Electromagnetic Modeling of Photolithography Aerial Image Formation Using the Octree Finite Element Method

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ELECTROMAGNETIC MODELING OF PHOTOLITHOGRAPHY AERIAL IMAGE FORMATION USING THE OCTREE FINITE ELEMENT METHOD

A Thesis Presented
by
SETH JACKSON

Submitted to the Graduate School of the University of Massachusetts Amherst in partial fulfillment of the requirements for the degree of

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Electrical and Computer Engineering
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ABSTRACT

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MAY 2011

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Modern semiconductor manufacturing requires photolithographic printing of sub-illumination wavelength features in photoresist via electromagnetic energy scattered by complicated photomask designs. This results in aerial images which are subject to constructive and destructive wave interference, as well as electromagnetic resonances in the photomask features. This thesis proposes a 3-D full-wave frequency domain nonconformal Octree mesh based Finite Element Method (OFEM) electromagnetic scattering solver in combination with Fourier Optics to accurately simulate the entire projection photolithography system, from illumination source to final image intensity in the photoresist layer. A rapid 1-irregular octree based geometry model mesher is developed and shown to perform remarkably well compared to a tetrahedral mesher. A special set of nonconformal 1st and 2nd order hierarchal OFEM basis functions is
presented, and 1st order numerical results show good performance compared to tetrahedral FEM. Optical and modern photomask phenomenology is examined, including optical proximity correction (OPC) with thick PEC metal layer, and chromeless phase inversion (PI) masks.
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CHAPTER 1
INTRODUCTION

1.1 Overview

This thesis work proposes a full wave electromagnetic field (EMF) simulation methodology for projection-based photolithography systems. The modeling of the complete photolithography system is attained by combining Fourier optics [3] and 3-D full wave electromagnetic simulation in the mask and photoresist regions. The crux of this thesis is in developing a nonconformal meshing algorithm and a Finite Element Method (FEM) formulation based on octrees. The presented octree meshing algorithm is extremely fast and robust, but necessitates special FEM basis functions to account for the mesh nonconformity. In this thesis a tangentially continuous vector FEM (TVFEM) basis for octree mesh is precomputed, allowing nonconformal mesh FEM matrix assembly to occur more rapidly than competing methods, which calculate the nonconformal basis at run-time. The resulting photolithography simulator has been used to study the basic phenomenology of various lithography technologies such as binary masks (BIM), optical proximity correction (OPC), phase shifting masks (PSM), and chromeless phase shifting masks.

A typical 193nm projection optics lithography system sketch is shown in Figure 1.1, which details the appropriate physics required to simulate each portion of this system. The photomask and photoresist regions are critical parts of this system, and require full-wave electromagnetic modeling to accurately capture the intricacies of modern masks and resists. In this thesis the model photoresist and photomask region geometries are meshed with octrees, and full wave Octree Finite Element
Method (OFEM) electromagnetic scattering simulations are performed. The illumination source, and the condenser and projection optics are all simulated via Fourier Optics [3].

![Diagram of photolithography system](image.png)

**Figure 1.1.** An illustration of a photolithography system. Electromagnetic radiation is directed through a condenser optic to a photomask, and the scattered light is projected via the objective lens onto a layer of photoresist atop a wafer substrate. For the proposed work, this system is modeled using successive Fourier optics and full wave electromagnetic models, as shown in the right side of the figure.

### 1.2 Motivation

Modern semiconductor technology is dependent on ever shrinking transistor size to keep pace with Moore’s Law. One critical phase of the semiconductor fabrication process is the transfer of the intended circuit pattern onto the wafer substrate via photolithography. Figure 1.2 shows the steady decrease in feature size with time, with only occasional updates to the illumination source wavelength due to the technical challenges and expense of switching fabrication plants to operate with new...
illumination sources. The challenge of semiconductor photolithography is to create nanometer feature sized images of integrated circuit (IC) patterns in photoresist (PR) layers by illuminating photomasks with electrically small features, at the illumination wavelength. At such electrically small photomask feature sizes optical theory fails to predict the image formation, due to electromagnetic resonances and constructive/destructive wave interference, that ultimately distort images. Distorted images in the photoresist lead to undesirable transistor and other IC feature shapes and sizes. These undesirable printed features ultimately degrade electrical performance, increase heat due to high leakage currents, or contribute to low IC yield [4].

Figure 1.2. The effect of Moore’s Law on photolithography: the steady decrease of features size has resulted in printed features which are smaller than the the illumination wavelength.

Over the years a number of advanced lithographic printing techniques such as phase shifting masks (PSM) and optical proximity correction (OPC) have made current printed lithography possible [5], but at the expense of very large scale integration (VLSI) design freedom. Rules-based design is the norm [6], [5], where layouts such as
Figure 1.3 must adhere to patterns which are known to print well with respect to idealized scalar based calculations. Each new technology node brings considerations of new mask materials, laser radiation sources, photoresists, etc., and requires updating the rules.

Figure 1.3. A portion of a VLSI layout, and a possible OPC mask for a small section of it. (a) A VLSI layer layout; (b) Layout zoom in; (c) OPC’d photomask for the zoomed-in section.

The cost of experimentation in assessing new lithography technologies and new technology nodes is prohibitively high, and photolithography system simulation offers a cheaper alternative. Design complexity has progressed, and automated methods have been developed to create OPC designs which rely on the repeated calculation of aerial images [7], [8]. Approximate methods for calculating the aerial image cannot account for full effects of the electromagnetic fields scattered by photolithography masks, and according to the International Technology Roadmap for Semiconductors (ITRS), rigorous full-wave (vectorial) electromagnetic simulation of photomask scattering is now a requirement for the advancement of the semiconductor industry [9].
1.3 Previous Work

In this section various methods for the simulation of the photomask and photoresist layer regions are discussed, since Fourier Optics [3] is well established. In the past, the rigorous coupled wave algorithm (RWCA) [10] and waveguide method (WM) [11], [12] have been used to model EMF photolithography. These methods model the electromagnetic fields in a geometry model as a truncated sum of all possible modes in neighboring regions, and so large eigenvalue problems must be solved. The full wave photolithography simulation of the photomask and resist regions via the Finite Difference Time Domain (FDTD) was first proposed by Wong [13], which was then extended to account for PSM [14] and thick mask effects [15]. The FDTD is currently the most popular full wave method for photolithography because of its simplicity and efficiency. However, FDTD is a time domain method, and time domain simulations require many time steps to capture electromagnetic resonances. Since photomask features are on the order of the radiation source wavelength $\lambda$, frequency domain simulation may be a better choice. Another major drawback of the FDTD technique is the reliance on uniform grid meshes. A preferable method is one which allows a nonuniform mesh that enables the mesh to conform to fine features without constraining all elements to have the same size throughout the computational domain, thus significantly reducing computational requirements. The Finite Element Method (FEM) [16] and [17], and Method of Moments (MoM) [16] and [5], both allow for general, unstructured meshes. The MoM is quite efficient for modeling the scattering from binary thin or thick masks, but when chromeless, material phase shifting, or assist features are present in a mask, the method becomes inefficient. On the other hand, the FEM readily handles any material or geometry complications.

One area of difficulty in FEM, or any method that allows unstructured meshes, is appropriate mesh generation [18]. In FEM the computational region surrounding the volume of the photomask or PR layer must be discretized with simplicial
or non-simplicial meshes, which are used to approximate the electromagnetic fields. The uniform grid mesh of FDTD excels in its simplicity, but stair casing errors are common because a grid cannot capture angled features or curves without much $h$ refinement. Unstructured tetrahedral and semi-structured hexahedral meshes overcome this problem, but are difficult to create. The refinement of a single mesh element can cause smoothing algorithms to propagate to every other element in the mesh. Meshing programs which create the unstructured meshes are either slow, non-robust, or require human intervention at multiple steps during mesh creation [19].

Much of the work in creating meshes [18] can be alleviated by allowing mesh nonconformity, where a mesh node does not necessarily only intersect other mesh nodes. Unfortunately arbitrarily nonconformal meshes greatly complicate finite element methods, often leading to inefficient implementations. Hill et al. [20] proposed a specialized non-conformal FEM method, where the nonconformal mesh is constructed by the recursive subdivision (halving tetrahedron edges) of an initial tetrahedron mesh. In this method special FEM basis are constructed at run-time that enforce the required tangential electric field continuity, even when the mesh is nonconformal. Demkowicz, Kurtz, et al. [21] have worked on a similar idea, but with general non-conformal hexahedral meshes. In both methodologies FEM matrix assembly requires slow run-time calculation in order to preserve field continuity across non-conformal element boundaries. In contrast this thesis presents a nonconformal basis which is precalculated, and does not need the time consuming initial tetrahedron or hexahedron mesh.

An alternative to the full blown meshing required by all approaches described thus far is to use an octree as a mesh. While the use of octrees in meshing is not a new idea, through for much of their history they have been considered as a preprocessing stage for the creation of hexahedral or tetrahedral meshes [22]-[25]. Before computing power allowed 3-D simulations, Yerry and Shephard used 2-D quadtrees for FEM triangle
meshing [26]. More recently the octree is used directly as the mesh in \( \text{div} \) conforming FEM to solve wave propagation due to earthquakes [27], and in computational fluid dynamics [28], [29] with adaptive mesh refinement (AMR). In each case of the use of octrees in meshing, whether as an intermediary or as the final mesh, the nonconformal octree was restricted to a 2:1 nonconformity as discussed in the octree meshing portion of this thesis.

1.4 Summary of Contributions

This work focuses on the creation of an octree geometry mesh generator and a tangential vector finite element (TVFEM) formulation which can handle the nonconformal octree mesh. To the best of the author’s knowledge, OFEM for electromagnetic scattering is unique in the handling of the nonconformal basis functions. The 1st and 2nd order OFEM basis functions are precomputed for all possible nonconformal mesh configurations which arise in the 2:1 octree mesh, and hence differ from the works of Demkowicz. The precomputed basis allows the nonconformal mesh OFEM matrix assembly to proceed at the pace of conformal mesh FEM assembly. However only the 1st order basis code is fully implemented in code.

This thesis also develops algorithms for the generation of the octree geometry mesh, which is relatively unknown in the field of computational electromagnetics (CEM). The robust and rapidly created octree mesh has the potential to drastically reduce the user time required for CEM and computational lithography simulation. Additionally the octree mesh promises a smoother eventual transition to parallelized computational methods.

The application of the Octree Finite Element Method to the simulation of electromagnetic scattering due to photolithography masks, coupled with Fourier optics for the simulation of lens elements and illumination sources, has never been done to the best of our knowledge. Additionally this thesis applies the aerial images calcu-
lated via OFEM and Fourier Optics as source fields for photoresist OFEM scattering simulation.

In list form, the contributions of this thesis are as follows:

1. OFEM for electromagnetic scattering formulation,

2. 2:1 balanced Octree Mesher,

3. Photomask electromagnetic scattering,

4. Aerial image formation via Fourier Optics,

5. Photoresist electromagnetic scattering.

1.5 Thesis Outline

The theory and formulation for OFEM are developed in Chapters 2. The first section of Chapter 2 focuses on the octree mesh generation algorithms, and then the electromagnetic scattering formulation for OFEM is discussed. The last section of Chapter 2 presents a study of two canonical scatters, validating the OFEM method for 1st order basis functions. Aerial image formation via Fourier optics is discussed in Chapter 3, as is the method of dealing with EMF scattering in the photoresist. Chapter 4 presents a study of various photomasks, and Chapter 5 discusses conclusions and future work. Appendix A presents the analytical form of the hierarchal 2nd order basis functions, and Appendix B discusses the OFEM element matrices. Finally Appendix C presents the precomputed restriction operator values used to create nonconformal OFEM element matrices, and discusses the special case of the 2nd order edge which spans two “source” faces.
CHAPTER 2
ELECTROMAGNETIC FIELD MODELING VIA THE OCTREE FEM

This chapter will outline the theory and formulation of the Octree Finite Element Method (OFEM) for electromagnetic scattering. The method is developed to model the electromagnetic interactions around the photomask region, and later on for the photore sist region. OFEM is an extension of the traditional hexahedral or brick tangential vector FEM (TVFEM) that is modified to handle nonconformal mesh generated by the octree data structure. More specifically this chapter describes the procedure for generating an octree mesh around the photomask and the photore sist regions, a general FEM scattering formulation, and then the combination of the two to form OFEM. Finally, numerical results validating OFEM for some canonical benchmark electromagnetic scattering problems are presented.

2.1 Octree Meshing

The traditional mesh choice for FEM is a tetrahedral mesh, due to the excellent geometry modeling properties of the simplex tetrahedron collections. Unfortunately the speed, memory, and robustness of tetrahedral meshers are considerably worse than those of structured grid meshers, and often become the bottleneck of large computations. A stark contrast to tetrahedral meshes are structured, uniform grid meshes, which are fast and simple to generate, but suffer greatly from poor geometry modeling. Minimizing “stair-casing” model errors (shown in yellow in Figure 2.1 (a)) requires uniform meshes with small element size, causing unmanageably large
FEM matrices. As seen in Figure 2.1 (b), octree (or in 2-D, quadtree) meshes offer a middle ground. The octree mesh combines fast, robust performance, while allowing mesh nonconformity in order to reduce stair-casing without adding unknowns where they are not required.

The octree mesh is a natural choice for photomask modeling, because of the “Manhattan” layout of photomask features. Curves and diagonal lines are rarely if ever used, and therefore in these type of geometries, an octree mesh would not have stair-casing errors. However, the octree mesh is nonconformal (nodes of a mesh element could touch the edges or faces of their neighboring mesh elements), thus enforcement of the tangential electric field continuity of the basis functions across these elements with ”hanging” nodes is more complicated that traditional conforming mesh FEM. The later parts of this chapter discribe special FEM basis functions that ensure this field continuity at octree meshes.

![Structured Mesh](image1) ![Quadtree Mesh](image2) ![Unstructured Mesh](image3)

**Figure 2.1.** Comparison of different meshing schemes that could be used to discretize the space around the photomask in EMF computations.: (a) Structured grid mesh; (b) Quadtree (2-D version of octree) mesh; (c) Unstructured mesh. Octree and quadtree meshes combine positive features of structured and unstructured meshes.

### 2.1.1 Octree Data Structure

The octree is a tree data structure where the members of the tree (octants) may have up to eight children. Octants with no children are referred to as leaves, and the
original octant is called the root. Figure 2.2 shows an example octree, where the child octants represent partitions of a 3-D space. A child octant is positioned to the left or right, front or back, and top or bottom of the center coordinate of its parent octant. As each child is located relative to its parent, the path from root octant to any given leaf octant is described by the series of child selections. As each subdivision halves the length of an octant in each dimension, the tree depth \( \ell \) of a particular octant \( O_\ell \) effectively fixes its size as \( (\frac{h}{2})^\ell \), where \( h \) is the length of the root octant.

\[ \text{Figure 2.2. Space-partitioning properties of the octree data structure.} \]

Other popular tree data structures include quadtrees, which can be viewed as partitioning 2-D space, and binary trees, which partition a line. Like these other trees, octrees with \( n \) leaves offer \( O(log_2(n)) \) insertion and search performance [30]. This rapid performance is extremely beneficial when searching for neighboring mesh elements. Without spatial partitioning such as an octree, locating neighbors could require much more computationally intensive searches of the mesh.

\section*{2.1.2 Octree Adressing}

The relative positioning of child octants to the left or right, front or back, and top or bottom of the center coordinate of its parent octant allows for a simple method of
child octant addressing. The positions within the parent octant are identified by zero indexed position \( ids (0, 7) \), as seen in Figure 2.2 at the \( O_1 \) position. In binary this is the range \((0b000, 0b111)\). The least significant bit position denotes the child octant is on the \(+ \hat{x} (1)\) or \(- \hat{x} (0)\) side of the parent center, the next least significant bit refers to the \(+ \hat{y} (1)\) or \(- \hat{y} (0)\) side of the parent center, and the most significant bit refers to the \(+ \hat{z} (1)\) or \(- \hat{z} (0)\) side of the parent center.

Using this 3 bit encoding scheme for a child octant address within its parent octant, the path to any octant is encoded as a stream of 3 bit clusters. With knowledge of the final octree level of a desired octant, and the bit stream address, the octant is located via the computationally rapid bit-shift and modulus operations.

