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Boundary Element Analysis of Dielectric Waveguides

by
Tao Lu

A thesis submitted to the Department of Electrical and Computer
Engineering in conformity with the requirements for
the degree of Master of Science

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Abstract

To enhance the performance of integrated optical devices, low modal reflectivities are often required. There are several numerical techniques to calculate the modal reflectivities of such devices. The bidirectional Beam Propagation Method (BPM) is successful for structures with paraxial electric fields and small refractive index differences but is less accurate for wide angle propagation or strongly-guiding structures. The Finite Element Method (FEM) is highly accurate and can treat inhomogeneous and wide angle structures easily, but often requires a fine discretization grid over the entire computational grid. In addition, this method often demands considerable memory and computation time.

In this thesis we consider the application of the Boundary Element Method (BEM) to waveguide calculations. This method is based on solving boundary integral equations by discretizing only boundaries of regions. It requires far less computation time than the Finite Element Method (FEM) and is particularly applicable to piecewise homogeneous optical structures and wide angle field propagation. In addition, it can handle unbounded fields as easily as bounded ones. This technique, however, is not particularly suited to waveguides with continuously varying refractive index distributions, which are generally better analyzed with the FEM. A large number of optical devices, such as rectangular, ridge and rib waveguides, semiconductor lasers, laser amplifiers, optical switches and directional couplers, have piecewise continuous refractive indices. Thus the Boundary Element Method is potentially a powerful tool for the analysis and design of a wide class of integrated optical structures.

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Symbol Notation

Symbol	Definition
$ M_i >$	Vector Presentation of Backward Bounded Mode i
$ R_\gamma >$	Vector Presentation of Backward Radiative Mode γ
$ \Phi >$	Vector Presentation of Reflected Field
$< M_i $	Forward bound propagation mode
$< R_\gamma $	Forward radiating propagation mode
a_i	Amplitude of state $ M_i >$ in $ \Phi >$
B	Magnetic Induction
b_γ	Amplitude of state $ R_\gamma >$ in $ \Phi >$
c	speed of light in vacuum
D	Electric displacement
E	Electric Field Vector
$E_{y }(\mathbf{r})$	E_y component where $\mathbf{n}(\mathbf{r}) \perp \hat{y}$
$E_{y\perp}(\mathbf{r})$	E_y component where $\mathbf{n}(\mathbf{r}) \parallel \hat{y}$
E_x, E_y, E_z	Components of Electric Field
$G^{(i)}(\mathbf{r}, \mathbf{r}')$	Green's function in subregion i
G_l, G_r	Green's function in left/right region
$g_{ij}^{l,r}$	Matrix element of submatrix $G^{l,r}$
H	Magnetic Field Vector
H_x, H_y, H_z	Components of Magnetic Field
$h_{ij}^{l,r}$	Matrix element of submatrix $H^{l,r}$
$I_0(\Theta, l)$	$\frac{1}{4\pi} \int_0^\Theta i_1(\theta) d\theta$

$I'_0(l_1, l_2)$	$I_0(\tan^{-1} \frac{l_2}{l_1}, l_1) + I_0(\tan^{-1} \frac{l_1}{l_2}, l_2)$
$i_1(\theta)$	$\int_0^{\frac{1}{\cos \theta}} \exp(-jkr) dr$
$I_1(\Theta, l)$	$\frac{1}{4\pi} \int_0^\Theta \cos \theta i_2(\theta) d\theta$
$I'_1(l_1, l_2)$	$\frac{1}{l_1} I_1(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_2} I_2(\tan^{-1} \frac{l_1}{l_2}, l_2)$
$i_2(\theta)$	$\int_0^{\frac{1}{\cos \theta}} \exp(-jkr) r dr$
$I_2(\Theta, l)$	$\frac{1}{4\pi} \int_0^\Theta \sin \theta i_2(\theta) d\theta$
$I'_2(l_1, l_2)$	$\frac{1}{l_2} I_2(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_1} I_1(\tan^{-1} \frac{l_1}{l_2}, l_2)$
$i_3(\theta)$	$\int_0^{\frac{1}{\cos \theta}} \exp(-jkr) r^2 dr$
$I_3(\Theta, l)$	$\frac{1}{4\pi} \int_0^\Theta \sin \theta \cos \theta i_3(\theta) d\theta$
$I'_3(l_1, l_2)$	$\frac{1}{l_1 l_2} I_3(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_1 l_2} I_3(\tan^{-1} \frac{l_1}{l_2}, l_2)$
$\mathbf{J}_f$	Free current density
$\mathbf{J}_t$	Total current density
$\mathbf{J}(\eta_1, \eta_2)$	Jacobian matrix
j	$\sqrt{-1}$
j_f	Free surface current density
k	Wave Vector in medium
k_0	Wave Vector in vacuum
L	Length of Fabry-Perot cavity
$\mathbf{M}$	Magnetic polarizability
m	Integer
N_{c1}	Refractive index of Waveguide Cladding Region 1
N_{c2}	Refractive index of Waveguide Cladding Region 2
N_{eff}	Effective Refractive Index
N_g	Refractive index of Waveguide Guiding Region
$\mathbf{n}$	Normal Vector of Boundary
$\mathbf{n}_{12}$	Normal vector of boundary between medium 1 and medium 2
n	Refractive Index
n_{ac}	Refractive Index of AR coating
n_{eff}^i	Effective index of mode i

n_i	Refractive index in subregion i
$\mathbf{P}$	Electric polarizability
P_{min}, P_{max}	Minimum/Maximum Optical Power
$p_n(\theta_1, \theta_2)$	$\int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta+\theta_1)}$
Q'	Electric Quadrupole Moment
R_1, R_2	Reflectivity of first and second facets in Fabry-Perot Cavity
$\mathbf{r}'$	Field Point
$\mathbf{r}$	Observation Point
S_e	Infinitesimal sphere at observation point
SR, SL	Source function in the right/left region
t	Time
t_c	Coating thickness of the waveguide
U	Scalar Potential
U_{e1}, U_{e2}, U_{e3}	Field component on the edges of element e
$U_e(x, y)$	Field distribution in element e
v	speed of light in medium
x, y, z	Axis of Cartesian Coordination
α	Internal Loss
$\alpha_i(x, y), i = 1..3$	Interpolation coefficients of triangular element in FEM
$\alpha_F^{l,r}$	Semi-Vector Coefficient. F can be TE, TM or SC
$\alpha_{SC}^{l,r}$	Semi-Vector Coefficient for Scalar Formalism
$\alpha_{TE}^{l,r}, \alpha_{TM}^{l,r}$	Semi-Vector Coefficient for TE/TM mode
β	Waveguide Propagation Constant
β^i	Propagation constant of mode i
$\gamma, \gamma^{l,r}$	Waveguide Geometry Coefficient
γ^E	Euler Constant
$\Delta f(\mathbf{r})$	Variation of refractive index
Δt	Uncertainty in Coating thickness
ϵ	Dielectric Permittivity

ϵ_0	Vacuum Permittivity
ϵ_r	Relative Permittivity
(η_1, η_2)	Interpolation Coefficient
θ	Angle
λ_0	Wavelength in vacuum
λ	Wavelength in medium
μ	Magnetic Permeability
μ_0	Vacuum Magnetic Permeability
μ_r	Relative Magnetic Permeability
ρ_ϵ	Radius of S_ϵ
ρ_f	Free charge density
ρ_t	Total charge density
σ_f	Free surface charge density
ϕ_k	Interpolation coefficients for the Linear Element BEM
Ω	Solid Angle
ω	Angular Frequency
∇	Differential operator
$\nabla_\perp^2$	$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$

Chapter 1

Introduction

Dielectric waveguides and other optical devices are central components in the rapidly expanding fiber communication industry. As the fabrication of these devices is costly, numerical simulation models are widely applied in the design process. These involve many different approaches to the solution of Maxwell's equations with appropriate boundary conditions. The numerical methods can be generally divided into two groups. The first of these considers the modal field problem in isolation and involves the calculation of the waveguide propagation constants and modal field distributions. The second group models the actual field propagation in a waveguiding structure.

