} \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} j \right) \sqrt{\pi} \exp(jz^2) \text{erfc} \left[z \left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} j \right) \right] \text{ for } \text{Abs}(z) \geq 0.3$$

$$F_C(z) = 0.5\sqrt{\pi} \exp(-j\pi/4) \exp(jz^2) - \left[z + z^3 \left(\frac{2}{3} j - \frac{4}{15} z^2 \right) \right] \text{ for } \text{Abs}(z) < 0.3$$

B.3 Gamma function, $\Gamma(x)$

$$\Gamma(x) = \int_0^\infty t^{x-1} \exp(-t) dt \quad \text{Re}(z) > 0$$

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi},$$

$$\Gamma\left(q + \frac{1}{2}\right) = \frac{1 \cdot 3 \cdot 5 \cdot 7 \dots (2q-1)}{2^q} \Gamma(\sqrt{\pi})$$

Appendix C Proofs and Detailed Evaluations

C.1 Derivative of $G(\mu=0)$ in Equation (3.11)

$$G(\mu=0) = f(\alpha_s) \sqrt{\frac{-2\pi}{k\rho f''(\alpha_s)}}$$

$$G''(\mu=0) = \sqrt{\frac{-2}{f''(\alpha_s)}} \left[\left\{ \frac{g(\alpha_s)}{6\{f''(\alpha_s)\}^3} \left(3f^{(IV)}(\alpha_s)f''(\alpha_s) - 5\{f^{(III)}(\alpha_s)\}^2 \right) \right. \right. \\ \left. \left. + \frac{2g'(\alpha_s)f^{(III)}(\alpha_s)}{\{f''(\alpha_s)\}^2} - \frac{2g''(\alpha_s)}{f''(\alpha_s)} \right\} \right]$$

$$G^{(IV)}(\mu=0) = \sqrt{\frac{-2}{f''(\alpha_s)}} \left[\left\{ \frac{4g^{(IV)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^2} - \frac{40}{3} \frac{g^{(III)}(\alpha_s)f^{(III)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^3} \right. \right. \\ \left. \left. + \frac{g^{(II)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^3} \left[\frac{70}{3} \frac{\{f^{(III)}(\alpha_s)\}^2}{f^{(II)}(\alpha_s)} - 10f^{(IV)}(\alpha_s) \right] \right. \right. \\ \left. \left. + g'(\alpha_s) \left[\frac{70}{3} \left(\frac{f^{(III)}(\alpha_s)f^{(IV)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^4} - \frac{\{f^{(III)}(\alpha_s)\}^3}{\{f^{(II)}(\alpha_s)\}^5} \right) - \frac{4f^{(V)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^3} \right] \right. \right. \\ \left. \left. + g(\alpha_s) \left[\frac{385}{36} \frac{\{f^{(III)}(\alpha_s)\}^4}{\{f^{(II)}(\alpha_s)\}^6} - \frac{2}{3} \frac{f^{(VI)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^3} + \frac{14}{3} \frac{f^{(V)}(\alpha_s)f^{(III)}(\alpha_s)}{\{f^{(II)}(\alpha_s)\}^4} \right. \right. \right. \\ \left. \left. \left. - \frac{315}{18} \frac{f^{(IV)}(\alpha_s)\{f^{(III)}(\alpha_s)\}^2}{\{f^{(II)}(\alpha_s)\}^5} + \frac{35}{12} \frac{\{f^{(IV)}(\alpha_s)\}^2}{\{f^{(II)}(\alpha_s)\}^4} \right] \right\} \right]$$

C.2 Prove for $f_1^a(\alpha + \Phi_1)$ in Equation (4.9)

By applying the boundary conditions (4.4) and (4.5) into the Sommerfeld contour integrals (4.2) and (4.3), the following equations are obtained,

$$\int_{L_{\text{ext}}} \exp(jk_1 \rho \cos \alpha) f_1(\alpha - (-1)^m \Phi_1) d\alpha = \int_{L_{\text{int}}} \exp(jk_2 \rho \cos \beta) f_2(\alpha + (-1)^m \Phi_2) d\beta \quad (\text{C.1})$$

$$\int_{L_{\text{ext}}} \exp(jk_1 \rho \cos \alpha) f_1'(\alpha - (-1)^m \Phi_1) d\alpha = \nu \int_{L_{\text{ext}}} \exp(jk_2 \rho \cos \beta) f_2'(\alpha + (-1)^m \Phi_2) d\beta \quad (\text{C.2})$$

where $m = 1, 2$ and $\Phi_2 = \pi - \Phi_1$.