### 2.1.3 Octree Geometry Modeling

The function of a mesh in a computational electromagnetics setting is to divide the computational region (in this case region around the mask) into a collection of elements that provide an approximation of a model geometry, while preserving its topological properties. An octree mesh approximates a geometry by surrounding entire model with the root octant, and then recursively subdividing until the corners (nodes), edges, surfaces, and volumes of the model reside inside leaf octants. The topological consistency between geometrical model and octree mesh is preserved by assigning a material \( id \) to each leaf octant, depending on which the octant’s center coordinate is inside or outside of the model geometry. Boundary conditions are assigned at the transitions between materials. It is important to note that an octree mesh is a pseudo mesh since only the minimum information to recreate the full mesh is stored. This is in contrast to other meshing methods, where typically each mesh element node, edge, and face is explicitly computed and written to file.

In practice the complete meshing of a model is an extension of the meshing of a geometry node. To create a mesh of a node, the coordinates of the node are
Figure 2.3. A 2-D (quadtree) example of node and edge meshing: (a) A node is surrounded by an octant at the desired refinement level; (b) A straight edge exists between its two end nodes; (c) The seed nodes are placed in neighboring mesh elements along the best approximation of the edge path.

compared to the center coordinate of the root octant, and the node is assigned to the appropriate child octant. A recursive process of comparison and subdivision continues until a desired octree level or mesh control parameter (MCP) is reached. This mesh control parameter is a user defined input that dictates the density of the mesh and the geometry fidelity in case of slanted or curved geometries. MCP is given to every geometrical entity in the model e.g. nodes, edges, faces and volumes. With each subdivision the volume of the octant enclosing the node reduces to \( \frac{1}{8} \) that of the parent, so finely detailed meshing is achieved rapidly. The final result of this node meshing procedure is depicted in Figure 2.3 (a) for the 2D quadtree equivalent of the 3D octree.

Straight geometry edges are meshed by starting at the octant containing the first node of the edge, and seeding new nodes along the approximated path of edge. The location for the first seed node is chosen by examining the neighbors of the octant enclosing the first node of the edge. The straight line path of the edge will pass through either a single face, edge, or corner node of the octant. In the event that the path crosses through a face, the neighbor octant which shares that face is chosen to
contain the seed node. In the event that the path goes through an edge, a choice must be made between the neighbors which share either face which includes that edge. The straight line path from the center of each neighbor to the end node is compared to the true path of the edge, and the neighbor with the minimum angle is chosen for the seed node. The same process occurs for a node intersection, only now the three neighbors which share the node must be considered.

Once a neighbor is chosen, the seed node is assigned the coordinate of the center of the octant and inserted into the mesh, similar to any other node. The octant housing the seed node is then “made current” and checked against the edge path, as the original octant had been. The process completes when the seeding process arrives at the octant which already contains the final edge node, as seen in Figure 2.3.

Each geometry face is meshed by laying a uniform grid of nodes in the plane of the face, and inserting them into the octree mesh, as seen in Figure 2.4. Volumes are meshed by checking whether the centers of the leaf octants equate to inside or outside of the model, and material \textit{ids} are assigned accordingly.

\textbf{Figure 2.4.} A 2-D (quadtree) example of face meshing: (a) Seed nodes are uniformly placed within the boundaries of the face; (b) The resulting mesh of the face. Stair-casing occurs for nongrid features, but arbitrary refinement is allowed.
2.1.4 Enforcement of 2:1 Mesh Balancing

Octree meshes have no requirement concerning neighboring octants and their respective refinement levels. A two dimensional example of this case is depicted in Figure 2.5 (a). In order to ease the construction of the FEM basis function later on, and to create a graded mesh, an additional restriction must be imposed on the octree. A 2:1 nonconformity restriction is imposed, where no octant is allowed to differ more than one level away from any of its direct neighbors [27]. As seen in Figure 2.5, the 2:1 condition leads to larger number of elements, but serves to both smooth the mesh grading, and to reduce the set of nonconformal octant patterns that can occur in a mesh.

![Figure 2.5](image)

Figure 2.5. A comparison of 2-D (quadtree) mesh of a disc geometry: (a) Quadtree without balancing restriction; (b) Quadtree with 2:1 balancing restriction.

While restricting the mesh to a single octree level of difference between neighbors increases the overall number of octants in the mesh, it does not greatly effect the speed at which the mesh is generated. To avoid the task of checking the entire mesh for balancing violations, the 2:1 condition is enforced recursively at every octant subdivision via the algorithms outlined in Figure 2.6. The recursive algorithm starts by checking the refinement level of the neighbor octants of the parent octant at hand. In the case that a neighbor is not at the required level, it is then subdivided, and the
Algorithm 1 Subdivide (parent, id)
\textbf{Input:} parent: octant, id: childId
\textbf{Output:} child: octant
1: \textbf{if} child(id) \neq 0 \textbf{then}
2: \quad \textbf{return} child(id)
3: \textbf{else}
4: \quad \textbf{for} i \in [0, 7] \textbf{do}
5: \quad \quad \text{create new child}(i)
6: \quad \textbf{end for}
7: \quad \textbf{for each parent neighbor direction do}
8: \quad \quad \textbf{call Ensure} (neighborOctant)
9: \quad \textbf{end for}
10: \textbf{return} child(id)
11: \textbf{end if}

Algorithm 2 Ensure (neighbor)
\textbf{Input:} neighbor: octant
\textbf{Output:} void
1: \text{cLevel} \leftarrow 0
2: \text{cOctant} \leftarrow \text{rootOctant}
3: \textbf{while} \text{cLevel} \neq \text{Level}(neighbor) \textbf{do}
4: \quad \text{cOctant} \leftarrow \text{Subdivide} (\text{cOctant}, \text{closestChoice})
5: \quad \text{cLevel} \leftarrow \text{Level}(\text{cOctant})
6: \textbf{end while}

Algorithm 3 Level( cOctant )
\textbf{Input:} cOctant: octant
\textbf{Output:} int
1: \textbf{return} \text{octree depth of} \text{cOctant}

Figure 2.6. Algorithms for 2:1 balancing condition enforcement at each octant subdivision: Each call to Subdivide returns the desired child immediately if it exists. Otherwise the parent octant creates 8 new children, and then calls Ensure for each of the parents neighbors. Ensure traverses from the root octant down to the desired neighbor octant, by repeated calls to Subdivide until the required octree level is reached.

process propagates outward. Figure 2.7 illustrates this concept in two dimensions. Upon the subdivision of an octant, the 8 children are instantiated. Because the check is performed at every subdivision, and returns immediately if an octant exists at the desired level, the balancing condition becomes an additional constant to geometry insertion and \(O(\log_2(n))\) performance is maintained.

Figure 2.8 shows the CPU time vs. number of octants for the example of a Predator drone aircraft. It is shown that even with 2:1 enforcement, the proposed algorithm scales as \(O(n\log_2(n))\) for \(n\) leaf octants. This highlights that the balancing condition does not disrupt the expected performance of the octree. The method is simple and robust: the Predator drone airplane model of Figure 2.9 was meshed to 12 million elements in 5.56s, while a traditional tetrahedral mesh [1] could take approximately
Figure 2.7. A 2-D illustration of 2:1 balancing condition enforcement. Upon the subdivision of a parent, the neighbors of the parent are required to match the parent’s refinement level.

48hrs for the same discretization level. It is worth noting that the octree mesher takes considerably longer to write the octree mesh onto a hard disk than to create the octree mesh itself.

Figure 2.8. 3-D octree meshing with 2:1 balancing vs tetrahedral meshing [1] of a Predator drone. The $O(\log_2(n))$ insertion time for each of the $n$ elements in the octree mesh far outpaces the performance of the tetrahedral mesher, to the point that writing the octree mesh to file is slower than the creation of the octree mesh.
Figure 2.9. A cut away of a 2:1 balanced octree meshed Predator drone aircraft. The mesh nonconformity allows for fine detail without excessive meshing of empty areas.
2.2 Octree Finite Element Method

Now that the 2:1 balanced (or 1-irregular) octree mesh is defined, the Octree Finite Element Method formulation for electromagnetic scattering can be obtained. This is a traditional FEM scattering formulation, with adaptations to the basis formation and matrix assembly to account for the mesh nonconformity.

2.2.1 Electromagnetic Boundary Value Problem

Electromagnetic scattering invariably includes some incident wave traveling through a medium and impinging upon a scatterer, be it an airplane or a photomask. The goal is then to find the electric field \( \mathbf{E} \in \Omega \), where \( \Omega \) is the computational region e.g. photomask region, that is a valid solution to the time-harmonic curl-curl form of Maxwell’s Equations.

\[
\text{Find } \mathbf{E} \in H(\text{curl}; \Omega) \text{ such that:}
\begin{align*}
\nabla \times \frac{1}{\mu_r} \nabla \times \mathbf{E} - k^2 \epsilon_r \mathbf{E} &= 0, \quad \text{in } \Omega \\
\hat{n} \times \mathbf{E} &= 0, \quad \text{on } \Gamma_{\text{pec}} \\
\hat{n} \times \nabla \times \mathbf{E} + jk \hat{n} \times \hat{n} \times \mathbf{E} &= \hat{n} \times \nabla \times \mathbf{E}^i + jk \hat{n} \times \hat{n} \times \mathbf{E}^i, \quad \text{on } \partial \Omega
\end{align*}
\]

where \( \partial \Omega \) is the outer boundary of domain \( \Omega \), and the total electric field \( \mathbf{E} = \mathbf{E}^i + \mathbf{E}^s \) is the sum of the (known) incident and (unknown) scattered fields respectively. \( \Gamma_{\text{pec}} \) denotes the surface of a perfect electrically conducting (PEC) scatterer, \( k = \omega \sqrt{\mu_0 \epsilon_0} \) is the wave number, \( \mu_0, \epsilon_0 \) are the permittivity and permeability of free space, \( \epsilon_r, \mu_r \) are the relative permittivity and permeability of a given material, and \( \omega \) is the angular frequency of the field oscillations. The second equation in (2.1) ensures zero tangential electric field on PEC. The third equation is a first order absorbing boundary condition (ABC) [31] and is used at the outer surface of the computational domain to emulate the infinite space. The admissible solution vectors will be those which are tangentially continuous. Therefore we seek \( \mathbf{E} \) in \( H_0(\text{curl}; \Omega) \) [31].
2.2.2 Variational Statement

To set up a variational formulation for finite elements, the residual functional

$$r(E) = \nabla \times \frac{1}{\mu_r} \nabla \times E - k^2 \epsilon_r E \in H_0(\text{div}; \Omega)$$  \hfill (2.2)

is convolved with a test function $V$ to form a weighted residual. The residual functional above resides in the space of normally continuous functions in domain $\Omega$, $H_0(\text{div}; \Omega)$ [31].

To obtain solutions with minimal energy, the inner product of $r(E)$ and $V$ is set to zero:

$$\langle V, r(E) \rangle = 0 \quad \forall V \in H_0(\text{div}; \Omega)' \equiv H_0(\text{curl}; \Omega),$$  \hfill (2.3)

where the test space is dual to the space of the residual, and

$$\langle A, B \rangle = \int_{\Omega} A(r) \cdot B(r) dr.$$  \hfill (2.4)

Integration by parts and a series of vector identities are employed to include the absorbing boundary condition, after which we arrive at the following variational (weak) form:
Find $\mathbf{E} \in \mathcal{H}_0(\text{curl}; \Omega)$ such that:

$$
\begin{align*}
&b(\mathbf{V}, \mathbf{E}) = l(\mathbf{V}) \quad \forall \, \mathbf{V} \in \mathcal{H}_0(\text{curl}; \Omega) \\
&\text{where:} \\
&\begin{aligned}
b(\mathbf{V}, \mathbf{E}) &= \int_{\Omega} \nabla \times \mathbf{V}(r) \cdot \frac{1}{\mu_r} \nabla \times \mathbf{E}(r) \, dr^3 - k^2 \int_{\Omega} \mathbf{V}(r) \cdot \epsilon_r \mathbf{E}(r) \, dr^3 \\
&\quad + jk \oint_{\partial \Omega} \hat{n} \times \mathbf{V}(r) \cdot \hat{n} \times \mathbf{E}(r) \, dr^2,
\end{aligned} \\
l(\mathbf{V}) &= \oint_{\partial \Omega} \hat{n} \times \mathbf{V}(r) \cdot \hat{n} \times \left\{ jk \mathbf{E}^i(r) - \hat{n} \times \frac{1}{\mu_r} \nabla \times \mathbf{E}^i(r) \right\} \, dr^2
\end{align*}
$$

(2.5)

### 2.2.3 Discrete Variational Statement

Let $\mathcal{W} = \{ \mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_n \}$ form a finite basis for finite dimensional space $\mathcal{V}_h \subset \mathcal{H}_0(\text{curl}; \Omega)$. Using $\mathcal{V}_h$ as both the trial and test space, we now seek $\mathbf{E}_h \in \mathcal{V}_h \subset \mathcal{H}_0(\text{curl}; \Omega)$ to satisfy the discretized variational problem:

$$
b(\mathbf{V}_h, \mathbf{E}_h) = l(\mathbf{V}_h), \forall \, \mathbf{V}_h \in \mathcal{V}_h,
$$

(2.6)

where:

$$
\mathbf{E}_h = \sum_{i=1}^{n} \alpha_i \mathbf{w}_i, \quad (2.7)
$$

$$
\mathcal{V}_h = \text{span} \{ \mathbf{w}_1, \mathbf{w}_2, ..., \mathbf{w}_n \}. \quad (2.8)
$$

### 2.2.4 Conformal Mesh Basis Formation

The individual $\mathbf{w}$ mentioned above must be defined. For $p^{th}$ order basis functions, the vector shape functions are vector tensor product polynomials of the form $Q^{p-1,p,p} \times Q^{p,p-1,p} \times Q^{p,p-1}$, where $Q^{n,m,r} = q^n(x) \cdot q^m(y) \cdot q^r(z)$ is the tensor product of 1-dimensional polynomial functions of order $n$, $m$, and $r$, respectively [32]. The conformal basis space is then:

$$
\mathcal{V}_h^c = \{ \mathbf{w} \in \mathcal{V}_h^c \mid \forall \, K \in \mathcal{M}, \mathbf{w}|_K \in Q^{p-1,p,p} \times Q^{p,p-1,p} \times Q^{p,p-1} \}.
$$

(2.9)

It is noted that for higher order $\mathcal{H}(\text{curl}; \Omega)$ basis, many specific polynomial choices $Q$ could be made, and in this case hierarchical polynomials have been used in order to facilitate $p$–type multi-grid solvers [32].
The support $\text{supp}(w_i)$ of basis function $w_i$ is the set of regular hexahedral elements $K = [0, h]^3$ with edge length $h$, in an octree mesh $\mathcal{M}$, which share the edge, face, or volume degree-of-freedom (dof) that $w_i$ is associated with. The degrees-of-freedom for higher order systems are the electric field circulation along edges, faces, and inside of volumes. Figure 2.11 shows the support for a first order edge dof (only edges have dofs in a first order system) across two neighboring elements. Following Munk [33], the degree-of-freedom functional for an edge is:

$$\ell_{i,e}(u) = \int_{\text{edge } i} q u \cdot dL \quad \forall q \in \mathcal{Q}^{p-1}(\text{edge } i), \quad (2.10)$$

and for a face is:

$$\ell_{j,f}(u) = \int_{\text{face } j} q \times u \cdot dA \quad \forall q \in \mathcal{Q}^{p-2,p-1}(\text{face } j) \times \mathcal{Q}^{p-1,p-2}(\text{face } j). \quad (2.11)$$

The dof functional for a volume is:

$$\ell_{k,v}(u) = \int_{\text{volume } k} u \cdot q dV \quad \forall q \in \mathcal{Q}^{p-1,p-2,p-2} \times \mathcal{Q}^{p-2,p-1,p-2} \times \mathcal{Q}^{p-2,p-2,p-1}. \quad (2.12)$$

The explicit form and plots for the $p = 1$ and $p = 2$ basis functions are given in Appendix A.