In this thesis we consider the optimization waveguiding structures with low facet reflectivity, which is a problem closest to that of evaluating modal field distributions. Accordingly in this introduction, after a short discussion of the experimental motivation for low reflectivity waveguide coatings, we present a short introduction to the boundary element method, which is the procedure applied for modeling waveguide reflectivities in the remainder of the thesis.

1.1 Advantages of Low Reflectivity Waveguide Coatings

There are several reasons that a low reflectivity is advantageous

- To minimize the impedance mismatch between optical components.

For example, in the coupling of a semiconductor laser to a modulator, the reflected laser output power at the front end of optical modulator downgrades the performance of the laser. This effect is caused by the standing wave pattern that is formed by the reflected output light inside the laser device. This standing wave pattern causes frequency and intensity instabilities in the output power.

- To suppress Fabry-Perot resonance in single pass active devices such as traveling wave amplifiers (TWA) or EDFA.

The gain medium inside these devices amplifies the reflected light and adds noise to the output signal.

- To maximize the output signal.

While of particular interest in, for example, long haul fiber communications where the loss between fiber interconnections limits the transmission distance this topic is not a concern of the present thesis.

1.2 Numerical Evaluation of Reflectivity

Several numerical techniques have been developed to calculate the modal reflectivity of integrate optical structures. In the next chapter, we will briefly review these methods. As discussed later, numerical methods for two dimensional structures are simply formulated, but these are generally not easily extended to three dimensional structures. On the other hand, many techniques for three dimensional numerical techniques require excessive computer memory or computational time for the following reasons.

- If the optical wavelength is small compared to the device size a fine discretization grid must be employed.
- Unlike metallic waveguides, dielectric waveguides are open and the electric fields can spread out of the guiding region. Thus artificial boundary conditions must

either be placed in the cladding region or the discretization region must be sufficiently large that the fields are effectively zero at the boundary. Those two methods either reduce the accuracy of the result or increase the computational requirements of the numerical technique.

1.3 Boundary Element Method (BEM)

The numerical method on which this thesis is based is labeled the boundary element method. The efficiency of this procedure in our applications rests on the observation that most dielectric waveguides have a piece wise homogeneous refractive index profile to construct efficient techniques for the calculation of modal reflection. We can then calculate the electric field of the waveguide by considering each homogeneous volume and integrating over the electrical field along boundary with the aid of the numerical Boundary Element Method (BEM).

Historically, this method dates back to 1903 when Fredholm demonstrated the existence of solutions to fundamental boundary value problems. The first detailed discussion of the BEM did not however appear until in 1963 when Jaswon [1] and Symm [2] presented a numerical technique to solve boundary integral equations. With the development of modern computer technology, the BEM has found increasing application in mechanics where it was pioneered by Brebbia [3] in the late 70s and early 80s. The method has recently been frequently used to solve microwave problems in metallic and subsequently optical waveguides. In the optical domain, the BEM has been applied to dielectric waveguide scattering problems[4] as well as Fresnel propagation problems[5]. In this thesis, the author will apply the BEM to the optimization of the modal reflectivity of dielectric waveguides with respect to the properties of a dielectric coating at their end facet.

The BEM is based on the assumption that the waveguide is piecewise homogeneous and that the field distribution inside a homogeneous waveguide region can be related to the field on the waveguide boundaries through an appropriate Green's function. Thus,

instead of discretizing the entire problem region, only the region boundaries need to be considered as elements. By integrating the Helmholtz equation on the boundary of these regions and applying certain boundary conditions, the fields on the boundary nodes form a $(2N \times 2N)$ linear system

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (1.1)$$

where $\mathbf{V}$ is a vector of the field distribution and its directional derivative on the boundary nodes and $\mathbf{S}$ is the source function. The matrix $\mathbf{H}$ is highly banded and the system is much smaller than that in FD-TD and FEM method discussed subsequently in Chapter 2. As a result, the BEM is often a particularly fast and efficient algorithm. For example, unlike the FD-TD algorithm, an exact boundary condition can in many cases be employed for the open boundary problem as the Green's function can be computed exactly so that a fictitious boundary layer is not required. Further, unlike the BPM algorithm, the BEM can be immediately applied to arbitrarily wide angle problems. Unfortunately, as noted earlier, the BEM can be difficult to apply if the waveguide does not have a piece wise homogeneous refractive index profile, although there is considerable interest in integrating the procedure with other numerical techniques to extend its applicability to general profiles.

1.4 Contributions of the Thesis

This section outlines the contributions of the author to the work described in this thesis.

- A Boundary Element Method (BEM) is introduced for dielectric waveguides. Constant and linear boundary element algorithms are applied for both the two and three dimensional cases. In the three dimensional case, we consider both triangular and quadrilateral discretization and present a series solution for the diagonal elements that greatly improves the accuracy of the BEM. The author then extends the scalar formalism to the more accurate semi-vectorial formalism.
- A new recursive procedure is further presented which would evaluate some of the integrals encountered in the implementation of the BEM.

- Matlab programs are developed for the two dimensional constant element and linear element boundary element methods. With the aid of these programs, two dimensional integrate optical structures are analyzed. The program can be used to evaluate the modal reflectivity as well as the electric fields inside the dielectric waveguides and can also be used to generate the E-M modal field profile given the propagation constant of a specific mode.
- A C++ program based on the constant element algorithm is presented for the three dimensional case. This program is based on a sparse matrix library splib++.

1.5 Organization of the thesis

The outline of this thesis is as follows: In the first chapter, the author introduces the thesis. Chapter 2 provides a review of Dielectric waveguide analysis methods. Chapter 3 presents three dimensional BEM while Chapter 4 presents the two dimensional case. In this thesis, the author presents 3-D BEM first since 2-D BEM can be considered as a special case of the 3-D theory. BEM Algorithms based on both the constant and linear element algorithms are presented for both the scalar and semi-vectorial fields. Chapter 5 examines the implementation of BEM while Chapter 6 and Chapter 7 apply it to several two and three dimensional dielectric waveguides. The reflection is here examined for waveguides with both coated and uncoated end facets. As well, we discuss the accuracy of the BEM results compared to those of other numerical techniques and we perform a formal error analysis. Finally, conclusions are presented in Chapter 8.

Chapter 2

Dielectric Waveguide Analysis Methods

This chapter outlines basic waveguide analysis methods with emphasis on numerical methods to evaluate reflectivity. It begins by describing basic dielectric waveguide structures in Section 2.1. Section 2.2 and 2.3 then describe the fabrication of AR coating and reflection measurement devices. In Section 2.4, basic wave propagation theory is introduced together with a discussion of the Maxwell's equations and its continuity relations, the Helmholtz equation, normal modes and modal reflectivity. Section 2.5 reviews the existing numerical techniques such as the beam propagation method (BPM), finite-difference time-domain method (FD-TD), and finite element method (FEM).

2.1 Dielectric Waveguides

In this section we introduce the waveguides with which the thesis is concerned. These are the two dimensional slab waveguides discussed in Section 2.1.1 followed by three dimensional rectangular, rib and ridge waveguide structures which are introduced in Section 2.1.2.

Figure 2.1: Illustration of two dimensional step-index slab waveguide

2.1.1 Two Dimensional Slab Waveguide

We examine first the two dimensional step-index slab waveguide shown in Fig. 2.1. This waveguide has a discontinuous refractive index profile such that the guiding region with refractive index N_g is sandwiched between cladding layers with refractive indices N_{c1} and N_{c2} . We assume that both the refractive index profile and the E-M fields are invariant along the y axis. If the cladding regions have equal values of the refractive index (i.e $N_{c1} = N_{c2}$), the waveguide is called symmetrical, otherwise it is called asymmetrical. In order for a waveguide to guide electrical waves, the refractive index, N_g , in its guiding region must be higher than in the cladding regions. A two dimensional slab waveguide usually serves as a simplified model of a three dimensional waveguide structure. This results in a considerable reduction in computing time and computer memory requirements. Another benefit from two-dimensional methods is that the guided modes and the modal reflectivities can often be obtained analytically, permitting the simple estimation

Figure 2.2: Three dimensional dielectric waveguide examples: (A) Rectangular Waveguide (B) Rib Waveguide (C) Ridge Waveguide

of the accuracy of numerical reflection techniques.