With the use of inverse cosine functions, (4.6) and (4.7), and the inversion theorem of Sommerfeld integral*, (C.1) and (C.2) are reformulated to

$$f_1(\alpha - (-1)^m \Phi_1) + f_1(-\alpha - (-1)^m \Phi_1) = \nu \left\{ f_2(b(\alpha) + (-1)^m \Phi_2) + f_2(-b(\alpha) + (-1)^m \Phi_2) \right\} \quad (\text{C.3})$$

$$f_1(\alpha - (-1)^m \Phi_1) - f_1(-\alpha - (-1)^m \Phi_1) = A(\alpha) \left\{ f_2(b(\alpha) + (-1)^m \Phi_2) - f_2(-b(\alpha) + (-1)^m \Phi_2) \right\} \quad (\text{C.4})$$

where

$$A(\alpha) = \frac{\gamma \sin \alpha}{\sqrt{1 - \gamma^2 \cos^2 \alpha}}$$

*A. V. Osipov and A. N. Norris, "The Malyuzhinets theory for scattering from wedge boundaries: a review," *Wave Motion*, Vol. 29, p. 313-340, 1999.

Apply $m = 1$ and 2 to (C.4),

$$f_1(\alpha + \Phi_1) - f_1(-\alpha + \Phi_1) = \frac{\gamma \sin \alpha}{\sqrt{1 - \gamma^2 \cos^2 \alpha}} \left\{ f_2(b(\alpha) - \Phi_2) - f_2(-b(\alpha) - \Phi_2) \right\} \quad (C.5)$$

$$f_1(\alpha - \Phi_1) - f_1(-\alpha - \Phi_1) = \frac{\gamma \sin \alpha}{\sqrt{1 - \gamma^2 \cos^2 \alpha}} \left\{ f_2(b(\alpha) + \Phi_2) - f_2(-b(\alpha) + \Phi_2) \right\} \quad (C.6)$$

(C.5) + (C.6) gives the asymmetric functional equation,

$$f_1^a(\alpha + \Phi_1) + f_1^a(\alpha - \Phi_1) = \frac{\gamma \sin \alpha}{\sqrt{1 - \gamma^2 \cos^2 \alpha}} \left\{ f_2^a(b(\alpha) - \Phi_2) + f_2^a(b(\alpha) + \Phi_2) \right\} \quad (C.7)$$

Apply $m = 1$ and 2 to (C.3),

$$f_1(\alpha + \Phi_1) + f_1(-\alpha + \Phi_1) = \nu \left\{ f_2(b(\alpha) - \Phi_2) + f_2(-b(\alpha) - \Phi_2) \right\} \quad (C.8)$$

$$f_1(\alpha - \Phi_1) + f_1(-\alpha - \Phi_1) = \nu \left\{ f_2(b(\alpha) + \Phi_2) + f_2(-b(\alpha) + \Phi_2) \right\} \quad (C.9)$$

(C.8)-(C.9) gives the another asymmetric functional equation,

$$f_1^a(\alpha + \Phi_1) - f_1^a(\alpha - \Phi_1) = \nu \left\{ f_2^a(b(\alpha) - \Phi_2) - f_2^a(b(\alpha) + \Phi_2) \right\} \quad (C.10)$$

Multiply (C.7) by $\nu \sqrt{1 - \gamma^2 \cos^2 \alpha}$ + Multiply (C.10) by $\gamma \sin \alpha$

$$\begin{aligned} f_1^a(\alpha + \Phi_1) \left\{ \nu \sqrt{1 - \gamma^2 \cos^2 \alpha} + \gamma \sin \alpha \right\} = \\ f_1^a(\alpha - \Phi_1) \left\{ \gamma \sin \alpha - \nu \sqrt{1 - \gamma^2 \cos^2 \alpha} \right\} + 2\nu \gamma f_2^a(b(\alpha) - \Phi_2) \sin \alpha \end{aligned}$$