### 2.2.5 Nonconformal Mesh Basis Formation

The basis functions are valid for the conforming region of the mesh, but cannot enforce tangential continuity across mesh nonconformities. These standard basis functions must be modified to work at the boundaries between differing levels of mesh. The hexahedral elements of an octree mesh which are smaller than their neighbors are said to “hang” from them. In this way, we can view the octree mesh as a series
of conformal meshes at varying octree levels $\mathcal{O}_t$, connected to each other via nonconformal hanging interfaces. The conformal basis space is then the union of conformal basis spaces associated with different octree mesh levels:

\[ \mathcal{V}_c^h = \bigcup_{i=1}^{l} \mathcal{V}^{c,\mathcal{O}_i}_h \]  \hspace{1cm} (2.13)

Likewise for the hanging basis space:

\[ \mathcal{V}^{\text{hang}}_h = \bigcup_{i=2}^{l} \mathcal{V}^{\text{hang},\mathcal{O}_i}_h \]  \hspace{1cm} (2.14)

The complete nonconformal basis space is then:

\[ \mathcal{V}_{nc}^h = \mathcal{V}_c^h \oplus \mathcal{V}^{\text{hang}}_h \]  \hspace{1cm} (2.15)

Tangential field continuity across finite element interfaces is required at all locations in the mesh. Due to the 2:1 condition, mesh nonconformities only exist between a coarse hexahedral element at a given octree level, and the neighboring fine hexahedral elements of the next octree level, as in Figure 2.13. In a 3D octree mesh, the edges, faces, and volumes that make up a continuous level of refinement are all
members of the conformal mesh space. When two differing levels abut, the more refined portion of the mesh has some edge and face members which contact edge and face members of the more coarse mesh portion. Only these hanging edges and faces are members of the nonconformal mesh space. A two dimensional example is shown in Figure 2.12, where only the red edges are considered nonconformal, and all other members are conformal. The degrees-of-freedom associated with these nonconformal interfaces require special attention.

![Figure 2.12](image)

**Figure 2.12.** A 2D representation of the mesh nonconformities. The solid blue and solid green regions are considered conformal meshes, joined by the nonconformity at the location of the red lines. The more refined red edges will require special basis functions to ensure that tangential continuity is preserved across the nonconformal boundary.

For the nonconformal OFEM, the hanging degrees-of-freedom are constrained so that the basis functions on the coarse side of the nonconformal interface are met with the equivalent of basis functions from a conformal neighbor element. The hanging dofs (shown red in Figure 2.12) are restricted to form a tangentially continuous transition between mesh refinement levels.

To construct the basis functions for the hanging elements in the $V_{nc}^h$, the notion of the transition element is introduced. A transition element $K_{trans}$, shown in Fig-
Figure 2.13. Some possible configurations of hanging elements. The 2:1 mesh nonconformity restriction reduces all nonconformities in the octree mesh to situations such as these.

Figure 2.14. The transition element is made of the superposition of 4 hanging hexahedral elements. The dotted lines represent the edges of the hanging elements.

Figure 2.14 has size $2h \times 2h \times h$, where $h$ is the edge length of a fine hexahedral element, and is neighboring a coarse hexahedron of size $2h$. Each interface shape function in a transition element is projected onto the set of shape functions available in each fine hexahedral element that comprise the transition element. For instance the first order element basis function of coarse edge $e^{2h} = \{1,3\}$ in Figure 2.14 would have contributions the fine edges $e^h_1 = \{1,10\}$, $e^h_2 = \{10,4\}$, $e^h_3 = \{8,12\}$, and $e^h_4 = \{12,11\}$. The relationship between the associated basis functions is then:

$$w^{2h} = w^h_1 + w^h_2 + \frac{1}{2} w^h_3 + \frac{1}{2} w^h_4.$$  (2.16)

where the superscript refers to the length of the associated edge. From (2.16) it clear that $w^h_1$ has a coefficient $\gamma_1 = 1$, where $w^h_4$ has a coefficient $\gamma_4 = \frac{1}{2}$. Figure 2.15
further illustrates this process, where the edge $e^{2h}$ has been highlighted with dashed yellow. The linear combination of basis functions at the fine level provides tangential continuity at the coarse level.

**Figure 2.15.** Edge dof basis formation across mesh nonconformity: Tangential continuity is enforced by constraining fine element basis functions to match those of a conformal transition element.

The coefficients $\gamma$ for a given hanging hexahedral element are separated into those acting on hanging dofs, and those acting on conformal dofs. They are grouped into matrix form $\bar{\gamma}_{\text{hang}}$ and $\bar{\gamma}_{c}$, respectively such that:

$$w^{2h} = \sum_{K=1}^{4} \begin{bmatrix} \bar{\gamma}_{\text{hang},K} \\ \bar{\gamma}_{c,K} \end{bmatrix}^T \begin{bmatrix} w^h_{\text{nc}} \\ w^h_c \end{bmatrix}$$  \hspace{1cm} (2.17)$$

where $w^h_{\text{nc}}$, $w^h_c$ are the vectors of hanging and conformal basis functions in each hanging hexahedral element $K$, respectively, and $w^{2h}$ is the transitional basis functions.

The coefficient matrices are grouped, and a nonconformal to conformal $N \times N$ mapping restriction operator is obtained:

$$G = \begin{bmatrix} \bar{\gamma}_{\text{hang}} & 0 \\ \bar{\gamma}_c & \mathcal{I} \end{bmatrix}$$  \hspace{1cm} (2.18)
where $\mathcal{I}$ is the identity matrix, and $N$ is the number of degrees-of-freedom per element. Because a conformal basis is created across nonconformal interfaces by the restriction of the hanging degrees of freedom, the hanging dofs are eliminated from the OFEM matrix and replaced by the conformal dofs from the coarser side. Interaction with the hanging dofs is in fact interaction with the coarse dofs at the interfaces, and the size of the nonconformal OFEM basis space is then:

$$\dim(\mathcal{V}_{nc}^h) \equiv \dim(\mathcal{V}_c^h).$$  (2.19)

Appendix C provides listings of all values $\gamma$ required to form $G$ for each hexahedral element in the OFEM mesh, as well as addresses the situations where a single source edge spans two source faces. In $1^{st}$ order basis OFEM this is not a problem, but for the $2^{nd}$ order basis OFEM the edge presents a significant challenge. The complete solution to this challenge is not presented in this thesis, and is an area of possible future research. For this reason all numerical results presented are for $1^{st}$ order basis OFEM.

### 2.2.6 FEM Matrices

With the above basis functions for the subspace $\mathcal{V}_h$, the discretized variational formulation in (2.6) reduces to the FEM matrix equation for electromagnetic scattering in domain $\Omega$ over $n$ unknown degrees-of-freedom:

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$  (2.20)

where:

$$\mathcal{A}_{i,j} = S_{i,j} - k^2 T_{i,j} + jk D_{i,j} \quad i = 1, ..., n \quad j = 1, ..., n$$  (2.21)

and the matrices $S, T, D$ are defined:

$$S_{i,j} = \int_{\text{supp}(w_j) \cup \text{supp}(w_i)} \nabla \times w_j(r) \cdot \frac{1}{\mu_r} \nabla \times w_i(r) dr^3,$$  (2.22)
\[ T_{i,j} = \int_{\text{supp}(w_j) \cup \text{supp}(w_i)} w_j(r) \cdot \epsilon_r w_i(r) dr^3, \]  
\[ D_{i,j} = \oint_{\text{supp}(\tilde{w}_j) \cup \text{supp}(\tilde{w}_i)} \hat{n} \times w_j(r) \cdot \hat{n} \times w_i(r) dr^2 \]  
where \( w_i(r) \) is the \( i^{th} \) basis function as defined previously, and \( \tilde{w} = \hat{n} \times w \times \hat{n} \). The right hand side vector \( b \) for scattering problems is given by:

\[ b_j = \sum_{i=1}^{n} D_{i,j} f_i \]  

where:

\[ f_i = \ell_i \left( jk E_i(r) - \hat{n} \times \frac{1}{\mu_r} \nabla \times E_i(r) \right), \]

and \( \ell_i \) is the degree-of-freedom functional for each degree of freedom \( i \) in the finite element mesh.

**2.2.7 OFEM Matrix Assembly**

To assemble the OFEM matrix, the traditional element-by-element FEM matrix assembly procedure, wherein local (elemental) dof numbering is mapped to global numbering via:

\[ n A^n = \sum_{\mathcal{K}} n M^n \cdot N A^N_{\mathcal{K}} \cdot N M^n, \]

is modified by the inclusion of the precomputed restriction operators \( G \). The restriction operators map the hanging elements from a nonconformal to conformal local id, resulting in the following modified assembly approach:

\[ n A^n = \sum_{\mathcal{K}} n M^n \cdot \left[ N G^N_{\mathcal{K}} \cdot N A^N_{\mathcal{K}} \cdot N G^N_{\mathcal{K}} \right] \cdot N M^n \]
total number of degrees of freedom in the system. The matrix inside the braces in
(2.28) could be thought as a modified element matrix that readily takes care the
non-conformity of the mesh. Element matrices for $1^{st}$ and $2^{nd}$ order basis OFEM
are presented in Appendix B, and the generation of $\mathbf{G}$ is discussed in Appendix C.
Because of the 2:1 mesh nonconformity restriction, there are a finite number of modified element matrices possible. These are therefore computed only once, allowing the
OFEM assembly procedure to proceed at the same rate as conformal FEM matrix
assembly.
2.3 Numerical Studies

Since the goal is to simulate the scattering of light due to photomasks, the OFEM code is validated against canonical benchmark electromagnetic scatterers. Presented here are two OFEM scattering results, computed with first order basis functions. First the scattering due to a wavelength long PEC cube, and then scattering due to a PEC sphere of radius 0.25m are presented.

All simulations were conducted serially on either a MacBook laptop with a 2.4 GHz Intel dual-core processor and 2 GB of RAM, or a MacPro with 2 2.8 GHz Xeon quad-core processors and 32 GB of RAM. Resource requirements are plotted in Figure 2.16, showing the expected $O(\log(n))$ growth of mesh related quantities, as well as the characteristic $O(n)$ FEM sparse matrix growth. Discontinuous lines in Figure 2.16 are from uniform meshes due to an octree with all leaves at the same level. The lines then progress as individual octants are refined.

![Figure 2.16](image)

**Figure 2.16.** OFEM resource requirements: (a) OFEM memory usage; (b) OFEM assembly times.

2.3.1 Scattering due to PEC Cube

The PEC cube geometry of Figure 2.17 represents a best-case scenario for octree meshes, because the cube geometry is a perfectly modeled by hexahedral elements.
Scattering due to an $\hat{x}$ polarized, $-\hat{z}$ directed wave incident on a PEC cube was simulated. The size of the cube is one freespace $\lambda$ per side. Bistatic radar cross section (RCS) results are compared to Method of Moments (MoM) and tetrahedral mesh FEM (TFEM) in Figure 2.18. There is good visual agreement between the tetrahedral mesh based FEM and the OFEM RCS pattern in Figure 2.18 (a), as well as with MoM results. The $L_2$ error for various OFEM bistatic RCS solutions are compared to a converged first order tetrahedral FEM reference solution are shown in Figure 2.18 (b). Starting from uniform meshes of regular hexahedral elements, octree refinements decrease the error. At no point does the addition of mesh nonconformity increase error. However, the extra refinement of the mesh did little to improve the answer. This is due to the blind (non-AMR) refinement chosen, which placed additional unknowns regardless of whether those dofs would better capture the solution. These local improvements of the modeled fields do not necessarily get communicated to the outer boundaries of the domain, which the RCS is calculated from.

Table 2.1 compares computational requirements for the octree and tetrahedral mesh FEM approaches. OFEM compares favorably with tetrahedral FEM for approxi-
Figure 2.18. PEC cube scattering: (a) Octree FEM, tetrahedral FEM, and method of moments bistatic RCS; (b) OFEM RCS error relative to tetrahedral FEM is not improved by arbitrary mesh refinement.

imately the same number of unknowns, and is considerably faster that tetrahedral FEM when meshing time is considered.

Table 2.1. Computational statistics for PEC cube scattering.

<table>
<thead>
<tr>
<th>Method</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>Time [s], mesh+FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>OFEM</td>
<td>112,758</td>
<td>877</td>
<td>0.1+64.1</td>
</tr>
<tr>
<td>TFEM</td>
<td>116,344</td>
<td>1049</td>
<td>62+68.3</td>
</tr>
</tbody>
</table>

2.3.2 Scattering due to PEC Sphere

The sphere geometry represents a worst-case scenario for octree meshes. Curved surfaces can never be fully captured by cubic elements, as highlighted by Figure 2.19. Octants whose center coordinates reside within the curvature of the model are deigned members of the sphere. While tetrahedral meshes quickly take on the spherical form, the octree mesh with element sizes comparable to those of the tetrahedral mesh exhibits large stair casing error.

Scattering due to an \( \hat{x} \) polarized, \( +\hat{z} \) directed wave incident on the sphere model was simulated. In this study the model radius was set to 0.25 meters and a frequency
sweep was performed. Data points are taken every 10MHz over the range 250MHz to 450MHz, where the first Mie resonance occurs. In addition to a standard tetrahedral mesh of a sphere, a tetrahedral mesh constructed from the outline of an octree mesh of a sphere was used. This latter model will be used to highlight the effects of geometric modeling error (e.g. approximation or dispersion) as opposed to any error inherent to OFEM itself.

![Image: An overlay of octree and tetrahedral sphere meshes, both with the same effective grid size. While the tetrahedral mesh approximates the sphere nicely, the octree mesh of the same element size exhibits considerable stair casing error.](image)

**Figure 2.19.** An overlay of octree and tetrahedral sphere meshes, both with the same effective grid size. While the tetrahedral mesh approximates the sphere nicely, the octree mesh of the same element size exhibits considerable stair casing error.

Backscatter data are plotted along with values computed via the exact Mie series results in Figure 2.20(a). Again OFEM mesh nonconformity does not adversely effect the accuracy with respect to the uniform HFEM mesh. The tetrahedral meshed sphere exhibits no backscatter at $\lambda = 4 \times \text{radius}$, but with the tetrahedral FEM on the octree geometry, the resonance is shifted upwards in frequency to where $\lambda = 3.727 \times \text{radius}$. This suggests that the stair casing error as shown in Figure 2.20(b) creates an effective radius $r_{eff} = 0.2329\text{m}$, and not the intended $0.25\text{m}$, in the OFEM simulation. Despite this the OFEM simulated sphere scattering follows the Mie series across the frequency range fairly well.
Figure 2.20. PEC sphere scattering: (a) OFEM, hexahedral FEM, tetrahedral FEM, and tetrahedral FEM on the stair cased geometry compared to the exact Mie series answer; (b) the effective radius suggests that octree meshes under represent curves.

Table 2.2 compares computational requirements for the octree and tetrahedral mesh FEM approaches. As in the case of the PEC cube, OFEM compares favorably with tetrahedral FEM for approximately the same number of unknowns. However the octree mesh was created in less than a second, compared to the tetrahedral mesh time of nearly 3 minutes.

Table 2.2. Computational statistics for PEC sphere scattering.

<table>
<thead>
<tr>
<th>Method</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>Time [s], mesh+FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>OFEM</td>
<td>106,173</td>
<td>912</td>
<td>0.3+66.9</td>
</tr>
<tr>
<td>TFEM</td>
<td>105,205</td>
<td>982</td>
<td>229+79.3</td>
</tr>
</tbody>
</table>
CHAPTER 3
IMAGING SYSTEM MODELING

While a chief concern in modeling photolithography systems is the electromagnetic field modeling (scattering of incident radiation) of the photomask region, the fidelity of the final aerial image projected into the photoresist region strongly depends on the illumination, condenser optic systems and the interaction of the projected light with the photoresist. The image formed inside the photoresist by the scattered fields of the photomask determines the geometry of the chemical etch process, and hence effect the shape of IC figures, which in turn effect parasitics, yield, and device variation. This chapter presents the approach used to model the illumination and condenser lens systems using the Fourier optics theory [3], and later outlines the electromagnetic field (EMF) modeling of the image formation inside the photoresist. First an overview of the photolithography system model is discussed, and then the formation of aerial images is presented, beginning with a discussion of coherent and partially coherent illumination. Next the imaging equations used in this thesis are presented, followed by a study of the effects of numerical aperture (NA). The computation methodology for aerial image formation is then discussed, including how to adjust the image plane relative to the focal plane. A study of the effect of partially coherent illumination is then presented. Finally, the phenomenology of focusing aerial images inside of the photoresist layer is presented.
3.1 Overview

A photolithography system is designed to facilitate the scattering of incident radiation off of a photomask, and the collection and guiding of the scattered fields to the image plane inside of the photoresist. A simplified photolithography system is shown in Figure 3.1. The condenser lens and its aperture together form the condenser optic, which guides the incident light to the photomask scatterer at the object plane. The projection lens and its aperture form the projection optic, which directs the scattered fields to the image plane.