2.1.2 Three Dimensional Waveguides

In this subsection, we discuss three dimensional dielectric waveguide structures. Commonly used three dimensional dielectric waveguides include rectangular dielectric waveguides, dielectric strip waveguides, rib waveguides, strip loaded waveguides and ridge waveguides. In this thesis, we consider the modal reflectivities of the three waveguide structures shown in Figure 2.2. These are

- Rectangular Waveguides

In a rectangular waveguide, the rectangularly shaped guiding region forms a buried structure in the cladding region. Some semiconductor laser amplifiers and buried heterostructure lasers can be approximated by this model. Although theoretically easy to analyze, such waveguides are relatively difficult to fabricate. We thus employ this waveguide profile solely to verify the accuracy of our numerical technique.

- Rib Waveguides

In a rib waveguide[6]-[11], the lateral confinement of light is achieved by changing the shape of the guiding region. The lateral guiding mechanism can be well modeled by the effective index method (EIM). Physically, the effective index of the guiding region depends on the thickness of the guiding layer. The thicker the guiding layer, the higher the value of the effective index. Therefore the light is confined to the center of the guiding region.

Rib waveguides are relatively simple to fabricate and are widely used in most passive integrate optical structures as they can be designed to exhibit low bending losses. Accordingly many of electro-optic devices such as Mach-Zehnder modulators, directional couplers, etc. are implemented using this type of waveguide profile.

- Ridge Waveguides

These are used in active devices such as the traveling wave laser amplifiers (TWA) and multiquantum well lasers. Ridge waveguides operate similarly to rib waveguides except that the lateral confinement of light is achieved in the cladding region instead of the active region thus enabling a thin active layer. A rib layer is formed either above or below the active layer to guide the electromagnetic field in the transverse direction.

2.2 Techniques to Minimize Modal Reflectivity

Two techniques are commonly employed to minimize the reflectivity at end-facets [12]. In the first case, an anti-reflection coating is applied and in the second case the facet is tilted with respect to the propagation axis. This section will address the principles of both methods.

2.2.1 Anti-Reflection (AR) Coating

Anti-reflection coatings are commonly applied to a wide range of optical structures such as cameras and eyeglasses and are used in waveguides as well [13]. The coating is based on the destructive interference of the reflected waves from the front and end facets of the coating to suppress the modal reflectivity. Usually it is desirable to use multi-layer coatings to achieve lower reflectivity and larger dynamic range. AR coatings can be deposited on waveguide by methods like electron cyclotron resonance (ECR) plasma chemical vapor deposition (CVD) method [14]-[16].

In Fig. 2.3 we display the ECR Plasma CVD unit used at NORTEL to generate AR coatings such as those considered in this thesis. In this apparatus, a $2.45GHz$ microwave power source is introduced into the plasma chamber that contains the reactive gases through a rectangular microwave waveguide that enters the chamber at a quartz plate window. This source excites a plasma in the chamber, which is $20cm$ in diameter and $20cm$ in height and forms a microwave cavity resonator. To obtain the desired chemically active species in the plasma, the plasma is further bombarded by electrons. To reduce the collision of the electrons with chamber walls and thus increase their average life time, a longitudinal static current is induced in electro-magnetic coils that are placed around around the chamber. This static field causes the electrons to rotate in helixes along the chamber axis and thus decreases the chance of recombination on the chamber wall. The reactive gases used to generate the SiO_2 coating are introduced through two respective inlets into the plasma chamber (O_2, N_2) and specimen chamber (SiH_4).

ECR plasma CVD has several advantages:

Figure 2.3: Electron Cyclotron Resonance (ECR) Plasma Chemical Vapor Deposition (CVD)

- **Low Temperature.** Unlike other coating techniques, which require temperatures above 700°C [17], the ECR process is carried out at temperatures less than 120°C , thereby avoiding thermal damage to the waveguide.
- **Low Energy.** Since the ion energies in the plasma are typically less than 40eV , bombardment damage to the waveguide facet is minimized. Other similar processes require ion energies that are higher than 300eV and they introduce more damage to the device.
- The deposited AR-coating is stable and displays a minimal drift of refractive index over time.

The uncertainties in the experimentally predicted refractive index and coating thickness for AR-films deposited by ECR are estimated to be $\Delta n = \pm 0.01$ and $\Delta t = \pm 61\text{\AA}$, respectively.

2.2.2 Tilted End Facets

Often the end facets of waveguide devices are tilted by an angle with respect to the propagation axis [18]-[19]. This decreases the reflected power which is coupled back opposite to the direction of propagation and thus avoids Fabry-Perot resonances as well. In practice, tilted facets are usually combined with AR coating to further minimize modal reflection.

2.3 Reflection Measurements

There are several methods to experimentally measure waveguide reflections in both the time-domain and the frequency-domain. These methods include time domain pulse train measurements, time domain modulation procedures, time domain low coherence measurements, the cut-back method and reflection measurements in Fabry-Perot cavities [20]-[24]. This section provides a brief description of the Fabry-Perot method[25].

Fabry-Perot measurements employ the fact that the end facets of the waveguide form the parallel mirrors of a Fabry-Perot cavity. Provided that the loss is known, the reflectivity can be determined from the fringe visibility. Assuming an internal loss α and a cavity length L we have

$$\frac{P_{min}}{P_{max}} = \frac{(1 - Re^{-\alpha L})^2}{(1 + Re^{-\alpha L})^2}. \quad (2.1)$$

In the above equation, P_{min} and P_{max} are the minimum and maximum optical power in the fringe while $R = \sqrt{R_1 R_2}$ where R_1, R_2 are the reflectivities for both facets. R is the reflectivity provided that $R_1 = R_2$. By measuring the optical power extrema we can therefore find the reflectivity.

The experimental setup for the reflection measurement constructed at NORTEL to measure end facet reflectivities is shown in Figure 2.4. In this realization, a DFB laser is provided as the light source. The output wavelength varies with the temperature of the laser. The laser is initially cooled to $5.0^\circ C$ and is then allowed to relax to room temperature, providing a wavelength scan of around $1.55\mu m$. The output beam is divided at a power splitter such that 10% of the power is sampled by the detector as a

Figure 2.4: Reflection measurement by Fabry-Perot apparatus

feedback controller to stabilize the output power. The rest of the power passes through the polarizer and it illuminates the sample waveguide through a fiber. The transmitted power is then collimated and modulated by a chopper. 90% of the modulated signal is detected, pre-amplified, lock-in amplified, A/D converted and fed into a computer. The computer collects the data and prints out the reflectivity according to Equation 2.1.

2.4 Basics of Electromagnetic Theory

This section provides brief background knowledge of electromagnetic theory. We start from Maxwell's Equations and briefly discuss the continuity relations. We also review Helmholtz equation and basic waveguide theory.