Rearrange and $f_1^a(\alpha + \Phi_1)$ is obtained,

$$f_1^a(\alpha + \Phi_1) = R(\alpha, \gamma, \nu) f_1^a(\alpha - \Phi_1) + \nu T(\alpha, \gamma, \nu) f_2^a(b(\alpha) - \Phi_2) \quad (C.11)$$

C.3 Residues for Higher Level Poles

Table C.1 Geometrical Optics Field and their corresponded poles and residues

Geometrical Optics Field	Zero Level Poles	Higher Level Poles	Residues for Higher Level Poles
Reflected, $U_z^r(k\rho, \phi)$	$\alpha = -\phi'_o$	$\alpha = -\phi_o \pm 2\Phi_1 - \phi'$	$R(-\phi'_o \pm \Phi_1, \gamma) \equiv R(\Phi_1 \mp \phi'_o, \gamma)$
Transmitted, $U_z^t(k_1\rho, \bar{\phi})$	$\alpha = \phi'_o$	$\alpha = b(\phi'_o \mp \Phi_1) \mp \Phi_2 + \bar{\phi}$	$\frac{\nu^{-1} T(b(\phi'_o \mp \Phi_1), \gamma^{-1})}{a'(b(\phi'_o \mp \Phi_1))} \equiv \nu^{-1} T(\Phi_1 \mp \phi'_o, \gamma)$
Transmitted-transmitted, $U_z^{tt}(k\rho, \phi)$	$\alpha = \phi'_o$	$\alpha = \mp \Phi_1 + a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2) - \phi'$	$\frac{\nu T(a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2), \gamma)}{b'(a(b(\phi'_o \mp \Phi_1) \mp 2\Phi_2))} \frac{\nu^{-1} T(b(\phi'_o \mp \Phi_1), \gamma^{-1})}{a'(b(\phi'_o \mp \Phi_1))} \equiv \nu T(2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1}) \nu^{-1} T(\Phi_1 \mp \phi'_o, \gamma)$
Transmitted-reflected, $U_z^{tr}(k_1\rho, \bar{\phi})$	$\alpha = -\phi'_o$	$\alpha = \pm 3\Phi_2 + b(-\phi_o \pm \Phi_1) + \bar{\phi}$	$-\frac{\nu^{-1} T(b(-\phi'_o \pm \Phi_1), \gamma^{-1})}{a'(b(-\phi'_o \pm \Phi_1))} R(\pm 2\Phi_2 + b(-\phi'_o \pm \Phi_1), \gamma^{-1}) \equiv T(\Phi_1 \mp \phi'_o, \gamma) R(\pm 2\Phi_2 + b(\Phi_1 \mp \phi'_o), \gamma^{-1})$

C.4 Location of Reflection Point, $Q_r(x_r, y_r)$

Incident ray that hit a wedge produces diffracted ray emanating from the corner. When this diffracted ray hit the bottom surface as shown in Figure C.1, it will be reflected from a specular point. For an observation point of $P(x, y)$, the location of this reflection point is given as $Q_r(x_r, y_r)$. It can be determined as follows.

Figure C.1 Geometry for the derivation of reflection point.

The origin at the wedge corner is acting as the phase reference point. Law of reflection states that

$$\hat{n} \cdot \hat{s}^i = -\hat{n} \cdot \hat{s}^r \quad (C.12)$$

where

$\hat{n}$ = unit normal at the bottom surface given as $\hat{y}$

$\hat{s}^i$ = unit vector in the direction of incident ray, given as $\frac{x_r \hat{x} + y_r \hat{y}}{\sqrt{x_r^2 + y_r^2}}$

$\hat{s}^r$ = unit vector in the direction of reflected ray, given as $\frac{(x - x_r) \hat{x} + (y - y_r) \hat{y}}{\sqrt{(x - x_r)^2 + (y - y_r)^2}}$

Substitute $\hat{n}$, $\hat{s}^i$ and $\hat{s}^r$ into (C.12),

$$\frac{y_r}{\sqrt{x_r^2 + y_r^2}} = \frac{-(y - y_r)}{\sqrt{(x - x_r)^2 + (y - y_r)^2}}$$

Rearrange,

$$(y^2 - 2y y_r) x_r^2 + 2x y_r^2 x_r - y_r^2 x^2 = 0$$

Given $y = h_1$, $y_r = -h_2$ and the location of x_r can be obtained by solving the following quadratic equation.

$$(h_1^2 + 2h_1 h_2) x_r^2 + 2x h_2^2 x_r - h_2^2 x^2 = 0 \quad (C.13)$$

C.5 Location of Transmission Point, $Q_{t2} (x_{t2}, y_{t2})$

Incident ray that hit a penetrable wedge will also produce internal diffracted ray. This ray follows the path as shown in Figure C.2. For an observation point of $P(x, y)$, the location of $Q_{t1} (x_{t1}, y_{t1})$ and $Q_{t2} (x_{t2}, y_{t2})$ can be determined as follows.