![Diagram of photolithography system]

**Figure 3.1.** The photolithography system can be viewed as the manipulation of source illumination before the photomask by the condenser optic, and after the photomask by the projection optic. In this thesis, the illumination is always placed in the $+z$ direction, and only waves which propagate in the $-z$ direction, and not the $+z$ direction, are considered in image formation.

In this thesis, the illumination is always traveling from the $+\hat{z}$ direction downward in the $-\hat{z}$ direction. All images are in the $x, y$ plane at some vertical location $z$. Plane
waves with wave vector \( \mathbf{k} \), and directional components \( k_x, k_y, \) and \( k_z \), are assumed to propagate in the \(-\hat{z}\) direction whenever there is a \( k_z \) component is non-zero.

### 3.2 Aerial Image Formation

The process of forming an aerial image due to photomask scattering requires consideration of both the condenser optic, on the illumination side of the mask, and of the projection optic on the photoresist side of the mask. Abbe’s theory of coherent image formation bypasses the condenser optic, or rather assumes the condenser optic outputs a single incident plane wave which is scattered into a multitude of new plane waves by the object (photomask), as seen in Figure 3.2. The Fourier transforming properties of the lens converts the plane waves to converging spherical waves, and reconstitutes the final image [3].

In Fourier optics, the lens is recognized as performing the inverse Fourier transform of the plane waves scattered from the object plane. The 3-D Fourier transform pair \( F \) of some function \( f(x, y, z) \) and its inverse is:

\[
\mathcal{F}\{f(x, y, z)\} = F(k) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z) \cdot e^{-j k_0 (k_x x + k_y y + k_z z)} \, dx dy dz, \\
\mathcal{F}^{-1}\{F(k)\} = f(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(k_x, k_y, k_z) \cdot e^{j k_0 (k_x x + k_y y + k_z z)} \, dk_x dk_y dk_z.
\]

(3.1)

where terms \( k_x, k_y, k_z \) refer to the normalized components of the wave vector \( \mathbf{k} = k_0(\hat{x} + \hat{y} + \hat{z}) \) as seen in Figure 3.4 (a), and \( k_0 = \frac{2\pi}{\lambda} \) and:

\[
k_x^2 + k_y^2 + k_z^2 = 1,
\]

(3.2)

is the free space dispersion relation.
Figure 3.2. The Abbe image model: coherent illumination is scattered by an object. The lens converts the resulting plane waves into converging spherical waves, centered at the focal plane, and viewed at the image plane.

3.2.1 Illumination

In practical photolithography, coherent (plane wave) illumination is not always possible or often desirable. Repeating structures benefit from either incoherent light, or a mixture of incoherent and coherent illumination termed partially coherent. Hopkins [34] showed that the minimum resolvable dimension changes with the ratio of partial coherence factor \( \sigma = \frac{N_{Ac}}{N_{Ap}} \), where NA is the numerical aperture, and the subscript refers to the condenser and projection optics, respectively. The numerical aperture relates the physical size of the aperture to the propagation wavelength \( \lambda \) via the relative permittivity \( \varepsilon_r \), such that:

\[
NA = \sqrt{\varepsilon_r} \sin(\theta). \tag{3.3}
\]

Simply put, larger NA means more light may pass through the aperture. When the pupil function has no phase dependance, and is either fully transparent or fully opaque, the system is said to be diffraction limited. Figure 3.5 shows k-space diagrams of different illumination schemes in photolithography, where the blue regions represent allowable values of \( k_x, k_y \), for the incident plane waves. The black outer ring is the
Figure 3.3. Numerical aperture: (a) NA relates the acceptance half-angle $\theta$ to the wavelength in a medium, via the relative permittivity $\epsilon_r$. (b) Both the condenser and objective optics have apertures, and hence numerical apertures.

maximum line $k_x^2 + k_y^2 = 1$, outside of which the waves evanesce. The dependent $k_z$ direction is not shown. Viewed from the perspective of Fourier optics, the aperture clearly performs the function of a low-pass filter in the spatial frequency domain. Figure 3.4 (b) illustrates the relationship between the radius of the circle in the $k_x, k_y$ plane and the numerical aperture.

Figure 3.4. Diagrams in k-space: (a) When magnitude $|k| = k_0$ is known, fixing $k_x$ and $k_y$ determines the length, but not direction, of $k_z$. (b) The circular pupil function in k-space is a low pass spatial filter. Only $k$ with $\sqrt{k_x^2 + k_y^2} \leq NA$ are allowed to propagate.
Figure 3.5 shows the k-space layouts of different source illumination strategies. Figure 3.5 (a) shows a circular illumination method, where the radius of the blue circle equates to the NA of the condenser lens aperture. It is in this case that the partial coherence factor $\sigma = \frac{NA_c}{NA_p}$. Figure 3.5 (b) shows an annular ring layout, which equates to a band-pass filter in k-space. Figure 3.5 (c) shows a quadrupole layout, and Figure 3.5 (d) shows the quasar layout. Both (c) and (d) are further restrictions on the annular ring illumination.

![k-space diagrams](image)

**Figure 3.5.** Source illumination k-space diagrams: (a) Circular illumination is similar to a pupil function; (b) Annular ring illumination; (c) Quadrupole illumination; (d) Quasar illumination.

The k-space illumination diagrams of Figure 3.5 say nothing of the polarization of the source plane waves. In simulation, the polarization are chosen to be orthogonal to each other, at each sample point. Figure 3.6 shows a possible discretization of an annular ring illumination scheme. Here each sample point in k-space yields 2 plane waves, polarized in the orthogonal spherical coordinate directions $\hat{\phi}$ and $\hat{\theta}$. Each individual plane wave requires a complete simulation of photomask scattering, aerial image formation, and then photoresist scattering, to form the final incoherent sum of all fields due to the source waves.

### 3.2.2 Imaging Equations

The simplest imaging model is geometric optics, where the effect of the projection optic is merely a rescaling of a scalar distribution at the object plane. The complex scalar distribution $U_g$ at the image plane coordinates $(u, v)$ is predicted simply as [3]:

\[ U_g(u, v) = \text{const} \times U_o \left( \frac{u}{f} \right) \]
Figure 3.6. An example of samples in k-space to form an annular ring illumination pattern. To ensure incoherent waves, the polarizations are \( \hat{\phi} \) and \( \hat{\theta} \) directed at each sample point, signified by the blue vectors. Here the red lines denote values of k-space radii of 0.85 for the outer ring and 0.3 for the inner ring.

\[
U_g(u, v) = \frac{1}{M} U_o \left( \frac{u}{M}, \frac{v}{M} \right)
\]  

(3.4)

where \( M \) is a demagnification factor, ie: \( M = 4 \) for the typical 4× demagnification in photolithography, and \( U_o \) is the complex field at the object plane. However in reality a lens is not infinitely large, and the effects of the extreme edges of the lens are avoided by blocking light transmission with an aperture. Diffraction due to the aperture of the projection optic effects the image \( U_i \), expressed as the following convolution:

\[
U_i(u, v) = \tilde{h}(u, v) \otimes U_g(u, v),
\]  

(3.5)

where:

\[
\tilde{h}(u, v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(x, y) \cdot e^{-j\frac{2\pi}{\lambda}(ux + vy)} dxdy
\]  

(3.6)

is the Fraunhofer diffraction pattern due to the aperture pupil function \( p \).
The pupil function can be any shape, but is typically a circle function:

\[
p(x/r, y/r) = \begin{cases} 
1 & \sqrt{x^2 + y^2} \leq 1 \\
0 & \sqrt{x^2 + y^2} > 1 
\end{cases},
\]

where \( r \) is the radius of the aperture. This radius is more commonly referred to in terms of the numerical aperture (NA), as seen in Figure 3.3(a).

Two diffraction pattern magnitudes \( |\tilde{h}| \) are plotted in Figure 3.7. A circular pupil function is most common in imaging, and is plotted in Figure 3.7 (a). A less common square pupil function magnitude is plotted in Figure 3.7 (b). In both cases the dimension of the aperture is arbitrarily chosen to be one free-space wavelength \( \lambda \). Diffraction limited aerial images are formed as convolutions on the object plane distribution with diffraction patterns such as these.

\[ F\{a \otimes b\} = F\{a\} \cdot F\{b\}, \] 

(3.8)

Figure 3.7. Diffraction patterns due to pupil functions: (a) A \( \lambda \) diameter circle. (b) A \( \lambda \times \lambda \) square.

From Fourier theory, it is known that the Fourier transform of the convolution of two functions is the product of the Fourier transforms of each function:
and so:

\[ a \otimes b = \mathcal{F}^{-1}\{\mathcal{F}\{a\} \cdot \mathcal{F}\{b\}\}, \quad (3.9) \]

for some arbitrary functions \( a \) and \( b \).

The imaging convolution of (3.5) is performed by taking the inverse Fourier transform of the product of the Fourier transformed field distribution, and the Fourier transform of the diffracted pupil function:

\[ U_i(xM, yM, zM) = \mathcal{F}^{-1}\{P(k_x, k_y, k_z) \cdot \mathcal{F}\{U_0(x, y, z)\}\}, \quad (3.10) \]

where:

\[ P(k_x, k_y) = \mathcal{F}\{\tilde{h}(x, y, 0)\} = \begin{cases} 1 & \sqrt{k_x^2 + k_y^2} \leq \frac{NA}{M} \\ 0 & \sqrt{k_x^2 + k_y^2} > \frac{NA}{M} \end{cases} \quad (3.11) \]

is the Fourier transformed, and thus scaled, pupil function. The magnification factor \( M \) has been shifted to the pupil function, and the dependent \( k_z \) term is ignored [15].

### 3.2.3 Numerical Aperture Study

For imaging, the usual quantity of interest is usually the image intensity:

\[ I(x, y) = |\mathbf{E}_i \cdot \mathbf{E}_i^*| = |\mathbf{E}_i|^2, \quad (3.12) \]

where \( \mathbf{E}_i^* \) is the complex conjugate of the field at the aerial image plane. The image intensity due to coherent illumination is:

\[ I(x, y) = \left| \sum_n \mathbf{E}_n(x, y) \right|^2, \quad (3.13) \]

where the intensity is formed from the total electric field, and the subscript \( n \) refers to the image fields due to each incident wave \( n \). The incoherent summation is:

\[ I(x, y) = \sum_n (|\mathbf{E}_n(x, y)|^2), \quad (3.14) \]
or rather a sum of the individual intensities of each electric field, due to each wave.

This section shows the effects of reduced numerical aperture on aerial image quality. For this study, the aerial images due to an infinitely thin binary mask with minimum feature size one illumination wavelength $\lambda$ was simulated, where the field distribution at the mask apertures were taken as samples of a normally incident plane wave, polarized along the axis of the longer features of the mask.

Figure 3.8 shows the aerial image intensity results of the simulation. Images were formed for $NA = 1$, $NA = 0.85$, $NA = 0.707$, $NA = 0.5$, $NA = 0.38$, and $NA = 0.259$. All images are normalized, and plotted on the same logarithmic scale. The behavior of the numerical aperture as a spatial frequency low pass filter is evident in the non-feature background of the images, where the noise patterns are seen increasing in wavelength.

The printability of a design is a chief concern in photolithography, and the aerial image intensity can offer good insight into the eventual success of a design. In Figure 3.8 (a), the aerial image is strong and crisp, leading to the conclusion that this image will print well. As the numerical aperture decreases to $NA = 0.85$ in (b), the image exhibits some softening around the edges, but the overall form remains. In (c), at $NA = 0.707$, the beginnings of features separation have occurred: the "L" pattern in the lower right corner and its neighboring features have begun to show the pulsing pattern of constructive and destructive interference. At $NA = 0.5$, Figure 3.8 (d) exhibits these patterns even more severely, where it is now evident that feature separation is imminent. At $NA = 0.38$ image (e) shows interference based fusing and separation of image features, and is no longer usable as an electrical circuit pattern. Strong secondary features have begun to appear between intended primary features, and the lower right corner feature has separated. At $NA = 0.259$, the aerial image of Figure 3.8 (f) is unrecognizable.
Figure 3.8. The effect of numerical aperture on aerial image intensity: A binary mask pattern is illuminated by an normally incident plane wave, and the scattered fields assembled into normalized aerial images: (a) At \( NA = 1.0 \), the intended pattern is clear; (b) At \( NA = 0.85 \), the image shows some rounding at the corners, but is still well defined; (c) At \( NA = 0.707 \), the beginnings of feature separation are evident; (d) At \( NA = 0.5 \), the features are now made of connected blobs, rather than continuously filled regions; (e) At \( NA = 0.38 \), separation in some areas and fusing in others; (f) At \( NA = 0.259 \), the image is unrecognizable. As more spatial frequencies are excluded from the final image by the reduced numerical aperture, deviations from the intended pattern increase. All images are plotted on the same scale.

Because of truncation of \( NA \) associated with demagnification, Figure 3.8 (e) is approximately equivalent of a \( 4 \times \) reduction image of Figure 3.8.

3.2.4 Image Formation with OFEM

In practice the Fourier transform of the fields at the photomask object plane is equivalent to the near-to-far field transformation. The equivalence principle is applied to the infinite PEC mask results in a half-space, as seen in Figure 3.9. Because \( \mathbf{E} \times \mathbf{n} = 0 \) on PEC, only \( \mathbf{J} \) currents are present outside of the apertures in the mask, as seen in Figure 3.9(b). As the fields are already zero behind the mask, the area is re-filled with PEC. Due to image theory, this produces \( -\mathbf{J} \) and \( +\mathbf{M} \) current images.
As the PEC is moved to the original plane of the mask PEC, the \( J \) goes to zero and \( M \) becomes \( 2M \). The Fourier transform of the fields at the mask plane becomes:

\[
E_{\text{far}}(\hat{r}) = \frac{-jk_0}{4\pi} \oint_{\partial \Omega} \{ 2M(r') \times \hat{r} \} e^{-jk_0 \hat{r} \cdot r'} dr',
\]

where \( M = 0 \) in areas other than the apertures in the PEC.

After an OFEM scattering simulation, the fields at the mask apertures are sampled uniformly, and the aerial image is calculated. This method can be applied to photomasks without PEC but only phase shifters. For this method to be accurate, either the side walls of the photomask must be infinite repeating boundaries, or the mask pattern must rest in an opening in a PEC plane.

\begin{figure}[h]
\centering
\includegraphics[width=\linewidth]{image}
\caption{Electromagnetic image theory applied to apertures in half-space: (a) An infinitely long \textit{pec} exists in a region of electric and magnetic fields. (b) The equivalence surface is chosen at the position of the PEC, and so \( E \times \hat{n} = M = 0 \) in areas other than the apertures. (c) The region of zero field is filled with PEC, shorting out the \( J \) currents everywhere, and doubling the \( M \). The PEC is then removed, leaving only \( 2M \).}
\end{figure}
3.2.5 Image Focus

The minimum resolvable feature size is for partially coherent systems is:

\[ d = \frac{1}{(1+\sigma)NA}, \]  

which reduces to Abbe’s result for coherent systems when \( \sigma = 0 \), and completely incoherent systems when \( \sigma = 1 \) [34]. The critical dimension, often referred to as twice the half pitch in photolithography, is often expressed as:

\[ d = k_1 \frac{\lambda}{NA}, \]  

where the \( k_1 \) term now accounts for various process factors in addition to the diffraction limited value of 0.5, and as such is sometimes given in the range 0.3 – 0.4.

The expression for critical dimension relates to the image behavior at the focal plane. When the image plane is located away from the focal plane, the relative focus changes. The depth of focus describes the distance from the focal plane where the image is still acceptably sharp, and is expressed:

\[ DOF = k_2 \frac{\lambda}{(NA)^2}, \]  

where \( k_2 \) is also a conglomerate term, typically around 0.5 [5]. It is apparent that larger NA leads to a shorter depth of focus, and so critical dimension and depth of focus are at odds.

To allow place a focal plane inside of a computational domain, the image must be first defocused such that the fields at the outer boundary of the domain converge inside of it, as seen in Figure 3.10. A benefit of the Fourier optics approach is that the focus of an aerial image is easily manipulated. During the forward Fourier transform
of the fields in the $x - y$ plane, that plane is placed at $z = 0$, and the exponentials due to $k_z$ and $z$ become equal to 1:

$$E_0(k_x, k_y) = \frac{-jk_0}{4\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left\{ 2M(x, y, 0) \times \hat{k} \right\} e^{-jk_0(k_x x + k_y y)} dx dy. \quad (3.19)$$

When defocus is desired, the image plane can be located anywhere in space during the following inverse Fourier transform calculation:

$$E_i(x, y, z_i) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(k_x, k_y) E_0(k_x, k_y) e^{jk_0(k_x x + k_y y + z_i \sqrt{1-k_x^2-k_y^2})} dk_x dk_y, \quad (3.20)$$

where $z_i$ is the offset distance from the focal plane, and $-\hat{z}$ wave propagation is assumed. In this way the image fields are located away from the focal plane, suitable as input fields for a secondary OFEM simulation.