2.4.1 Maxwell's Equations and Continuity Relations

The Maxwell's equations in a vacuum are [26]

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (2.2)$$

$$\nabla \times \mathbf{B} = \mu_0(\mathbf{J}_t + \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}) \quad (2.3)$$

$$\nabla \cdot \mathbf{E} = \frac{\rho_t}{\epsilon} \quad (2.4)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.5)$$

in which $\mathbf{E}$ is the electric field and $\mathbf{B}$ is the magnetic field, ρ is the total charge density and $\mathbf{J}$ is the total current density. ϵ_0 is the vacuum dielectric permittivity and μ_0 is the vacuum permeability. In the presence of macroscopic media, Maxwell's Equations are reformulated in terms of the four fields $\mathbf{E}$, $\mathbf{D}$, $\mathbf{B}$, $\mathbf{H}$ defined by

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} - \sum_j \frac{\partial Q'_{\alpha j}}{\partial x_j} + \dots \quad (2.6)$$

$$\mathbf{H} = \frac{\mathbf{B}}{\mu_0} - \mathbf{M} + \dots \quad (2.7)$$

In this expression $\mathbf{E}$, $\mathbf{B}$ represent the average over the microscopic fields. $\mathbf{D}$ is the electric displacement and $\mathbf{H}$ is the magnetic field. $\mathbf{B}$ is then called the magnetic induction. $\mathbf{P}$

is the electric polarizability and $\mathbf{M}$ is the magnetic polarizability. These are first order response of the material to the E-M field. $\mathbf{Q}'$ is the electric quadrupole tensor and is related to the second order response of the medium. The macroscopic Maxwell's Equations then become

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad (2.8)$$

$$\nabla \times \mathbf{H} = \mathbf{J}_f + \frac{\partial \mathbf{D}}{\partial t} \quad (2.9)$$

$$\nabla \cdot \mathbf{D} = \rho_f \quad (2.10)$$

$$\nabla \cdot \mathbf{B} = 0 \quad (2.11)$$

In the above equation, ρ_f is free electric charge density, and $\mathbf{J}_f$ is the free electric current density. In a dielectric medium, the following assumptions can be made

- **Linear**

We first neglect quadrupole and higher order terms in Equations (2.6) and (2.7) so that

$$\mathbf{D} = \epsilon_r \epsilon_0 \mathbf{E} \quad (2.12)$$

$$\mathbf{B} = \mu_r \mu_0 \mathbf{H} \quad (2.13)$$

where ϵ_r is the relative permittivity and μ_r is relative permeability. Generally ϵ_r , μ_r are first order tensors or 3×3 matrix with (i, j) component representing the material response to the x_j field component at x_i direction.

- **Isotropic**

In an isotropic medium, ϵ_r and μ_r are scalars. We then define $\epsilon_r = n^2$, where n is called refractive index.

- **Nonmagnetic**

In a non-magnetic medium $\mathbf{M} = 0$, which leads to $\mu_r = 1$.

- **Charge and Current free**

Assuming that there is no free charge and current in the dielectric media as well on the media boundary we have $\rho_f = 0$, $\mathbf{J}_f = 0$.

Under the above assumptions the Maxwell's Equations become

$$\begin{aligned}\nabla \times \mathbf{E} &= -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \\ \nabla \times \mathbf{H} &= \epsilon_0 \frac{\partial n^2 \mathbf{E}}{\partial t} \\ \nabla \cdot (n^2 \mathbf{E}) &= 0 \\ \nabla \cdot \mathbf{H} &= 0\end{aligned}\tag{2.14}$$

Further, for a monochromatic electric field distribution.

$$\mathbf{E} = \mathbf{E}(\mathbf{r})e^{-j\omega t}\tag{2.15}$$

$$\mathbf{H} = \mathbf{H}(\mathbf{r})e^{-j\omega t}\tag{2.16}$$

results in the time-independent Maxwell's equations

$$\nabla \times \mathbf{E} = j\sqrt{\frac{\mu_0}{\epsilon_0}}k_0\mathbf{H}\tag{2.17}$$

$$\nabla \times \mathbf{H} = -j\sqrt{\frac{\epsilon_0}{\mu_0}}k_0n^2\mathbf{E}\tag{2.18}$$

$$\nabla \cdot (n^2 \mathbf{E}) = 0\tag{2.19}$$

$$\nabla \cdot \mathbf{H} = 0\tag{2.20}$$

Here $k_0 = \omega/c = \omega\sqrt{\mu_0\epsilon_0}$ is the wavevector of the E-M wave travelling the vacuum while $k = nk_0$ is the corresponding wavevector in the material.

At the boundary of two different dielectric media 1 and 2, the continuity relations can be derived by applying Stokes theorem to the first two Maxwell's Equations and Gauss Theorem to the last two equations [26]. This leads to

$$\begin{aligned}\mathbf{n}_{12} \cdot (\epsilon_2 \mathbf{E}_2 - \epsilon_1 \mathbf{E}_1) &= \sigma_f \\ \mathbf{n}_{12} \times (\mathbf{E}_2 - \mathbf{E}_1) &= 0 \\ \mathbf{n}_{12} \cdot (\mathbf{H}_2 - \mathbf{H}_1) &= 0 \\ \mathbf{n}_{12} \times (\mathbf{H}_2 - \mathbf{H}_1) &= \mathbf{j}_f\end{aligned}\tag{2.21}$$

where $\mathbf{n}_{12}$ is the normal vector from the interface directed from medium 1 to medium 2, σ_f is surface free charge density and j_f is surface free current density. In dielectric media, each of these quantities are zero.

2.4.2 Helmholtz's Equation

Maxwell's Equations lead to Helmholtz equation for any of the ($\mathbf{E}, \mathbf{H}$) components by taking the curl of the first two equations in Equations (2.17) and (2.18) and applying

$$\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \quad (2.22)$$

where $\mathbf{A}$ can be either $\mathbf{E}$ or $\mathbf{H}$. Hence,

$$\begin{aligned} \nabla \times \nabla \times \mathbf{E} &= j\sqrt{\frac{\mu_0}{\epsilon_0}}k_0 \nabla \times \mathbf{H} \\ \nabla(\nabla \cdot \mathbf{E}) - \nabla^2 \mathbf{E} &= n^2 k_0^2 \mathbf{E} \end{aligned} \quad (2.23)$$

From Maxwell's Equation (2.19) we then obtain

$$(\nabla n^2) \mathbf{E} + n^2 \nabla \cdot \mathbf{E} = 0 \quad (2.24)$$

$$\nabla \cdot \mathbf{E} = -\nabla \ln n^2 \mathbf{E} \quad (2.25)$$

Substituting the above expression into Equation (2.23) we have

$$\nabla^2 \mathbf{E} + n^2 k_0^2 \mathbf{E} = -\nabla(\nabla \ln n^2 \mathbf{E}) \quad (2.26)$$

$$= (\nabla \times \mathbf{E}) \times \nabla \ln n^2 - (\nabla \ln n^2 \cdot \nabla) \mathbf{E} - (\mathbf{E} \cdot \nabla) \ln n^2 \quad (2.27)$$

Similarly

$$\nabla^2 \mathbf{H} + k^2 \mathbf{H} = (\nabla \times \mathbf{H}) \times \nabla \ln n^2 \quad (2.28)$$

where the refractive index profile can be expressed as

$$n(\mathbf{r}) = n_0(1 + \Delta f(\mathbf{r})) \quad (2.29)$$

For weakly guided waveguides $\Delta f(\mathbf{r}) \ll 1$, thus we obtain the scalar Helmholtz equation

$$\begin{aligned} \nabla^2 \mathbf{E} + n^2 k_0^2 \mathbf{E} &= 0 \\ \nabla^2 \mathbf{H} + n^2 k_0^2 \mathbf{H} &= 0 \end{aligned} \quad (2.30)$$

2.4.3 Normal Modes and Modal Reflectivity

The normal modes of a z -independent dielectric waveguide propagate according to

$$\begin{aligned} \mathbf{E}(x, y, z) &= \mathbf{E}(x, y) \exp(j\beta z) \\ \mathbf{H}(x, y, z) &= \mathbf{H}(x, y) \exp(j\beta z) \end{aligned} \quad (2.31)$$

For these modes, Maxwell's equations reduce to

$$\begin{aligned} \frac{\partial E_z}{\partial y} - j\beta E_y &= j\omega\mu H_x \\ j\beta E_x - \frac{\partial E_z}{\partial x} &= j\omega\mu H_y \\ \frac{\partial H_z}{\partial y} - j\beta H_y &= -j\omega\epsilon E_x \\ j\beta H_x - \frac{\partial H_z}{\partial x} &= -j\omega\epsilon E_y \end{aligned} \quad (2.32)$$

If we rearrange the equations above, we can express the transverse field components in terms of the longitudinal components

$$\begin{pmatrix} H_x \\ E_y \end{pmatrix} = \frac{1}{\beta^2 - k^2} \begin{pmatrix} j\omega\epsilon & -j\beta \\ -j\beta & j\omega\mu \end{pmatrix} \begin{pmatrix} \frac{\partial E_z}{\partial y} \\ \frac{\partial H_z}{\partial x} \end{pmatrix} \quad (2.33)$$

$$\begin{pmatrix} E_x \\ H_y \end{pmatrix} = -\frac{1}{\beta^2 - k^2} \begin{pmatrix} j\omega\mu & j\beta \\ j\beta & j\omega\epsilon \end{pmatrix} \begin{pmatrix} \frac{\partial H_z}{\partial y} \\ \frac{\partial E_z}{\partial x} \end{pmatrix} \quad (2.34)$$

Therefore we need only consider the two fields (H_z, E_z) in Maxwell's equations. These can be obtained from the Helmholtz Equations by applying proper boundary conditions.