Figure C.2 Geometry for the derivation of transmission point.

The origin at the wedge corner is acting as the phase reference point. Law of refraction states that

$$-(\hat{n} \times \hat{s}^i) = -\frac{n_o}{n_1}(\hat{n} \times \hat{s}^t) \quad (C.14)$$

where

$\hat{n}$ = unit normal at the top surface, given as $\hat{y}$

$\hat{s}^i$ = unit vector in the direction of incident ray (in n_2), given as

$$\frac{(x_{t1} - x_{t2})\hat{x} + (y_{t1} - y_{t2})\hat{y}}{\sqrt{(x_{t1} - x_{t2})^2 + (y_{t1} - y_{t2})^2}}$$

$\hat{s}^t$ = unit vector in the direction of the transmitted ray (in n_o), given as

$$\frac{(x - x_{t1})\hat{x} + (y - y_{t1})\hat{y}}{\sqrt{(x - x_{t1})^2 + (y - y_{t1})^2}}$$

Substitute $\hat{n}$, $\hat{s}^i$ and $\hat{s}^r$ into (C.14),

$$\frac{(x_{t1} - x_{t2})}{\sqrt{(x_{t2})^2 + (y_{t1} - y_{t2})^2}} = \gamma \frac{(x - x_{t1})}{\sqrt{(x - 2x_{t2})^2 + (y - y_{t1})^2}}$$

From Law of Reflection, $x_{t1} = 2x_{t2}$ and given $\gamma = \frac{n_o}{n_1}$, $y = h_1$, $y_{t2} = -h_2$, $y_{t1} = 0$, the location of

x_{t2} can be obtained by solving the following equation.

$$4(1 - \gamma^2)x_{t2}^4 - 4x(1 - \gamma^2)x_{t2}^3 + (x^2 + h_1^2 - \gamma^2 x^2 - 4\gamma^2 h_2^2)x_{t2}^2 + 4\gamma^2 x h_2^2 x_{t2} - \gamma^2 h_2^2 x^2 = 0 \quad (C.15)$$

Appendix D List of Publications

JOURNAL

C. B. Tan, A. Khoh, and S. H. Yeo, "Electromagnetic Ray Tracing Model for Line Structures," *Optics Express*, Vol. 16, p. 3589-3603, 2008.

C. B. Tan, A. Khoh, and S. H. Yeo, "Higher Order Asymptotic Analysis of Impedance Wedge Using Uniform Theory of Diffraction," *Electromagnetics*, Vol. 27, p. 23-39, 2007.

S. H. Yeo, C. B. Tan, and A. Khoh, "Rigorous coupled wave analysis of front-end-of-line wafer alignment marks," *Journal of Vacuum Science and Technology B*, Vol. 23, p. 186-195, 2005.

CONFERENCE PROCEEDINGS

C. B. Tan, S. H. Yeo, and A. Khoh, "Modeling of wafer alignment marks using geometrical theory of diffraction (GTD)," *Proceeding of SPIE*, Vol. 5752, p. 977-986, 2005.

C. B. Tan, S. H. Yeo, H. P. Koh, C. K. Koo, Y. M. Foong, and Y. K. Siew, "Evaluation of alignment marks using ASML ATHENA alignment system in 90nm BEOL process," *Proceeding of SPIE*, Vol. 5038, p. 1211-1218, 2003.

SYMPOSIUMS

C. B. Tan, A. Khoh, and S. H. Yeo, "Imaging of line structures at wafer level using heuristic UTD solution," presented at the Symposium on Microelectronics 2005, Institute of Microelectronics, Singapore.

C. B. Tan, S. H. Yeo, and A. Khoh, "Simulation of wafer alignment marks for transverse electric (TE) polarization," presented at the Symposium on Microelectronics 2004, Institute of Microelectronics, Singapore.