**Figure 3.10.** Aerial image defocus: to position the focal plane within a computational domain, the input fields must represent a defocused image at the position of the green dotted line.

Figure 3.11 and Figure 3.12 show an example of focusing an aerial image. In this case a simple image of a $\lambda \times \lambda$ square was focused in a free-space domain surrounded
with absorbing boundaries, and the focal plane $1.5\lambda$ from the top of the domain. The focal plane is signified by the dotted line in Figure 3.11 (a). The magnitude plot of Figure 3.11 (a) clearly shows the spherical waves converging at the focal plane, and then diverging as the fields travel in the downward direction. The intensity plots

![Figure 3.11](image1.png)

**Figure 3.11.** Focusing aerial image electric field magnitude: (a) The spherical waves converge at the focal plane, located at the dashed line, $1.5\lambda$ from the top of the plot; (b) Multiple cuts of the air domain, including a horizontal cut at the focal plane.

of Figure 3.12 show that the area above and below the focal plane still contains an image, exemplifying the effect of depth of focus. The intensity softens as the image plane ventures above or below the focal plane.

![Figure 3.12](image2.png)

**Figure 3.12.** Focusing aerial image electric field intensity: (a) With the focal plane at the dotted line, the strong image intensity due to depth of focus is visible above and below; (b) Multiple cuts show that the depth of focus provides a decent rendering of the image even away from the plane of best focus. Here the focal plane cut has been rendered semi-transparent, to allow viewing the intensity below the focal plane.
3.3 Partial Coherence Study

The aerial image due to the scattering of plane waves incident on a repeating rectangular pattern was simulated, and the effects of increasing degrees of partial coherence factor $\sigma$ was investigated. The binary mask pattern of $193[\text{nm}] \times 289[\text{nm}]$ rectangles in Figure 3.13(a) was modeled using the full-wave (EMF) OFEM. The binary mask was modeled as an infinitely thin PEC coating beneath $100[\text{nm}]$ of quartz, above $100[\text{nm}]$ of air. The outer walls of the computational domain were truncated using absorbing boundaries. The free space illumination wavelength was chosen as $\lambda = 193[\text{nm}]$, consistent with the ArF laser source. The OFEM matrix in this example was inverted using Intel’s MKL Pardiso direct solver. In this case a direct solver is computationaly beneficial because many right-hand side solutions must be obtained due to the multiple plane waves forming of the incoherent illumination (Abbe summation). The OFEM system involved $N = 214,226$ unknowns, and the initial factorization of the matrix took 29s and 1113MB of RAM, and each forward-backward substitution took approximately 1s. The aerial imaged due to the scattering of each incident wave was calculated via the Fourier transform and its inverse. Each coherent image took 134s to calculate, and 3.70MB of RAM. The incoherent summation of the images took approximately 2s each. All image plots are normalized to the same logarithmic scale.

For all of the images in this section, the projection optic numerical aperture $NA_p = 0.85$. The image in Figure 3.13(b) was formed by only 2 illumination plane waves, normally incident on the mask, polarized in the $\hat{x}$ and $\hat{y}$ directions. This image clearly shows the intended intensity pattern relative to position, but does not fill in the dotted line rectangles. The small rounded features leave a large percentage of the desired pattern empty, leading to possible broken contacts in an IC.

In Figure 3.14 the illumination aperture radius is $NA_c = 0.2125$, for a partial coherence factor $\sigma = NA_c/NA_p = 0.25$. The noise patterns outside of the intended
design have begun to smooth, and the overall shapes are more uniform. In Figure 3.15 the illumination radius is widened to $NA_o = 0.425$, for a partial coherence factor $\sigma = 0.5$. Here the rectangles are mostly filled and the background noise from each feature has begun to smear into that of the next.

In Figure 3.16 the illumination radius is increased to $NA_c = 0.6375$ for $\sigma = 0.75$. The dotted rectangles are now near entirely filled, and the areas between the features still exhibit low intensity values, though they have begun to fill in. Finally in Figure 3.17, the objective NA is equal to the projection NA, leaving a partial coherence factor $\sigma = 1$, or completely incoherent. The features are well filled in, but at the expense of contrast. The areas between the features have filled in as well. While this is not an issue in the aerial image as presented, in the case of exposing photoresist, the contrast of the image can be important because of the finite range of energies in which the image is transferred to the photoresist.
Figure 3.14. Imaging of the repeating pattern with partial coherence factor $\sigma = 0.25$: (a) The k-space diagram of the circular illumination with radius 0.2125, with polarizations; (b) The aerial image resulting from an incoherent summation of scattered images due to 10 plane waves, polarized in the $\hat{\phi}$ and $\hat{\theta}$ directions.

Figure 3.15. Imaging of the repeating pattern with partial coherence factor $\sigma = 0.5$: (a) The k-space diagram of the circular illumination with radius 0.425, with polarizations; (b) The aerial image resulting from an incoherent summation of scattered images due to 26 plane waves, polarized in the $\hat{\phi}$ and $\hat{\theta}$ directions.
Figure 3.16. Imaging of the repeating pattern with partial coherence factor $\sigma = 0.75$: (a) The k-space diagram of the circular illumination with radius 0.6375, with polarizations; (b) The aerial image resulting from an incoherent summation of scattered images due to 58 plane waves, polarized in the $\hat{\phi}$ and $\hat{\theta}$ directions.
Figure 3.17. Incoherent imaging of the repeating pattern: (a) The k-space diagram of the circular illumination with radius 0.85, with polarizations; (b) The aerial image resulting from an incoherent summation of scattered images due to 98 plane waves, polarized in the $\hat{\phi}$ and $\hat{\theta}$ directions. The image fits the expected pattern well.

The illumination type was then changed from circular to annular. In Figure 3.18 the inner illumination radius is 0.425 and the outer radius is held at 0.85. Compared to the incoherent case in Figure 3.17 (b), Figure 3.18 (b) shows similar intensity, but with less contrast between features. Additionally the beginnings of a separation of the feature into two separate lobes of intensity is faintly visible. With the inner radius increased to 0.6375 as in Figure 3.19, the slight separation is still evident but is eclipsed by the even increased lack of contrast between features. The intensity now over-fills the features, and the outer features are lopsided. Figure 3.20 (a) shows an intensity plot of the annular ring illumination inner radius 0.6375 case, and Figure 3.20 (b) shows the incoherent illumination image. Both images have been rescaled to the same logarithmic scale to highlight the difference between them. Figure 3.20 (b) exhibits smooth, even intensity while in Figure 3.20 (a) the separate lobes and lopsided distribution are evident.

From this study it is evident that a mostly coherent illumination system will yield higher contrast images, but with the side effect of feature resonances and wave inter-
ference distorting the intended pattern. Mostly incoherent illumination alleviates the feature fill-in problem, but reduces contrast. While the definition for partial coherence factor $\sigma$ is for circular illumination only, it appears that annular ring illumination leads to more coherent illumination for values of inner illumination radius which are nearer to the outer illumination radius.

The usefulness of partially coherent illumination is not limited only to repeating patterns. The cross pattern of Figure 3.21 (a) is an example of an isolated photomask feature which benefits from annular ring illumination. For this example the edge lengths of the cross are $0.5$ illumination $\lambda$ each, so that the length from end to end is $1.5\lambda$. Figure 3.21 (b) shows the aerial image resulting from the illumination of the binary mask pattern with normally incident $\hat{x}$ and $\hat{y}$ polarized plane waves. With $NA = 0.85$ and an incoherent summation of the two images, the defining features of the cross are missing. However under annular ring illumination with inner radius $0.94$ and outer radius $0.74$, the image is more clearly defined, as seen in Figure 3.21 (c).
Figure 3.19. Partially coherent imaging of the repeating pattern: (a) The k-space diagram of the annular ring illumination with inner radius 0.6375 and outer radius 0.85, with polarizations; (b) The aerial image resulting from an incoherent summation of scattered images due to 48 plane waves, polarized in the $\hat{\phi}$ and $\hat{\theta}$ directions. The rectangles are over-filled, and there is a tightening in the midsection.

Figure 3.20. Rescaled images due to annular and incoherent circular illumination: (a) The annular (inner radius 0.6375, outer radius 0.85) illuminated image shows a bias towards the middle feature, with lopsided intensities in the other features; (b) The incoherently illuminated image shows fairly uniform intensities within the features, with less intensity in the center feature.
Figure 3.21. Cross pattern with 0.5 illumination λ edges: (a) The intended binary mask pattern, used for the following aerial images with $NA = 0.85$; (b) Normally incident plane wave ($\hat{x}$ and $\hat{y}$ polarized) illumination yields an aerial image which poorly represents the intended pattern; (c) Partially coherent annular ring illumination (outer radius 0.94, inner radius 0.74) fills out the aerial image pattern more effectively.
3.4 Focus Inside Photoresist

The goal of photolithography is to form a desired image pattern inside of the photoresist layer on a wafer substrate. The aerial image formed in free space is useful for inspecting the effects of constructive and destructive wave interference, but it is not the final result. The image must be focused inside of the PR layer, and the effects of the different dielectric media considered.

The change in material properties from free-space, or the immersion medium, to the electric and magnetic properties of the photoresist causes a portion of the impinging wave to reflect off of the material interface, and the other portion to continue into the photoresist at a new propagation angle, as seen in Figure 3.22. From the tangential continuity of electric fields,

\[ k_i \sin \theta_i = k_r \sin \theta_r = k_t \sin \theta_t, \tag{3.21} \]

where \( k_i \) is the incident wavenumber, \( k_r \) is the reflected wavenumber, \( k_t \) is the transmitted wavenumber, and \( \theta_i \), \( \theta_r \), and \( \theta_t \) are the angles of incidence, reflection, and transmittance angles with respect to the normal vector of the material interface. Because the incident and reflected waves exist in the same medium, the associated wave numbers are equal. Therefore the reflected angle \( \theta_r \) is equal to the incident angle \( \theta_i \). However the incident and transmitted wave numbers are not equal, and are typically related in Snell’s law:

\[ \frac{\sin \theta_i}{\sin \theta_t} = \frac{k_t}{k_i} = \frac{\sqrt{\epsilon_2 \mu_2}}{\sqrt{\epsilon_1 \mu_1}}, \tag{3.22} \]

where \( \epsilon_2 = \epsilon_{r,2} \epsilon_0 \) is the permittivity, and \( \mu_2 = \mu_{r,2} \mu_0 \) is the permeability in the transmitted wave material, and \( \epsilon_1 = \epsilon_{r,1} \epsilon_0 \) is the permittivity, and \( \mu_1 = \mu_{r,1} \mu_0 \) is the
Figure 3.22. Snell’s law: due to the tangential continuity of electric fields, $k_i \sin \theta_i = k_r \sin \theta_r = k_t \sin \theta_t$. When the refractive index in medium 2 is greater than that of medium 1, the transmitted wave propagates at a smaller angle to the normal.

permeability in the incident wave material. Typically materials are non-magnetic and medium 1 is free-space. In this situation Snell’s law reduces to:

$$\frac{\sin \theta_i}{\sin \theta_t} = \sqrt{\epsilon_{r,2}}$$

(3.23)

where $\sqrt{\epsilon_{r,2}}$ is referred to as the refractive index of medium 2, commonly denoted $n_2$. In this form it is clear that when the incident wave refractive index is less that that of the transmitted wave, the angle $\theta_i > \theta_t$, and the direction of wave propagation is skewed towards the normal of the interface.

This effect is illustrated in Figure 3.23 and Figure 3.24. Again a single free space $\lambda \times \lambda$ square is illuminated by a normally incident plane wave, but the focal plane was located inside of a layer of photoresist on top of silicon dioxide. With freespace illumination $\lambda = 193[\text{nm}]$, the photoresist layer is $600[\text{nm}]$ thick, and then $150[\text{nm}]$ of silicon dioxide below it. The outer boundaries of the domain are all absorbing
boundaries. The relative dielectric constant of the photoresist is $\epsilon_r = 2.9238$ for an refractive index of $n = 1.7099$, and in the silicon dioxide $\epsilon_r = 2.4336$ for an refractive index of $n = 1.56$.

Figure 3.23. Focusing image electric fields inside of photoresist: (a) The waves converge on the focal plane at a decreased angle upon entering the photoresist dielectric layer from the air filled region; (b) Addition plane cuts show a funneling effect as the paths of the waves bend toward the normal axis.

As expected, the fields are most aligned along the vertical axis in the photoresist region, where the index of refraction is highest.

Figure 3.24. Focusing image intensity inside of photoresist: (a) A standing wave pattern is visible in the photoresist layer, sandwiched between air and silicon dioxide; (b) The more vertical wave pattern in the photoresist leads to a larger area of exposed image.
CHAPTER 4
NUMERICAL RESULTS

This chapter presents various numerical results of simulated electromagnetic scattering by photomasks and the subsequent intensity patterns that develop inside of photoresist using the OFEM and Fourier optics theories developed in Chapters 2 and 3. The first study presented examines the effect of decreasing technology size on the aerial image and photoresist intensity due to an infinitely thin PEC binary photomask, compared to an ideal scalar aerial image computation. Next the effect of adding realistic mask thickness is discussed, and then an optical proximity correction design. Finally, a chromeless phase shift mask design is explored.

All simulations were carried out on an Macbook with a 2.4 GHz Intel core-duo processor, and 6 GB of RAM. The direct solver Pardiso [35] from Intel’s math kernel library (MKL) was used to solve OFEM matrices. In cases of multiple incident plane waves for a single photomask mesh domain the OFEM matrix was first factorized with Pardiso and then the multiple RHS were solved via forward and backward substitution. For OFEM photoresist simulations, the number of unknowns sometimes exceeded the limit for a direct solver with the available memory, and so OFEM was solved via the conjugate gradient (CG) method with diagonal scaling preconditioner. The CG iterations were stopped at residual error $10^{-3}$. All idealized scalar aerial image computations were performed using a value of “1” inside of photomask apertures, and “0” outside of the apertures.
4.1 Infinitely Thin PEC Mask

An infinitely thin PEC layer binary photomask was simulated with OFEM at the 250[nm], 180[nm], and 130[nm] half-pitch technology nodes. The radiation source was \( \hat{x} \) and \( \hat{y} \) polarized, normally incident plane waves, with free space \( \lambda = 193[\text{nm}] \) consistent with a ArF laser source. The OFEM scattering simulation times, unknown degrees of freedom counts, and total computation times for forward and inverse Fourier transforms for all source waves are listed in Table 4.1. All domains consisted of 100[nm] of quartz above 100[nm] of free space, with outer boundaries truncated by absorbing boundary conditions.

![Diagram of photolithography pattern](image)

**Figure 4.1.** Simulation of the two “L” photolithography pattern: (a) The binary mask pattern used in this section; (b) A diagram of the computational domain for photoresist scattering simulations. The photoresist layer is 420[nm] deep, with 193[nm] of free space above it, and 193[nm] below it.

<table>
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<th>Technology</th>
<th>Unknowns</th>
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<th>OFEM Time [s]</th>
<th>Fourier Time [s]</th>
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<td>203.2</td>
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<tr>
<td>130[nm]</td>
<td>89,994</td>
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The aerial image intensity plots in Figure 4.2 show the result of the OFEM scattering solutions for (a) \( \hat{x} \) and (b) \( \hat{y} \) polarized, normally incident plane wave illumination, with \( \text{NA} = 0.85 \). The logarithmic scale highlights the interference pattern between
Figure 4.2. OFEM scattering of 250[nm] half-pitch technology node intensity plots: (a) Aerial image due to $\hat{x}$ polarized plane wave; (b) Aerial image due to $\hat{y}$ polarized plane wave.