In the two dimensional case, all fields are invariant along the y direction, that is,

$$\frac{\partial E_z}{\partial y} = 0 \quad (2.35)$$

$$\frac{\partial H_z}{\partial y} = 0 \quad (2.36)$$

We then obtain two sets of orthogonal fields in the waveguides,

$$\begin{pmatrix} H_x \\ E_y \end{pmatrix} = \frac{1}{\beta^2 - k^2} \begin{pmatrix} -j\beta \\ j\omega\mu \end{pmatrix} \frac{\partial H_z}{\partial x}; \quad \begin{pmatrix} E_x \\ H_y \end{pmatrix} = 0 \quad (2.37)$$

where we assume $E_z = 0$ and

$$\begin{pmatrix} E_x \\ H_y \end{pmatrix} = -\frac{1}{\beta^2 - k^2} \begin{pmatrix} j\beta \\ j\omega\epsilon \end{pmatrix} \frac{\partial E_z}{\partial x}; \quad \begin{pmatrix} H_x \\ E_y \end{pmatrix} = 0, \quad (2.38)$$

where we assume $H_z = 0$, namely *Transverse Electric (TE)* modes and *Transverse Magnetic (TM)* modes. In accordance with their names, *TE* modes do not have a longitudinal electric field component E_z , and thus only (E_y, H_x, H_z) fields exist in the waveguide. Similarly, *TM* modes only support (H_y, E_x, E_z) field components. In a two dimensional waveguide, the *TE* mode and *TM* mode are separable. Unlike two dimensional waveguides, three dimensional structures do not support pure TE or TM modes unless they are formed by a series of quasi-two dimensional layers. The modes are instead classified into two types depending on the polarization direction of the electric field. If $H_z > E_z$, it is called HE mode, otherwise the mode is an EH mode. If the main component of the electric field lies in the y direction, the mode is called a quasi-TE mode. If E_x is the main component of the electric field, the mode is called quasi-TM mode.

Generally there are an infinite number of independent normal modes in dielectric waveguides with distinct propagation constants β . The mode with the largest value of β is called the fundamental mode. A waveguide that can only support one guided mode is called a single mode waveguide. Several modes may be degenerate and possess the same propagation constant. Modes can be grouped into guided modes and radiation modes. Guided modes are discrete and are confined to the waveguide. Radiative modes have a continuous spectrum. Since the waveguide modes form a complete orthogonal set, any field can be expressed as a linear combination of these modes.

When an E-M wave propagates across the interface of two different media, part of its energy is reflected into the reverse direction. The modal reflectivity measures the ratio of the power reflected into the backward mode to the power of the incoming mode [20]. Active optical devices such as lasers and optical amplifiers generally require minimal external feedback caused by reflection to exhibit optimal performance under modulation. Consider reflection from a waveguide end-facet and define $|\Phi\rangle$ as the reflected field to be calculated, $|M_i\rangle$ as the i -th guided mode and $|R_\gamma\rangle$ as the γ -th radiative mode. Both $|M_i\rangle$, $|R_\gamma\rangle$ propagate in the reverse direction along the waveguide axis and are thus called backward propagating modes, while their complex

conjugates $\langle M_i |$ and $\langle R_\gamma |$ are forward propagation modes. We can express the reflected field in terms of the backward propagating modes as

$$|\Phi\rangle = \sum_{i=0}^k a_i |M_i\rangle + \sum_{\gamma=0}^{\infty} b_\gamma |R_\gamma\rangle \quad (2.39)$$

where $\sum_\gamma$ should be understood as an integration over the continuous spectrum. If we launch the input field $\langle M_j |$ and obtain a reflected $|\Phi^j\rangle$, then

$$a_k^j = \langle M_k | \Phi^j \rangle \quad (2.40)$$

is the modal reflection coefficient, where $|a_k^j|^2$ refers to the energy coupled to the k -th backward mode when excited with j -th mode. To derive the above equation, we have employed the orthogonality of the mode set $|M_k\rangle$ which gives

$$\langle M_j | M_k \rangle = \delta_{jk}. \quad (2.41)$$

In this thesis, unless otherwise specified, modal reflectivity refers to the reflectivity of the fundamental mode a_0^0 .

2.5 Numerical Techniques for Waveguide Problems

Recently, several computational techniques have been suggested in integrated optical structures[27],[28]. These include the Beam Propagation Method (BPM) [29]-[44], Time-Domain Finite Difference method (TD-FD) [45]-[55], Fast Fourier Transform method (FFT), Finite Element method (FEM) [56]-[59] and Boundary Element Method (BEM) [3]-[5], [46], [50], [55], [60]-[90]. In this thesis we will focus on the BEM, which can be considered as a special case of the FEM. The BEM is particularly efficient if the device under study has a piecewise homogeneous refractive index profile and is also amenable to large-angle reflection. The results are found to be in excellent agreement with other computational methods and the procedure is additionally found to be highly computationally efficient.

2.5.1 Effective Index Method (EIM)

The Effective Index Method approximates a three-dimensional dielectric waveguide by an equivalent two-dimensional model. The method is simple, fast and efficient but is not always sufficiently accurate. It divides the three-dimensional waveguide into several subregions along the transverse, $\hat{x}$ direction, each with refractive index that is invariant along that direction. By assuming each sub-waveguide i to be infinite along the $\hat{x}$ direction and applying conventional two-dimensional waveguide theory, approximate propagation constants β^i for the lowest-order electric field distribution guided by the transverse refractive index profile within each segment can be determined. The system is then modeled by a refractive profile that is invariant along the $\hat{y}$ direction and in which the refractive index of each subregion is replaced by the two-dimensional transverse effective indices $n_{eff}^i = \frac{\beta^i}{k_0}$ in each subregion. Again applying conventional two-dimensional waveguide analysis to this effective refractive index profile, we find the propagation constant β and approximate electric field distribution of the waveguide mode. This information can then be used to compute the reflectivity in the (x, z) plane using an effective index model of the refractive index profiles at both sides of the end facet.

Although the above method is described in step-index waveguide, it is equally valid for waveguides with any refractive index profile. To extend it to the generic case, however, the waveguide must first be discretized along the $\hat{x}$ direction and the propagation constant determined numerically for each of the sections. The resulting two dimensional model is then analyzed numerically.