For each technology node, the aerial images intensities due to the incident $\hat{x}$ and $\hat{y}$ polarized plane waves were combined via incoherent summation, as a corollary to double exposure patterning. Figure 4.5 shows the focal plane aerial image intensity for the 250[nm], 180[nm], and 130[nm] double pattering. The intensity plots in Figure 4.5 show that the effects of the illumination wave polarizations can be mitigated through double patterning. Compared to the idealized scalar aerial images shown in Figure 4.6,
Figure 4.3. OFEM scattering of 180[nm] half-pitch technology node intensity plots: (a) Aerial image due to $\hat{x}$ polarized plane wave; (b) Aerial image due to $\hat{y}$ polarized plane wave.

which are plotted at the same scale as the those in Figure 4.5, the OFEM plus Fourier optics aerial images exhibit much less clearly defined nulls in the intensity patterns.

The OFEM photoresist simulation was then performed with the vertical domain layout shown in Figure 4.1. For all simulations the vertical portion of the computational domain was the same, and the domain length and width changed with size of the source aerial image. Computational statistics are listed in Table 4.2. The 250[nm] and 180[nm] technology simulations were solved using CG, and the 130[nm] half-pitch technology simulation was solved via the direct solver Pardiso [35]. The photoresist layer was modeled as a dielectric with relative permittivity $\epsilon_r = 2.9238$, and the silicon dioxide was modeled as $\epsilon_r = 2.4336$.

Table 4.2. Computational statistics for photoresist scattering simulation.

<table>
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<tr>
<th>Technology</th>
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<th>Memory [MB]</th>
<th>Iterations</th>
<th>Time [s]</th>
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Figure 4.4. OFEM scattering of 130[nm] half-pitch technology node intensity plots:
(a) Aerial image due to $\hat{x}$ polarized plane wave; (b) Aerial image due to $\hat{y}$ polarized plane wave.

Figure 4.7 shows the incoherent sum of field intensities inside of the PR layer for the 250[nm] case. Figure 4.7 (a) is at the focal plane, inside of the photoresist. The image is weaker than the aerial image in free space because energy has reflected away at the dielectric interface. Figure 4.7 (b) shows a side cut of the intensity in the computational domain through a long axis of the smaller “L,” where the transition from air to photoresist is clearly visible. The pattern is strong. For the 180[nm] technology, the intensities in Figure 4.8 show that the small “L” pattern will not print the concave corner. Figure 4.8 (b) shows that the intensity within the PR layer is not evenly distributed. The images of Figure 4.9 are even worse, with the small “L” printing as a rotated block, and the ends of the large “L” showing likely separation.

Compared to images formed in free space, image intensities inside of photoresist layers are generally weaker. The dielectric impedance mismatch causes energy to leave the region of the PR. The features are also somewhat smoothed, as higher spatial frequency field components are skewed towards the normal as discussed in Section 3.4.
Figure 4.5. Aerial images due OFEM simulation and incoherent sum of $\hat{x}$ and $\hat{y}$ polarized normally incident plane wave on: (a) 250[nm] technology mask; (b) 180[nm] technology mask; (c) 130[nm] technology mask;

Figure 4.6. Aerial images due idealized scalar image calculation: (a) 250[nm] technology mask; (b) 180[nm] technology mask; (c) 130[nm] technology mask;
Figure 4.7. OFEM scattering for 250[nm] half-pitch technology node photoresist intensity plots: (a) Image in photoresist due to double-patterned exposure; (b) Side view of the same PR domain. The air-pr interface is visible in the wave patterns.

Figure 4.8. OFEM scattering for 180[nm] half-pitch technology node photoresist intensity plots: (a) Image in photoresist due to double-patterned exposure; (b) Side view of the same PR domain. The air-pr interface is visible in the wave patterns.
Figure 4.9. OFEM scattering for 130[nm] half-pitch technology node photoresist intensity plots: (a) Image in photoresist due to double-patterned exposure; (b) Side view of the same PR domain. The air-pr interface is visible in the wave patterns.
4.2 Thick Mask

The idealized concept of the infinitely thin PEC photomask cannot capture the electromagnetic scattering effects of mask metal layer thickness. The binary mask from Section 4.1 was again simulated, but with the metal layer an industry typical 85[nm] thick [5]. The extended aperture depth of the mask leads to more OFEM degrees-of-freedom than in the infinitely thin PEC case. Figure 4.10 shows are cut-away portions of the octree meshes for the thick mask. The thick PEC layer binary photomask was simulated with OFEM at the 250[nm], 180[nm], and 130[nm] half-pitch technology nodes. The radiation source was $\hat{x}$ and $\hat{y}$ polarized, normally incident plane waves, with free space $\lambda = 193$[nm] consistent with a ArF laser source. The OFEM scattering simulation times, unknown degrees of freedom counts, and total computation times for forward and inverse Fourier transforms for all source waves are listed in Table 4.3. All domains consisted of 100[nm] of quartz above 100[nm] of free space, with outer boundaries truncated by absorbing boundary conditions.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td>272,952</td>
<td>1.856</td>
<td>204.2</td>
<td>377.2</td>
</tr>
<tr>
<td>180</td>
<td>143,940</td>
<td>0.884</td>
<td>59.3</td>
<td>99.3</td>
</tr>
<tr>
<td>130</td>
<td>127,762</td>
<td>0.862</td>
<td>62.9</td>
<td>28.1</td>
</tr>
</tbody>
</table>

Figure 4.10. Cutaways of the octree mesh for 85[nm] thick binary photomask: (a) 250[nm] half-pitch; (b) 180[nm] half-pitch; (c) 130[nm] half-pitch. The red portion of the mesh is air beneath the mask.
Figure 4.11 shows the aerial image intensities due to the \( \hat{x} \) polarized incident wave scattered off of the photomasks. The intensity in Figure 4.11 (a) shows a marked increase in knobiness due to the 85[\text{nm}] PEC channel in the photomask, relative to the infinitely thin photomask from the previous section. Figure 4.11 (b) exhibits a similar effect. Figure 4.11 (c) shows the small “L” feature intensity is more horizontal than in the infinitely thin case. The perpendicular portions of both “L” features is poorly represented.

\[\begin{array}{ccc}
\text{(a)} & \text{(b)} & \text{(c)} \\
\end{array}\]

\textbf{Figure 4.11.} Aerial image intensity due to \( \hat{x} \) polarized normally incident plane wave on a thick binary photomask: (a) 250[\text{nm}] half-pitch; (b) 180[\text{nm}] half-pitch; (c) 130[\text{nm}] half-pitch.

\[\begin{array}{ccc}
\text{(a)} & \text{(b)} & \text{(c)} \\
\end{array}\]

\textbf{Figure 4.12.} Aerial image intensity due to incoherent sum of \( \hat{y} \) and \( \hat{x} \) polarized normally incident plane waves on a thick binary photomask: (a) 250[\text{nm}] pitch; (b) 180[\text{nm}] pitch; (c) 130[\text{nm}] pitch.

Double patterned aerial images were created through the incoherent summation of the image intensities due to the \( \hat{x} \) and \( \hat{y} \) polarized plane waves, and plotted in
Figure 4.12. For the 250[nm] half-pitch photomask, the features are distinct in the concave regions a mostly filled in, as seen in Figure 4.12 (a). There is a considerable periodic rounding to the edges. Figure 4.12 (b) retains the well defined concave corners, with less defined periodic rounding. The 130[nm] half-pitch image in Figure 4.12 (c) fails to reproduce the smaller “L” feature, as was the case for the infinitely thin photomask.

Table 4.4. Comparison of aerial images for different computational models, for three technology sizes. The full wave infinitely thin mask and thick mask models are both double patterned.

<table>
<thead>
<tr>
<th></th>
<th>250[nm]</th>
<th>180[nm]</th>
<th>130[nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scalar</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>Thin</td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
<tr>
<td>Thick</td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
<td><img src="image9.png" alt="Image" /></td>
</tr>
</tbody>
</table>

Table 4.4 shows a side by side comparison of the aerial images calculated from the idealized scalar model, the full wave OFEM infinitely thin photomask model from the previous section, and the full wave OFEM thick metal layer photomask model. The
The idealized scalar model produces extremely sharp, well-defined image intensity nulls. Both the infinitely thin and thick metal layer models produce softer, more blurred images.

The aerial images due to the electromagnetic scattering of incident plane waves by the thick PEC layer photomask were calculated at 1.5λ from the focal plane, and used as inputs to a photoresist modeling OFEM electromagnetic scattering simulation. The computation domain was defined as 193[nm] of air above 420[nm] of photoresist with $\varepsilon_r = 2.9238$, on top of 193[nm] of silicon dioxide with $\varepsilon_r = 2.4336$. The computational statistics for the PR OFEM scattering simulation were the same as those for the infinitely thin PEC photomask case, as seen in Table 4.5.

Table 4.5. Computational statistics for photoresist scattering simulation.

<table>
<thead>
<tr>
<th>Technology</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>Iterations</th>
<th>Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>250[nm]</td>
<td>1,099,074</td>
<td>1,036</td>
<td>517</td>
<td>1,151</td>
</tr>
<tr>
<td>180[nm]</td>
<td>568,830</td>
<td>552</td>
<td>385</td>
<td>734</td>
</tr>
<tr>
<td>130[nm]</td>
<td>232,064</td>
<td>2,586</td>
<td>(direct)</td>
<td>225</td>
</tr>
</tbody>
</table>

Figure 4.13 shows the images at the focal plane within the photoresist layer. Contrary to the infinitely thin PEC photomask, the 85[nm] thick PEC photomask is a physically realizable design. For the intensity images of Figure 4.13, 50% of the peak intensity was chosen as the photoresist exposure threshold. In Figure 4.13 (a) the intensity inside of the photoresist is plotted with 50% of peak intensity and above in solid red. The two “L” pattern is clearly visible, and the concave corners are not very rounded. Figure 4.13 (b) shows the 180[nm] PR intensity image, where the concave corners are now rounded. The outer lines of the features are still connected, but not evenly. The image of Figure 4.13 (c) has no recognizable small “L” and the large “L” is very rounded. Clearly the photoresist field intensity in the 130[nm] is not acceptable with regards to the intended design.

Table 4.6 shows a side by side comparison of the images formed in photoresist, according to three different computational models. The idealized scalar aerial image
Figure 4.13. Image intensity in photoresist due to incoherent sum of $\hat{y}$ and $\hat{x}$ polarized normally incident plane waves on a thick binary photomask: (a) 250[\text{nm}] pitch; (b) 180[\text{nm}] pitch; (c) 130[\text{nm}] pitch.

computation is translated to a photoresist image by scaling the computed scalar electric field values with the electromagnetic transmission coefficient calculated as:

$$T = \frac{2\eta}{\eta + \eta_0},$$  \hspace{0.5cm} (4.1)

where $\eta = \eta_0/\sqrt{\epsilon_r}$ is the wave impedance inside the photoresist, $\eta_0$ is the free-space wave impedance, and $\epsilon_r = 2.4336$ is the relative permittivity of the simulated photoresist. The infinitely thin mask simulation results are from the previous section of this chapter. There is a good visual agreement between the idealized scalar model images and the thick metal layer full wave OFEM images, especially for the 180[\text{nm}] technology. However at 130[\text{nm}] the idealized scalar model predicts a very different image from the full wave OFEM images. The 130[\text{nm}] thick metal layer OFEM simulation predicts better feature separation between the corners of the two “L” patterns than the infinitely thin metal layer OFEM simulation.
Table 4.6. Comparison of aerial images at the focal plane inside of photoresist for different computational models, for three technology sizes. The scalar model forms the image inside of the photoresist as a rescaling of the aerial image formed in free space. The full wave infinitely thin mask and thick mask models are both double patterned.

<table>
<thead>
<tr>
<th></th>
<th>250[nm]</th>
<th>180[nm]</th>
<th>130[nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scalar</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
</tr>
<tr>
<td>Thin</td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
<tr>
<td>Thick</td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
<td><img src="image9.png" alt="Image" /></td>
</tr>
</tbody>
</table>
4.3 Thick Mask With OPC

The decrease of feature sizes in photolithography necessitate special methods to ensure the intended image is printed in photoresist. Optical proximity correction (OPC) techniques are arrived at through a variety of methods, but the current methodology is generally an iterative error minimization scheme. Poonawala et. al [2] utilized one such method to create the binary mask pattern shown in Figure 4.14 (b) from the intended pattern of Figure 4.14 (a). However that pattern was optimized using an idealized scalar aerial image calculation. In this section, the electromagnetic scattering due to a 85[nm] thick binary photomask with OPC is simulated, and the resulting aerial image calculated. The scattered fields are then used to create a set of input fields for a photoresist scattering OFEM simulation to test the printability of the OPC mask design.

![Figure 4.14. Images of binary mask patterns from [2]: (a) The original intended rectangular pattern; (b) The calculated OPC pattern for the intended image.](image)

The mask layouts from [2] in Figure 4.14 were discretized via octree mesh, as seen in Figure 4.15. With source $\lambda = 193[\text{nm}]$, the fine OPC details in Figure 4.14 (b) were discretized to element size $\frac{\lambda}{24}$, and all other domain features discretized to $\frac{\lambda}{12}$. A preliminary idealized aerial image computation with $NA = 0.85$ was performed, where
\( \hat{x} \) and \( \hat{y} \) polarized plane waves were sampled at the locations of the mask apertures and Fourier transformed. The inverse Fourier transform was then performed and the resulting aerial image intensities were plotted in Figure 4.16. As seen in Figure 4.16 (a), the result of using the intended image pattern as the photomask results in severely rounded features, while the OPC photomask design yields the largely rectangular intensity pattern of Figure 4.16 (b).

![Figure 4.15. Cutaways of the octree mesh for thick mask: (a) The original intended pattern used as a binary mask; (b) The octree meshed OPC layout arrived at by Poonawala et. al [2]. The blue regions are meshed air below the mask mesh.](image)

<table>
<thead>
<tr>
<th>Mask</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>OFEM Time [s]</th>
<th>Fourier Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intent</td>
<td>143,076</td>
<td>870</td>
<td>58.9</td>
<td>84.2</td>
</tr>
<tr>
<td>OPC</td>
<td>270,772</td>
<td>2,070</td>
<td>143.9</td>
<td>146.2</td>
</tr>
</tbody>
</table>

Table 4.7. Computational statistics for 85[nm] thick photomask scattering and aerial image formation.

OFEM electromagnetic scattering simulation was then performed for 85[nm] thick PEC layer photomask models. The aerial images due to the scattering of \( \hat{x} \) and \( \hat{y} \) polarized, normally incident plane waves were calculated, and incoherently summed to form image intensity plots. The computational statistics for the OFEM scattering and Fourier calculations are listed in Table 4.7. As has been previously shown for
Figure 4.16. Aerial images due to idealized scalar computation in the apertures of infinitely thin PEC mask: (a) Intensity from intended rectangular pattern used as the photomask layout; (b) Intensity from OPC layout arrived at by Poonawala et. al [2].

Thick photomasks, the image intensity plot of Figure 4.17 (a) exhibit an increased bias along straight edges. However the plot of Figure 4.17 (b) also shows an increased field coupling between the intended rectangles, showing that the idealized calculation used to determine the OPC pattern is not sufficient. It must be mentioned that [2] does not claim that the OPC of Figure 4.14 is correct for real life photolithography. The purpose here is to highlight the necessity of EMF simulation such as OFEM electromagnetic scattering in the iterative process which develops the OPC pattern in the first place.

Table 4.8. Computational statistics for photoresist scattering simulation.

<table>
<thead>
<tr>
<th>Mask</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>Iterations</th>
<th>Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intent</td>
<td>492,033</td>
<td>481</td>
<td>382</td>
<td>338</td>
</tr>
<tr>
<td>OPC</td>
<td>666,533</td>
<td>641</td>
<td>372</td>
<td>433</td>
</tr>
</tbody>
</table>

The aerial images due to the electromagnetic scattering of incident plane waves by the photomasks were calculated at $1.5\lambda$ from the focal plane, and used as inputs to a photoresist modeling OFEM electromagnetic scattering simulation. The computation domain was again defined as 193[nm] of air above 420[nm] of photoresist with $\epsilon_r =$
Figure 4.17. Aerial images due to OFEM simulation and incoherent sum of $\hat{x}$, $\hat{y}$ polarized plane waves incident on 85[nm] thick PEC photomask: (a) Intensity from intended rectangular pattern used as the photomask layout; (b) Intensity from OPC layout arrived at by Poonawala et. al [2].

2.9238, on top of 193[nm] of silicon dioxide with $\epsilon_r = 2.4336$. The computational statistics for the PR OFEM scattering simulation are listed in Table 4.8.