2.5.2 Beam Propagation Method (BPM)

The Beam Propagation Method (BPM) is suitable for paraxial propagation problems. The starting point for the formalism is the Helmholtz equation (2.30),

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + k_0^2 n^2(x, y, z)\right)U(x, y, z) = 0 \quad (2.42)$$

where U can be any field component. Since the field of interest propagates along the optical axis z , this field component can be approximated as

$$U(x, y, z) = a(x, y, z) \exp(-jk_0 n_0 z) \quad (2.43)$$

where n_0 is the reference refractive index chosen such that $a(x, y, z)$ varies slowly along the z axis. Substitute the above expression into the Helmholtz equation yields

$$-\frac{\partial^2 a}{\partial z^2} + 2jk_0 n_0 \frac{\partial a}{\partial z} = (k_0^2(n^2 - n_0^2) + \nabla_\perp^2) a \quad (2.44)$$

Ignoring the second derivative with respect to z , leads to the Fresnel parabolic wave equation

$$\frac{\partial a}{\partial z} = \frac{1}{2jk_0 n_0} (k_0^2(n^2 - n_0^2) + \nabla_\perp^2) a \quad (2.45)$$

A numerical solution of this equation can be written as

$$\begin{aligned} a(x, y, z + \delta z) = & \exp\left(-\frac{j\delta z}{4k_0 n_0} \nabla_\perp^2\right) \exp\left(\int_z^{z+\delta z} -\frac{jk_0 n_0}{2} \left(\frac{n^2(x, y, z')}{n_0^2} - 1\right) dz'\right) \\ & \exp\left(-\frac{j\delta z}{4k_0 n_0} \nabla_\perp^2\right) a(x, y, z) + O(\delta z^3) \end{aligned} \quad (2.46)$$

This equation is employed to simulate the propagation of an optical field from z to $z + \delta z$. Solving the equation iteratively using either the split-step Fast Fourier Transform Beam Propagation Method (FFTBPB) or the split-operator finite difference method thus models the field evolution down the waveguide. Generally the latter of these procedures is more computationally efficient.

The BPM is far more efficient than either the TDFD and FEM and applies to arbitrary refractive index. However, the solution is less accurate especially for wide angle structures where the fresnel approximation fails.

2.5.3 Time-Domain Finite Difference Method (TD-FD)

The Time-Domain Finite Difference (TD-FD) method evaluates the full time dependent Maxwell's Equation in a discretized form. The waveguide is discretized into an N -point grid and the differential operator ∇ is expressed in discrete form. Starting from the initial field distribution, time evolution is then simulated by directly integrating the discretized Maxwell's equations from from $t = m$ to $t = m + 1$.

The TD-FD is one of the most versatile method to simulate three dimensional waveguide problems as no approximations are required except for that associated with the problem discretization. Also it is advantageous to solve time dependent problems such as pulse chirping in rapidly modulated laser sources. However, to discretize the full three dimensional structure requires considerable memory size and computational time. In addition, to avoid unphysical reflection at the computational window boundary, suitable absorbing boundary conditions must be applied. This is typically the problem we encounter in most other numerical methods except BEM. These limitations effectively restrict the applicability of the method to small-scale waveguide problems.

2.5.4 Finite Element Method (FEM)

The Finite Element Method is one of the most powerful methods in the area of numerical computation. Although first introduced by Courant [91] in the early 1940s, this method was not applied to electromagnetic problems until 1968. Since then, its applicability to optical waveguide problems has been established by many authors.

In the finite-element method the problem region is discretized into discrete finite elements. The vertices of the elements are called nodes. While the elements can be of any shape, they are generally triangular in two-dimensions and pyramids in three-dimensions. The field component in an element e is associated with the field component on the vertices of that element through a given interpolation (shape) function.

Accordingly, in two dimensions, the field component is expressed as

$$U_e(x, y) = \alpha_1(x, y)U_{e1} + \alpha_2(x, y)U_{e2} + \alpha_3(x, y)U_{e3} \quad (2.47)$$

where U_e is the field component inside element e and U_{ei} is the field component on the i -th vertex node of the element. α_i is the associated shape (or interpolation) function. By inserting the electric field expressed in terms of the $U_e(x, y)$ into Maxwell's Equations, each nodal field component can be expressed as the contribution from all discrete elements in the problem region. Constructing $\vec{U} = (U_1, U_2 \dots U_N)^T$ where U_i is

the field component on node i , we obtain an $(N \times N)$ linear system given by

$$\mathbf{C}\vec{U} = \mathbf{S} \quad (2.48)$$

In this equation, $\mathbf{S}$ is a source function due to the contribution of the external source. Solving this system numerically yields the field distribution $\vec{U}$, in the waveguide. Unfortunately, the matrix $\mathbf{C}$ is dense compared to TD-FD. Further, the entire problem region must be discretized which leads to large resource requirements. In addition, open boundaries are somewhat difficult to implement.

2.6 Conclusions

In this chapter, our the boundary element method was introduced. In particular, we have described the basics of dielectric waveguide structures, electromagnetic theory and some competing methods for solving the electric field propagation problems and some modal reflectivities. While the next chapters are devoted to the boundary element method, it is important to consider that this procedure is only particularly efficient for refractive index structures that do not have a substantial continuous transverse variation of their refractive index. Thus the methods outlined above as well as various approximate techniques have their particular region of applicability and should be understood in greater detail by serious practitioners in the guided-wave optics field.

Chapter 3

Three Dimensional BEM Method

3.1 Introduction

This chapter presents the theory of the three dimensional Boundary Element Method (BEM). We first derive the matrix representation of the Green's equation and we briefly review Green's theorem in Section 3.2. In Section 3.3, we derive and apply the Boundary Element Method to a dielectric waveguide. Section 3.4 and Section 3.5 discuss the scalar and semi-vector BEM formalisms respectively. In Section 3.6 we develop the constant element BEM algorithm, which is based on the assumption of uniform field distribution over a single discretized cell. The algorithm is based on a series solution for the diagonal matrix element, which makes our version of the algorithm accurate and efficient. In Section 3.7, we study the linear element algorithm and as in the case of constant elements, we develop the series solution for the diagonal matrix elements. In both algorithms, we consider two different computational meshes, namely a quadrilateral and a triangular mesh and present the matrix elements for both cases. In section 3.8 and section 3.9, we derive the recursive solution for the frequently used integral p_n and its convergence property. The conclusions of the chapter are presented in Section 3.10.

Figure 3.1: Cross section of integration region V in Green's Theorem. S is the surface boundary, A is the observation point. B is a singular point on surface. C is a hole in V

3.2 Boundary Element Method

The Green's Theorem is a direct consequence of the Divergence Theorem of Gauss [92].[93] The divergence theorem is given by

$$\int_V \nabla \cdot \mathbf{A} d\tau = \oint_S \mathbf{A} \cdot \mathbf{n} ds \quad (3.1)$$

where as in Figure 3.1, volume V is singly connected and bounded by the closed surface S , $\mathbf{n}$ is the normal vector of S directed outward. $\mathbf{A}$ can be any well-behaved vector field inside V , where a well-behaved vector has continuous first and second partial derivatives on the surface and throughout region V . The $\int_V d\tau$ operator is a volume integral over the region V and $\oint_S ds$ is the area integral on that surface. Also, two arbitrary scalar fields ϕ, ψ follow

$$\begin{aligned} \nabla \cdot (\phi \nabla \psi) &= \phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi \\ \nabla \cdot (\psi \nabla \phi) &= \psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi \end{aligned} \quad (3.2)$$

and the definition of the gradient

$$\phi \nabla \psi \cdot \mathbf{n} = \phi \frac{\partial \psi}{\partial n} \quad (3.3)$$

$$\psi \nabla \phi \cdot \mathbf{n} = \psi \frac{\partial \phi}{\partial n} \quad (3.4)$$

Replacing $\mathbf{A}$ in (3.1) with $\phi \nabla \psi$ and $\psi \nabla \phi$, using equation (3.2), we get

$$\int_V (\phi \nabla^2 \psi + \nabla \phi \cdot \nabla \psi) d\tau = \oint_S \phi \frac{\partial \psi}{\partial n} ds \quad (3.5)$$

$$\int_V (\psi \nabla^2 \phi + \nabla \psi \cdot \nabla \phi) d\tau = \oint_S \psi \frac{\partial \phi}{\partial n} ds \quad (3.6)$$

Subtracting the two equations above leads to Green's second identity or Green's theorem.

$$\int_V (\phi \nabla^2 \psi - \psi \nabla^2 \phi) d\tau = \oint_S [\phi \frac{\partial \psi}{\partial n} - \psi \frac{\partial \phi}{\partial n}] ds \quad (3.7)$$

Consequently once we know ϕ, ψ and their directional derivatives on the boundary surface, the volume integral in the form of (3.7) can be simplified into a surface integral.