The field intensity in the photoresist was calculated as an incoherent summation of the intensities due to the scattered photomask fields. The field intensity at the focal plane inside of the photoresist is plotted in Figure 4.18. Again the intensities in the PR layer are similar to the aerial image intensities, with reduced overall energy and a softening of the image. The curvature of the rectangular features in Figure 4.18 (b) illustrates the necessity of consideration of photoresist electromagnetic scattering in the calculation of optical proximity correction designs.
Figure 4.18. Intensity at the focal plane inside of the photoresist layer, due to OFEM simulation and incoherent sum of $\hat{x}$, $\hat{y}$ polarized plane waves incident on 85[nm] thick PEC photomask: (a) Intensity from intended pattern used as the photomask layout; (b) Intensity from OPC layout arrived at by Poonawala et. al [2].
4.4 Chromeless Phase Shift Mask

The automation of photomask design has led to the pixelization of photomasks. Often the chrome layer is completely removed in order to facilitate simplified mask layout calculations [36]. The chromeless pixelated phase shift masks are created through an iterative process where the phase shifter location and illumination pattern are both optimized.

![Chromeless phase shift mask diagram](image)

**Figure 4.19.** Chromeless phase shifting photomask: (a) The design layout of the $\pi$ phase shifters; (b) The k-space diagram of the annular ring illumination with outer radius 0.94 and inner radius 0.74, with polarizations.

In this section, a grid of $\pi$ phase shifters on a quartz substrate is presented. This design was chosen for its simplicity, as no detailed chromless photomask and illumination pattern was available for modeling. The pattern chosen was a $4 \times 4$ grid of $\pi$ phase shifters, illuminated with an annular ring pattern with outer radius 0.94 and inner radius 0.74, as seen in Figure 4.19. The height $d$ of the phase shifters is determined by the equation for optical path difference (OPD):

$$\text{OPD} = d(n_1 - 1), \quad (4.2)$$
where \( n_1 \) is the refractive index of the mask material, and the immersion material is assumed to be air. By this relation, the height of a \( \pi \) (or \( 180^\circ \)) phase shifter is 0.8929\( \lambda \) when the mask is composed of quartz with refractive index \( n_1 = 1.56 \) for the standard ArF 193[\text{nm}] wavelength illumination [5].

![Figure 4.20. A \( \lambda \) pitch chromeless phase shift mask, where \( \lambda \) is the free space wavelength of the illumination source: (a) 2D diagram of the computational domain; (b) Cutaway of an octree mesh of the photomask, with only the quartz portion shown.](image)

The first OFEM electromagnetic scattering simulation presented is for a pitch of \( \lambda \), such that the phase shifters were \( \frac{\lambda}{2} \) apart. Figure 4.20 (a) shows a side-view diagram of the computational domain, where all outer boundaries are absorbing. Figure 4.20 (b) shows a cutaway portion of the corresponding octree mesh, where the view is from the bottom up to show the \( \pi \) phase shifters. The octree was refined to mesh element size \( \frac{\lambda}{16} \). The OFEM simulation was run for each of the 40 incident plane waves, and the OFEM scattering matrix was solved using the Pardiso direct solver. The computational statistics are listed in Table 4.9.

**Table 4.9.** Computational statistics for chromeless photomask scattering and aerial image formation due to 40 incident plane waves.

<table>
<thead>
<tr>
<th>Pitch</th>
<th>Unknowns</th>
<th>Memory [MB]</th>
<th>OFEM Time [s]</th>
<th>Fourier Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda )</td>
<td>369,439</td>
<td>3,639</td>
<td>1,786</td>
<td>780</td>
</tr>
<tr>
<td>0.667( \lambda )</td>
<td>141,615</td>
<td>1,366</td>
<td>739</td>
<td>676</td>
</tr>
<tr>
<td>0.5( \lambda )</td>
<td>93,735</td>
<td>763</td>
<td>545</td>
<td>668</td>
</tr>
</tbody>
</table>
Each of the 40 aerial images due to electromagnetic scattering from the chromeless photomask were incoherently summed, and the resulting aerial image intensity plotted in Figure 4.21 (a). The image has a much lower dynamic range than previous aerial images because there is no PEC layer present to deflect most of the incoming plane waves. As a result it can be asserted that any exposure of photoresist using a chromeless mask must be extremely accurate. Figure 4.21 (b) shows a possible exposure cutoff of 90% of the peak aerial image intensity.

![Aerial images due to OFEM simulation of the $\lambda$ pitch chromeless phase shift mask: (a) The aerial image intensity exhibits a lower dynamic range than previous images due to binary photomasks; (b) The same image with all intensity above 90% in red, and below 90% in blue.](image)

Figure 4.21. Aerial images due to OFEM simulation of the $\lambda$ pitch chromeless phase shift mask: (a) The aerial image intensity exhibits a lower dynamic range than previous images due to binary photomasks; (b) The same image with all intensity above 90% in red, and below 90% in blue.

The process was repeated for a pitch of $\frac{2}{3}\lambda$, such that the phase shifters were $\frac{\lambda}{6}$ apart. Figure 4.22 (a) shows a side-view diagram of the computational domain, and Figure 4.20 (b) shows a cutaway portion of the corresponding octree mesh. As seen in Figure 4.23, the smaller pitch chromeless mask results in an even lower aerial image intensity dynamic range, due to the reduced amount of destructive wave interference.
The simple design philosophy of rescaling the mask pattern broke down when applied to $\frac{1}{2}\lambda$ pitch, such that the spacing between the $\pi$ phase shifters was $\frac{\lambda}{4}$ as seen in Figure 4.24. At this feature size the destructive wave interference between the phase shifters was not sufficient to eliminate electric field intensity, resulting in the aerial images of Figure 4.25. The familiar reduced dynamic range gave way to connected features. This is highlighted in Figure 4.25 (b), where all intensity above 95% is shown in red. The diagonal symmetry is very apparent, suggesting electromagnetic resonances across phase shifting elements.

The plots of this section show chromeless phase shift masks reduce the dynamic range of aerial image intensities. This is due to the lack of metal photomask features, which reflect electromagnetic energy back towards the illumination source and away from the image plane. As printed semiconductor technology shrinks, special measures must be taken to ensure destructive wave interference, and hence contrast, between desired image features.
Figure 4.23. Aerial images due to OFEM simulation of the $\frac{2}{3}\lambda$ pitch chromeless phase shift mask: (a) The aerial image intensity exhibits a lower dynamic range than previous images due to binary photomasks; (b) The same image with all intensity above 95% in red, and below 95% in blue.

Figure 4.24. A $\frac{1}{2}\lambda$ pitch chromeless phase shift mask, where $\lambda$ is the free space wavelength of the illumination source: (a) 2D diagram of the computational domain; (b) Cutaway of an octree mesh of the photomask, with only the quartz portion shown.
Figure 4.25. Aerial images due to OFEM simulation of the $\frac{1}{2}\lambda$ pitch chromeless phase shift mask: (a) The aerial image intensity exhibits a lower dynamic range than previous images due to binary photomasks; (b) The same image with all intensity above 95% in red, and below 95% in blue.
CHAPTER 5
CONCLUSIONS AND FUTURE WORK

5.1 Conclusions

This thesis proposed a simulation system capable of modeling a complete photolithography system, from illumination source to image intensity inside of the photoresist layer, based on the Octree Finite Element Method (OFEM) for full wave electromagnetic scattering and Fourier optics. The 2:1 nonconformal octree model geometry mesher developed was shown to be rapid and stable. When compared to the performance of a published tetrahedral mesher, the 2:1 balanced octree mesher was up to two orders of magnitude faster.

The special nonconformal basis and finite element assembly procedure was created to preserve tangential electric field continuity, and shown to behave as well as a conformal tetrahedral mesh element based FEM for 1st order basis functions. Arbitrary refinement of the nonconformal mesh did not lead to error in electromagnetic scattering simulations, but also did not necessarily decrease RCS error. Targeted adaptive mesh refinement is clearly a better strategy for octree mesh refinement.

When OFEM electromagnetic scattering simulations are compared to tetrahedral mesh based FEM electromagnetic scattering simulations the run times are approximately the same, due to the precomputing of the nonconformal octree element matrices. Additionally the accuracy is similar, even though the tetrahedral mesh based FEM used adaptive mesh refinement. Nearly all of the performance time gains over tetrahedral mesh FEMs are due to the extreme speed of the octree mesh generation.
The aerial image formation presented in this thesis proved to be a computational bottleneck, often taking longer to perform than the corresponding OFEM scattering simulations. The Fourier transforms were implemented in a brute force fashion and did not scale well. A better solution is to apply the fast Fourier transform (FFT) [30] to the Fourier Optics portions of the codes.

Simulation of photolithography systems with OFEM scattering and Fourier optics revealed that for simple features, full-wave simulation produced results similar to those from idealized calculation. However more complex photomask layouts resulted in aerial images which differed greatly from the idealized expectation. Simulation of photoresist scattering did little to effect the overall image. Automated iterative design systems which produce complicated OPC photomasks would likely benefit from OFEM simulation of the photomask scattering.

5.2 Future Work

This work encountered a number of areas for future research. These include:

1. Extend OFEM to work with domain decomposition finite element method (DDFEM) for parallelization [37].

2. Explore singular value decomposition (SVD) to reduce to number of source waves required to simulated incoherent illumination [38].

3. Formulate an adaptive mesh refinement (AMR) scheme to optimize octree mesh density.

4. Apply fast Fourier transform (FFT) [30] algorithm to alleviate the computational bottleneck caused by the brute force Fourier Optics implementation in this thesis.

5. Implement the assembly procedure for 2nd order hanging basis functions.
APPENDIX A

HIERARCHICAL BASIS FOR HEXAHEDRAL ELEMENTS

This thesis utilized a hierarchical vector basis as described by Zaglmayr [32]. Here the basis functions are divided into 1st order functions associated with edges, and 2nd order functions associated with edges, faces, and volumes. The nodes and edges are ordered lexicographically, as seen in Figure A.1. The reference element is a regular hexahedron with height, length and width equal to $h$. The basis functions are defined on transformed coordinates $x = \frac{u}{h}$, $y = \frac{v}{h}$, and $z = \frac{w}{h}$, within the reference element, and zero outside of it.

The edge vector basis functions $w$ are identified by zero-indexed edge id, followed by the zero-indexed order. The 1st order edge basis functions are:

\[ w_{e0,0} = (1 - y - x + xy)\hat{z}, \]
\[ w_{e1,0} = (1 - z - x + xz)\hat{y}, \]
\[ w_{e2,0} = (1 - z - y + yz)\hat{x}, \]
\[ w_{e3,0} = (z - xz)\hat{y}, \]
\[ w_{e4,0} = (z - yz)\hat{x}, \]
\[ w_{e5,0} = (y - xy)\hat{z}, \]
\[ w_{e6,0} = (y - yz)\hat{x}, \]
\[ w_{e7,0} = (yz)\hat{x}, \]
Figure A.1. The element features in this thesis are ordered lexicographically, with the \( \hat{u} \) direction varying most slowly, the \( \hat{v} \) direction varying second most slowly, and direction \( \hat{w} \) varying the fastest. Here the nodes are labeled in black. The edges are labeled in blue, and directed towards increasing nodes. The height of the element is \( h \), such that local coordinates \( x, y, z \) are \( \frac{u}{h}, \frac{v}{h}, \frac{w}{h} \), respectively.

\[
w_{e8,0} = (x - xy)\hat{z},
\]

\[
w_{e9,0} = (x - xz)\hat{y},
\]

\[
w_{e10,0} = (xz)\hat{y},
\]

and

\[
w_{e11,0} = (xy)\hat{z}.
\]

The 2\textsuperscript{nd} order edge basis functions are:

\[
w_{e0,1} = \begin{cases} 
    z(z - 1)(y - 1) \\
    z(z - 1)(x - 1) \\
    (2z - 1)(1 - y - x + xy)
\end{cases},
\]
Figure A.2. Edge vector basis functions: (a) 1\textsuperscript{st} order edge basis function; (b) 2\textsuperscript{nd} order edge basis function;

\[ w_{e1,1} = \begin{cases} 
  y(y-1)(z-1) \\
  (2y-1)(1-z-x+xz) \\
  y(y-1)(x-1) 
\end{cases}, \]

\[ w_{e2,1} = \begin{cases} 
  (2x-1)(1-z-y+yz) \\
  x(x-1)(z-1) \\
  x(x-1)(y-1) 
\end{cases}, \]

\[ w_{e3,1} = \begin{cases} 
  -yz(y-1) \\
  -z(2y-1)(x-1) \\
  -y(y-1)(x-1) 
\end{cases}, \]

\[ w_{e4,1} = \begin{cases} 
  -z(2x-1)(y-1) \\
  -xz(x-1) \\
  -x(y-1)(x-1) 
\end{cases}, \]

\[ w_{e5,1} = \begin{cases} 
  -zy(z-1) \\
  -z(z-1)(x-1) \\
  -y(2z-1)(x-1) 
\end{cases}, \]
The 2nd order functions associated with faces are ordered by the outward facing normal vectors \{-\hat{z}, -\hat{y}, -\hat{x}, \hat{x}, \hat{y}, \hat{z}\}, again, zero-indexed. Each face has 4 functions associated with it. The 2nd order face basis functions for the \(-\hat{z}\) directed face are:

\[ w_{e6,1} = \begin{cases} 
- y(2x - 1)(z - 1) \\
- x(z - 1)(x - 1) \\
- xy(x - 1)
\end{cases}, \]

\[ w_{e7,1} = \begin{cases} 
yz(2x - 1) \\
xz(x - 1) \\
xy(x - 1)
\end{cases}, \]

\[ w_{e8,1} = \begin{cases} 
- z(z - 1)(y - 1) \\
- xz(z - 1) \\
- x(2z - 1)(y - 1)
\end{cases}, \]

\[ w_{e9,1} = \begin{cases} 
- y(z - 1)(y - 1) \\
- x(2y - 1)(z - 1) \\
- xy(y - 1)
\end{cases}, \]

\[ w_{e10,1} = \begin{cases} 
yz(y - 1) \\
xz(2y - 1) \\
xy(y - 1)
\end{cases}, \]

\[ w_{e11,1} = \begin{cases} 
yz(z - 1) \\
xz(z - 1) \\
xy(2z - 1)
\end{cases}. \]

and

\[ w_{j0,0} = \begin{cases} 
-4y(y - 1)(2x - 1)(z - 1) \\
-4x(2y - 1)(x - 1)(z - 1) \\
-4y(y - 1)(x - 1)
\end{cases}. \]
The 2nd order face basis functions for the $-\hat{y}$ directed face are:

\[ w_{f0,1} = \begin{cases} 
-4y(y-1)(2x-1)(z-1) \\
4x(2y-1)(x-1)(z-1) \\
0 
\end{cases} , \]

\[ w_{f0,2} = \begin{cases} 
4y(y-1)(z-1) \\
0 \\
0 
\end{cases} , \]

\[ w_{f0,3} = \begin{cases} 
0 \\
0 \\
4x(x-1)(z-1) 
\end{cases} . \]

\[ w_{f1,0} = \begin{cases} 
-4z(2x-1)(y-1)(z-1) \\
-4xz(x-1)(z-1) \\
-4x(x-1)(y-1)(2z-1) 
\end{cases} , \]

\[ w_{f1,1} = \begin{cases} 
-4z(2x-1)(y-1)(z-1) \\
0 \\
4x(x-1)(y-1)(2z-1) 
\end{cases} , \]

\[ w_{f1,2} = \begin{cases} 
4z(y-1)(z-1) \\
0 \\
0 
\end{cases} , \]

\[ w_{f1,3} = \begin{cases} 
0 \\
0 \\
4x(x-1)(y-1) 
\end{cases} . \]
The 2\textsuperscript{nd} order face basis functions for the $-\mathbf{x}$ directed face are:

\[
\begin{align*}
\mathbf{w}_{f2,0} &= \begin{cases} 
-4yz(y - 1)(z - 1) \\
-4z(x - 1)(2y - 1)(z - 1) \\
-4y(x - 1)(y - 1)(2z - 1)
\end{cases}, \\
\mathbf{w}_{f2,1} &= \begin{cases} 
0 \\
-4z(x - 1)(2y - 1)(z - 1) \\
4y(x - 1)(y - 1)(2z - 1)
\end{cases}, \\
\mathbf{w}_{f2,2} &= \begin{cases} 
0 \\
4z(x - 1)(z - 1) \\
0
\end{cases}, \\
\mathbf{w}_{f2,3} &= \begin{cases} 
0 \\
0 \\
4y(x - 1)(y - 1)
\end{cases}.
\end{align*}
\]