3.3 Application to Guided-Wave Optics

In this section, we apply Green's Theorem to the electromagnetic wave propagation problem in dielectric waveguides. In a homogeneous dielectric medium, any field component of $(\mathbf{E}, \mathbf{H})$ satisfies the scalar Helmholtz equation. Denoting the coordinate of the field point by $\mathbf{r}'$ and the observation point by $\mathbf{r}$ (Figure 3.1), the scalar Helmholtz equation is

$$\nabla'^2 U(\mathbf{r}') + n(\mathbf{r}')^2 k_0^2 U(\mathbf{r}') = 0 \quad (3.8)$$

Here $U(\mathbf{r}')$ is any component of the E-M field at $\mathbf{r}'$, and $n(\mathbf{r}')$ is the refractive index at that point. In this thesis, unless otherwise specified, we assume that all the waveguide studied are piecewise homogeneous. Therefore, for each homogeneous subregion i with refractive index n_i , we can find a function $G^{(i)}(\mathbf{r}, \mathbf{r}')$ that satisfies

$$\nabla'^2 G^{(i)}(\mathbf{r}', \mathbf{r}) + n_i^2 k_0^2 G^{(i)}(\mathbf{r}', \mathbf{r}) = -\delta(\mathbf{r} - \mathbf{r}') \quad (3.9)$$

$G^{(i)}(\mathbf{r}', \mathbf{r})$ is called the Green's Function and Equation (3.9) is called Green's Equation. Multiplying the scalar Helmholtz Equation (3.8) by $G(\mathbf{r}', \mathbf{r})$, and Green's Equation (3.9) by $U(\mathbf{r}')$ and subtracting, we obtain

$$G(\mathbf{r}', \mathbf{r}) \nabla'^2 U(\mathbf{r}') - U(\mathbf{r}') \nabla'^2 G(\mathbf{r}', \mathbf{r}) = U(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') \quad (3.10)$$

Obviously, the Equation (3.10) has a singularity at $\mathbf{r} = \mathbf{r}'$. Removing this singularity as shown in Figure 3.1, integrating (3.10) over subregion V and applying Green's second identity yields

$$\begin{aligned} & \int_{V-V_\epsilon} [G(\mathbf{r}', \mathbf{r}) \nabla'^2 U(\mathbf{r}') - U(\mathbf{r}') \nabla'^2 G(\mathbf{r}', \mathbf{r})] d\tau' \\ &= \oint_{S+S_\epsilon} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' \\ &= \int_S [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' + \int_{S_\epsilon} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' \quad (3.11) \\ &= \int_{V-V_\epsilon} U(\mathbf{r}') \delta(\mathbf{r}', \mathbf{r}) d\tau' \\ &= 0 \end{aligned}$$

from which we obtain Green's theorem

$$-\int_{S_\epsilon} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' = \int_S [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' \quad (3.12)$$

In the limit when $S_\epsilon \rightarrow 0$ we can take $\frac{\partial U(\mathbf{r}')}{\partial n'}$, $U(\mathbf{r}')$ outside the integral.

$$-\frac{\partial U(\mathbf{r})}{\partial n} \int_{S_\epsilon} G(\mathbf{r}', \mathbf{r}) ds' + U(\mathbf{r}) \int_{S_\epsilon} \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'} ds' = \int_S [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] ds' \quad (3.13)$$

Equation (3.13) indicates that the form of Green's function $G(\mathbf{r}, \mathbf{r}')$ and the field on a closed boundary is known. The field can be determined throughout the region enclosed by the boundary. In the next subsection, we derive the analytic form of the Green's function.

3.3.1 Analytic Form of Green's Function

The Green's function $G^{(i)}(\mathbf{r}, \mathbf{r}')$ can be found by solving Green's equation (3.9). Define $\bar{\rho} = \mathbf{r}' - \mathbf{r}$ as the displacement between the field point and the observation point. Since $\frac{\partial}{\partial \bar{\rho}} = \frac{\partial}{\partial \mathbf{r}'} = -\frac{\partial}{\partial \mathbf{r}}$, we get

$$\nabla_{\bar{\rho}} = \nabla_{\mathbf{r}'} = -\nabla_{\mathbf{r}} \quad (3.14)$$

From the fact that $G^{(i)}(\mathbf{r}', \mathbf{r})$ is the solution of Green's equation for infinite homogeneous media, we conclude that the form of the function must be independent of the choice of origin and the coordinate orientation and therefore must be a function of ρ only. Thus,

$$G^{(i)}(\mathbf{r}', \mathbf{r}) = G^{(i)}(|\mathbf{r}' - \mathbf{r}|) = G^{(i)}(\rho) \quad (3.15)$$

Rewriting the Helmholtz equation in terms of ρ , we arrive at

$$\frac{\partial^2 G^{(i)}(\rho)}{\partial \rho^2} + n_i^2 k_0^2 G^{(i)}(\rho) = -\delta(\rho) \quad (3.16)$$

The boundary condition is that $G^{(i)}(\rho) \rightarrow 0$ as $\rho \rightarrow \infty$. To find the analytical solution, it is easier to solve (3.16) in Fourier space

$$-k_\rho^2 G^{(i)}(k_\rho) + n_i^2 k_0^2 G^{(i)}(k_\rho) = -\frac{1}{4\pi\sqrt{2\pi}} \quad (3.17)$$

and rearrange it in terms of $G^{(i)}(\rho)$

$$G^{(i)}(k_\rho) = \left(\frac{1}{2\pi}\right)^{3/2} \frac{1}{k_\rho^2 - n_i^2 k_0^2} \quad (3.18)$$

Performing an inverse Fourier Transformation on equation (3.18), we obtain the analytical solution for Green's Function

$$G^{(i)}(\rho) = \frac{1}{4\pi\rho} \exp(-jk\rho) \quad (3.19)$$

The directional derivative of G is then

$$\begin{aligned} \frac{\partial G^{(i)}(\rho)}{\partial n} &= \frac{\partial G^{(i)}(\rho)}{\partial \rho} \hat{\mathbf{n}} \cdot \hat{\rho} \\ &= -\frac{1 + jk\rho}{4\pi\rho^2} \exp(-jk\rho) \cos(\angle \hat{\rho}, \hat{\mathbf{n}}) \end{aligned} \quad (3.20)$$

3.3.2 Green's Formulation

Once the solution of Green's function $G^{(i)}(\rho)$ is determined, the left side of Green's Equation (3.13) terms $\int_{S_\epsilon} G^{(i)}(\mathbf{r}', \mathbf{r}) ds'$ and $\int_{S_\epsilon} \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial n'} ds'$ can be evaluated. In Figure 3.2, ϵ_A is an infinitesimal hole surrounding the singular point. Without loss of generality, we can take S_ϵ as a hemisphere centered at $\mathbf{r}'$, that spans a solid angle of $\Delta\Omega = \frac{S_\epsilon}{\rho_\epsilon^2}$, where ρ_ϵ is the radius of S_ϵ .