The 2\textsuperscript{nd} order face basis functions for the $\mathbf{x}$ directed face are:

\[
\begin{align*}
\mathbf{w}_{f3,0} &= \begin{cases} 
4yz(y - 1)(z - 1) \\
4xz(2y - 1)(z - 1) \\
4xy(y - 1)(2z - 1)
\end{cases}, \\
\mathbf{w}_{f3,1} &= \begin{cases} 
0 \\
4xz(2y - 1)(z - 1) \\
-4xy(y - 1)(2z - 1)
\end{cases}, \\
\mathbf{w}_{f3,2} &= \begin{cases} 
0 \\
-4xz(z - 1) \\
0
\end{cases}.
\end{align*}
\]
The 2\textsuperscript{nd} order face basis functions for the $\hat{y}$ directed face are:

\[
\mathbf{w}_f_{4,0} = \begin{bmatrix}
4yz(2x - 1)(z - 1) \\
4xz(y - 1)(z - 1) \\
4xy(x - 1)(2z - 1)
\end{bmatrix},
\]

\[
\mathbf{w}_f_{4,1} = \begin{bmatrix}
4yz(2x - 1)(z - 1) \\
0 \\
-4xy(x - 1)(2z - 1)
\end{bmatrix},
\]

\[
\mathbf{w}_f_{4,2} = \begin{bmatrix}
-4yz(z - 1) \\
0 \\
0
\end{bmatrix},
\]

\[
\mathbf{w}_f_{4,3} = \begin{bmatrix}
0 \\
0 \\
-4xy(x - 1)
\end{bmatrix}.
\]

The 2\textsuperscript{nd} order face basis functions for the $\hat{z}$ directed face are:

\[
\mathbf{w}_f_{5,0} = \begin{bmatrix}
4yz(2x - 1)(y - 1) \\
-4xz(x - 1)(2y - 1) \\
4xy(x - 1)(y - 1)
\end{bmatrix},
\]

\[
\mathbf{w}_f_{5,1} = \begin{bmatrix}
4yz(2x - 1)(y - 1) \\
-4xz(x - 1)(2y - 1) \\
0
\end{bmatrix}.
\]
Figure A.3. Face vector basis functions: (a) Type 0 face basis function; (b) Type 1 face basis function; (c) Type 2 face basis function; (d) Type 3 face basis function;

\[
\begin{align*}
\mathbf{w}_{f5,2} &= \begin{cases} 
-4yz(y-1) \\
0 \\
0 \\
0
\end{cases}, \\
\mathbf{w}_{f5,3} &= \begin{cases} 
0 \\
-4xz(x-1) \\
0 \\
0
\end{cases}.
\end{align*}
\]

Finally the 2\textsuperscript{nd} order vector basis functions associated with the volume of the reference element are:
\[ \mathbf{w}_{v,0} = \begin{cases} 
16yz(2x - 1)(y - 1)(z - 1) \\
16xz(x - 1)(2y - 1)(z - 1) \\
16xy(x - 1)(y - 1)(2z - 1) 
\end{cases}, \]

\[ \mathbf{w}_{v,1} = \begin{cases} 
16yz(2x - 1)(y - 1)(z - 1) \\
-16xz(x - 1)(2y - 1)(z - 1) \\
16xy(x - 1)(y - 1)(2z - 1) 
\end{cases}, \]

\[ \mathbf{w}_{v,0} = \begin{cases} 
16yz(2x - 1)(y - 1)(z - 1) \\
-16xz(x - 1)(2y - 1)(z - 1) \\
-16xy(x - 1)(y - 1)(2z - 1) 
\end{cases}, \]

\[ \mathbf{w}_{v,0} = \begin{cases} 
16yz(y - 1)(z - 1) \\
0 \\
0 
\end{cases}, \]

\[ \mathbf{w}_{v,0} = \begin{cases} 
16xz(x - 1)(z - 1) \\
0 
\end{cases}, \]

\[ \mathbf{w}_{v,0} = \begin{cases} 
16zy(x - 1)(y - 1) \\
0 
\end{cases}. \]
Figure A.4. Volume vector basis functions: (a) Type 0 volume basis function; (b) Type 1 volume basis function; (c) Type 2 volume basis function; (d) Type 3 volume basis function; (e) Type 4 volume basis function; (f) Type 5 volume basis function;
APPENDIX B
OFEM ELEMENT MATRICES

The OFEM matrix $\mathbf{A}$ is formed as a summation of individual element matrices, which are themselves a summation of the element stiffness matrix $\mathbf{S}$, mass matrix $\mathbf{T}$, and absorbing boundary condition matrix $\mathbf{D}$ defined on faces in contact with the outer surface of the computational domain. Each individual OFEM element matrix entry is found as an integration:

$$\mathbf{S}_{ij} = \int_{\text{element}} \nabla \times \mathbf{w}_i \cdot \nabla \times \mathbf{w}_j \, dr^3,$$  \hspace{1cm} (B.1)

$$\mathbf{T}_{ij} = \int_{\text{element}} \mathbf{w}_i \cdot \mathbf{w}_j \, dr^3,$$  \hspace{1cm} (B.2)

and:

$$\mathbf{D}_{ij} = \int_{\text{face}} \hat{n} \times \mathbf{w}_i \cdot \hat{n} \times \mathbf{w}_j \, dr^2,$$  \hspace{1cm} (B.3)

where $\hat{n}$ is the outward normal of the absorbing boundary condition face, and the $\epsilon_r$ and $\mu_r$ terms are ignored since material properties do not vary within a finite element.

For 1st order octree finite elements, the stiffness and mass element matrices are of dimension $12 \times 12$, and the absorbing boundary condition matrix is $4 \times 4$. For 2nd order octree finite elements, the stiffness and mass element matrices are of dimension $54 \times 54$, and the absorbing boundary condition matrix is $12 \times 12$. The degree-of-freedom index $i$ follows the order of Appendix A, where $i \in [0, 11]$ refers to 1st order edge dofs $0 - 11$, $i \in [12, 23]$ refers to 2nd order edge dofs $0 - 11$, $i \in [24, 47]$ refers to the type 0,1,2,3 dofs for faces $0 - 6$, respectively, and finally $i \in [48, 53]$ reference the type 0,1,2,3,4,5 dofs associated with the element volume.
Element Matrix Assembly

The integrations for reference element $\mathcal{K} = [0, h]^3$, where $h$ is the side length of the hexahedral element, were performed using the Maple software package. The value listings for the $S$ and $T$ OFEM element matrices are partitioned according to the scheme in Figure B.2 to allow all 2,916 values to appear on the page. The OFEM element matrices are reconstituted as follows: the $D$ OFEM element matrix is the listed values of Figure B.1 times the common term $h^{2/90}$, the $T$ OFEM element matrix is the listed values of Figure B.3 through Figure B.6 times $h^{3/540}$, and the $S$ OFEM element matrix is the listed values of Figure B.7 through Figure B.10 times $h^{8/810}$. Additionally, the values for 1st order OFEM element matrices are found as the first $12 \times 12$ portion of partition 1 for the $S$ and $T$ matrices, and the first $4 \times 4$ portion of the $D$ matrix.

\[
\begin{array}{cccccccccccc}
30 & 0 & 0 & 15 & 0 & 8 & -7 & 0 & 0 & 0 & 0 & 30 \\
0 & 30 & 15 & 0 & 8 & 0 & 0 & -7 & 0 & 0 & 30 & 0 \\
0 & 15 & 30 & 0 & 8 & 0 & 0 & -7 & 0 & 0 & 30 & 0 \\
15 & 0 & 0 & 30 & 6 & 8 & -7 & 0 & 0 & 0 & 30 & 0 \\
0 & 8 & 8 & 0 & 13 & 0 & 0 & 2 & -10 & 10 & 12 & 0 \\
8 & 0 & 0 & 8 & 0 & 13 & 2 & 0 & -10 & -10 & 0 & 12 \\
-7 & 0 & 0 & -7 & 0 & 2 & 13 & 0 & -10 & -10 & 0 & -12 \\
0 & -7 & -7 & 0 & 2 & 0 & 0 & 13 & -10 & 10 & -12 & 0 \\
0 & 0 & 0 & 0 & -10 & -10 & -10 & -10 & 32 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 10 & -10 & -10 & 10 & 0 & 32 & 0 & 0 \\
0 & 30 & 30 & 0 & 12 & 0 & 0 & -12 & 0 & 0 & 48 & 0 \\
30 & 0 & 0 & 30 & 6 & 12 & -12 & 0 & 0 & 0 & 0 & 48 \\
\end{array}
\]

Figure B.1. Calculating the $D$ OFEM element matrix: The listed values must be multiplied by $h^{2/90}$. 
Figure B.2. The partition scheme for the listing of the $54 \times 54$ 2nd order $T$ and $S$ OFEM element matrix values.

<table>
<thead>
<tr>
<th>0,0</th>
<th>0,26</th>
<th>0,27</th>
<th>0,53</th>
</tr>
</thead>
<tbody>
<tr>
<td>26,0</td>
<td>26,26</td>
<td>26,27</td>
<td>26,53</td>
</tr>
<tr>
<td>27,0</td>
<td>27,26</td>
<td>27,27</td>
<td>27,53</td>
</tr>
<tr>
<td>53,0</td>
<td>53,26</td>
<td>53,27</td>
<td>53,53</td>
</tr>
</tbody>
</table>

| 60 0 0 0 30 0 0 30 0 0 15 0 0 15 0 15 -15 -15 0 0 8 -7 0 0 -15 0 0 0 0 30 0 0 30 0 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 0 0 60 0 0 0 0 0 30 0 15 0 0 15 0 0 15 0 8 0 0 8 0 0 -15 -15 -7 -7 0 0 0 0 30 Figure B.3. Calculating the first portion of the $T$ OFEM element matrix: The listed values must be multiplied by $\frac{h^3}{540}$. 100
Figure B.4. Calculating the second portion of the $T$ OFEM element matrix: The listed values must be multiplied by $h^{3/540}$.

Figure B.5. Calculating the third portion of the $T$ OFEM element matrix: The listed values must be multiplied by $h^{3/540}$. 

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Figure B.6. Calculating the fourth portion of the $T$ OFEM element matrix: The listed values must be multiplied by $\frac{h^3}{540}$.

Figure B.7. Calculating the first portion of the $S$ OFEM element matrix: The listed values must be multiplied by $\frac{h}{810}$. 

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Figure B.8. Calculating the second portion of the $S$ OFEM element matrix: The listed values must be multiplied by $\frac{h}{810}$.

| -270 | 270 | 0 | -270 | 0 | 270 | 0 | 0 | -270 | 270 | 270 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | -270 | 270 | -270 | 270 | 0    | 0 | 0 | -270 | 270 | 270 | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 270 | -270 | 0 | 270 | 0 | 270 | 0 | 0 | 270 | -270 | 270 | 270 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0    | 0    | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0    | 0 | 0    | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Figure B.9. Calculating the third portion of the $S$ OFEM element matrix: The listed values must be multiplied by $\frac{h}{810}$.
Figure B.10. Calculating the fourth and final portion of the $S$ OFEM element matrix: The listed values must be multiplied by $\frac{h}{810}$.
APPENDIX C
OFEM RESTRICTION OPERATORS

The assembly of the OFEM matrix $\mathcal{A}$ proceeds as the summation over all elements $K$ of the mapped OFEM element matrix $\mathcal{A}_K$:

$$n\mathcal{A}^n = \sum_K nM^N \cdot \left[ N G^K_T N \cdot N A^K_N \cdot N G^K_N \right] \cdot N M^n,$$

(C.1)

where $N$ is the local degree-of-freedom count, $n$ is the global dof count, and $M$ is the local to global id mapping matrix. The restriction operator $G$ is assembled by choosing appropriate columns of values $\gamma$ from the precomputed projection listings for each hanging degree-of-freedom. The columns are chosen by the position of the hanging face on the hanging octant, and the particular local dof ids which are associated with the hanging face and its edges.

Operator Assembly

Figure C.1 (a) shows a single face made up of edges $\{A, B, C, D\}$ which contacts four hanging octants. The hanging octants are addressed as quadrants $q_0, q_1, q_2,$ and $q_3$, and are ordered lexicographically by the octant id number. For the sake of example, Figure C.1 (b) shows the edge dof ids which must be considered for the case of a $1^{st}$ order basis. By the face ordering scheme explained in Appendix B, the hanging octant is has a hanging face in the $\hat{-y}$ position, and the octant id combined with the face location leads to the designation quadrant $q_0$. The resulting restriction operator $G$ is shown in Figure C.2 (b). In a situation where an edge is a member of two source faces, and the hanging octants have multiple hanging faces,
Figure C.1. Identification of dofs to be mapped via the restriction operator $G$: (a) The octants which hang from a source face are lexicographically ordered via the hanging face quadrant they occupy; (b) Each hanging octant is then addressed individually.

$G$ is assembled by choosing the first required listing column, and then overwriting zeros in that column with values from the second required listing column. During the final mapping phase of OFEM matrix assembly, the local dofs which hang are indexed directly to the source dof ids.

However the combination method works only for 1st order edge basis functions which contact two source faces. The practice of assembling hanging basis from the linear combination of half-length reference elements does not hold for 2nd order edge basis functions. Figure C.3 (a) illustrates the failure of the method to maintain tangential continuity between the octants for the 2nd order $e_{0,1}$ basis function. A possible solution is shown in Figure C.3 (b), which is created as a projection of not a half-length reference element basis, but a full octant parent 2nd order edge basis function. A tradeoff of using this basis function is that the 2nd order edge basis function now excites the basis in all 8 child octants, and so element-by-element OFEM matrix assembly will require the additional information of diagonally offset source edges.
Figure C.2. The restriction operator $G$ is assembled from the value listings: (a) For each face and quadrant combination the values $\gamma$ are listed in the order shown, with each source dof shown in blue; (b) For the example hexa with quadrant 0 on the $-\hat{y}$ face, the assembled 1$^{st}$ order $G$ is shown.

Figure C.3. A top down view of the $e_{0,1}$ 2$^{nd}$ order edge (shown red) basis function: (a) Using the combination of two different listing columns, the recreated basis is not tangentially continuous between neighbors; (b) The alternate projection maintains tangential continuity, but must excite the concave corner edge because of the nonzero tangential vector field at $(0.5, 0.5)$, and so all of the 8 hexahedral elements associated with the octants must be involved in the creation of the tangentially continuous basis function.
Projection Values

The projection values for the four quadrants of each face are listed in Figure C.4 through Figure C.9. The common denominator 32 has been removed from each listing, and so all values must be divided by 32 before use. The combine-two-columns method described previously works for 1st order edge basis functions, and is not required for 2nd order face basis functions.

Figure C.11 and Figure C.12 list the projection values for 2nd order edge basis functions in the order described in Figure C.10. The values must be divided by their common denominator 8 before use. Because the 2nd order source edge basis functions are mapped onto all 8 hexahedral elements associated with the 8 octants, the listings are grouped by octant id, and values are given for all 12 possible source edges.
Figure C.4. The projection values for octants which hang in the $-\hat{z}$ direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by $\frac{1}{32}$.
Figure C.5. The projection values for octants which hang in the $-\hat{y}$ direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by $\frac{1}{32}$. 

(a) (b) (c) (d)
Figure C.6. The projection values for octants which hang in the $-\hat{x}$ direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by $\frac{1}{32}$. 

\[
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Figure C.7. The projection values for octants which hang in the \( \hat{x} \) direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by \( \frac{1}{32} \).
Figure C.8. The projection values for octants which hang in the $\hat{y}$ direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by $\frac{1}{32}$. 
**Figure C.9.** The projection values for octants which hang in the $\hat{z}$ direction: (a) Quadrant 0; (b) Quadrant 1; (c) Quadrant 2; (d) Quadrant 3. The listed values must be multiplied by $\frac{1}{32}$.

**Figure C.10.** The 2nd order edge basis listing order for each octant: The source edge ids are across the top in blue.
Figure C.11. The projection values due to 2nd order edge basis functions spanning 2 source faces: (a) Octant 0; (b) Octant 1; (c) Octant 2; (d) Octant 3. The listed values must be multiplied by $\frac{1}{8}$.

Figure C.12. The projection values due to 2nd order edge basis functions spanning 2 source faces: (a) Octant 4; (b) Octant 5; (c) Octant 6; (d) Octant 7. The listed values must be multiplied by $\frac{1}{8}$. 

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