Figure 3.2: Solid angle at different positions

Figure 3.3 shows the different values of the solid angles when the singular points are positioned at different places. When radius ϵ_0 approaches zero, the first term $\int_{S_\epsilon} G^{(i)}(\mathbf{r}', \mathbf{r}) ds'$ approaches zero since

$$\begin{aligned}
 & \int_{S_\epsilon} G^{(i)}(\mathbf{r}', \mathbf{r}) ds' \\
 &= \lim_{\rho \rightarrow 0} \int_{\phi=0}^{\phi_0} d\phi \int_{\theta=0}^{\theta_0} G^{(i)}(\rho) \rho^2 \sin \theta d\theta \\
 &= \lim_{\rho \rightarrow 0} \frac{\exp(-jk\rho)}{4\pi\rho} \rho^2 \int_{\Omega=0}^{\Delta\Omega_0} d\Omega \\
 &= \frac{\Delta\Omega_0}{4\pi} \lim_{\rho \rightarrow 0} \rho \exp(-jk\rho) \\
 &= 0
 \end{aligned} \tag{3.21}$$

Now consider the second term in equation (3.13), namely $\int_{S_\epsilon} \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial n'} ds'$. Notice that $\mathbf{n} \cdot \vec{\rho} = -1$ on the hemisphere S_ϵ , since the vector $\vec{\rho}$ is directed outward from the center of the sphere while the normal vector to the boundary surface, $\mathbf{n}$, points inward. From equation (3.20), we obtain the directional derivative

$$\frac{\partial G^{(i)}(\rho)}{\partial n} = -\frac{1 + jk\rho}{4\pi\rho^2} \exp(-jk\rho) \tag{3.22}$$

Figure 3.3: Singular integral on boundary and inside

Substituting equation (3.20) into the second term of equation (3.13) yields

$$\begin{aligned}
 & \int_{S_\epsilon} \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'} ds' \\
 &= -\lim_{\rho \rightarrow 0} \int_0^{\theta_0} \int_0^{\theta_0} \frac{1+jk\rho}{4\pi\rho^2} \exp(-jk\rho) \rho^2 \sin\theta d\theta d\phi \\
 &= -\lim_{\rho \rightarrow 0} (1+jk\rho) \frac{1}{4\pi} \int_0^{\Delta\Omega_0} d\Omega \\
 &= -\frac{\Delta\Omega_0}{4\pi}
 \end{aligned} \tag{3.23}$$

Inserting the results of (3.21) and (3.23) into Green's Equation (3.13) we obtain

$$\gamma U(\mathbf{r}) + \int_{S-S_\epsilon} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'} ds' = \int_{S-S_\epsilon} G^{(i)}(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'} ds' \tag{3.24}$$

Here the value $\gamma = \frac{\Delta\Omega_0}{4\pi}$ depends on the shape of the waveguide. We have

$$\gamma = \begin{cases} 1 & \text{inside the region} \\ \frac{1}{2} & \text{on the smooth boundary} \\ \frac{\Omega_0}{4\pi} & \text{on sharp corners of the boundary} \end{cases} \tag{3.25}$$

This is the Green's equation for a piecewise homogeneous waveguide which indicates that in a homogeneous region of a waveguide, the field distribution on the boundary of the region can be used to calculate the fields everywhere in that region. Accordingly the task of solving field values inside the waveguides can be transferred to that of determining the value of the field on the boundary.

3.3.3 Discretization of the Boundary Surface

Solving the integral equation (3.24) numerically requires that the boundary surface S be discretized into elements $S_1, S_2 \dots S_N$. The integral then becomes, if $\mathbf{r}$ is taken to be inside the integral region

$$U(\mathbf{r}) + \sum_{j=1}^N \int_{S_j} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'_j} ds' = \sum_{j=1}^N \int_{S_j} G^{(i)}(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'_j} ds' \quad (3.26)$$

If $\mathbf{r}$ is located on the boundary element S_{i_0} , then the integral (3.24) is given by

$$\gamma U(\mathbf{r}) + \sum_{j \neq i_0}^N \int_{S_j} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'_j} ds' = \sum_{j=1}^N \int_{S_j} G^{(i)}(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'_j} ds' \quad (3.27)$$

The term $\int_{S_{i_0}-S_\epsilon} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'} ds'$ can be eliminated since the discretized element is assumed to be planar and thus $\vec{\rho} \perp \mathbf{n}$, leading to

$$\frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'_j} = \frac{\partial G(\rho)}{\partial \rho} \hat{\mathbf{n}} \cdot \hat{\rho} = 0 \quad (3.28)$$

The S_{i_0} term on right hand side of Green's Equation (3.27) should be taken as the principal integral $\int_{S_{i_0}-S_\epsilon} G^{(i)}(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'_j} ds'$ due to the singularity of $G^{(i)}(\mathbf{r}', \mathbf{r})$ at the point ϵ .

The estimation of the discretized integrals in (3.27) further depends on the form in which $U(\mathbf{r}'_j)$ and $\frac{\partial U(\mathbf{r}'_j)}{\partial \mathbf{n}'_j}$ are discretized. We therefore separately consider various implementations of the Boundary Element Method, which we label constant element, linear element and higher order methods. In the following sections, we will focus on the study of constant element and linear element algorithms. On the other hand, if the variation of the refractive index is small, the components of E-M fields will be decoupled and we can simplify the problem through a scalar formalism, as the general vector solution is

Figure 3.4: Dielectric waveguide subregions. each boundary element belongs to both the left and the right region simultaneously

somewhat involved. In this thesis, we will consider instead a semi-vectorial formalism which is a trade-off between complexity and accuracy. In the rest of the chapter, we will discuss both scalar and semi-vector formalisms. Each will be provided with a constant and a linear element algorithm.

3.4 Scalar Formalism

Consider a dielectric waveguide formed from piecewise homogeneous refractive index regions. If the difference in refractive index is small, all the field components of $\mathbf{E}$ and $\mathbf{H}$ will be decoupled. Define U to be any field component. We know that U and its directional derivatives are continuous across any boundary. We can discretize the boundary into N elements. Nodes i , each of which is positioned at the center of element

i. In mathematical terms, $\mathbf{r}_i$ is determined by

$$\mathbf{r}_i = \frac{\int_{S_i} \mathbf{r} ds}{\int_{S_i} ds} \quad (3.29)$$

It is assume that each element has a uniform field distribution as illustrated in Figure 3.5. Since each boundary element i belongs to two different regions with different refractive indices as in Figure 3.4. In our context, we define a region as an area with uniform refractive index profile. From Green's formulation, its field satisfies the two equations

$$\begin{aligned} \gamma^r U^r(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial n_j^r} U_j^r(\mathbf{r}_j) ds + \sum_j \int_{S_j} G_r(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j^r(\mathbf{r}_j)}{\partial n_j^r} ds + SR \\ \gamma^l U^l(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial n_j^l} U_j^l(\mathbf{r}_j) ds + \sum_j \int_{S_j} G_l(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j^l(\mathbf{r}_j)}{\partial n_j^l} ds + SL \end{aligned} \quad (3.30)$$

where SR and SL are summations over the nodes with non-zero values of the excitation source function. The boundary conditions of the waveguides then determines the relationship between $U^l(\mathbf{r})$ and $U^r(\mathbf{r})$ on the boundary. In the scalar approximation, the field U and its directional derivative are continuous across the boundary, that is

$$\begin{aligned} U(\mathbf{r}) &= U^l(\mathbf{r}) = U^r(\mathbf{r}) \\ \frac{\partial U(\mathbf{r})}{\partial n} &= \frac{\partial U^l(\mathbf{r})}{\partial n^l} = -\frac{\partial U^r(\mathbf{r})}{\partial n^r} \end{aligned} \quad (3.31)$$

The negative sign in the second equation comes from the fact that $\mathbf{n}^l = -\mathbf{n}^r$ as the normal vector that is directed outward from the enclosed region. In the scalar formulation, we can therefore drop the l, r superscript of U , $\frac{\partial U}{\partial n}$.

3.5 Semi-Vector Formalism

3.5.1 Quasi-TE Mode

When the difference in refractive index is large the scalar formalism can be generalized to a semi-vectorial formalism[94]. That is, for a quasi-TE mode, $\mathbf{E} \approx (0, E_y, E_z)$, take E_y as the field component. We have from Maxwell's equations,

$$\begin{aligned} \frac{\partial E_y}{\partial x} &= j\omega\mu H_z \\ \frac{\partial E_y}{\partial y} &= -\frac{\partial E_z}{\partial z} \approx -j\beta E_z \\ \frac{\partial E_y}{\partial z} &\approx j\beta E_y \end{aligned} \quad (3.32)$$

E_z, H_z are continuous transverse to the boundary. That implies the directional derivative is continuous along transverse direction. At a longitudinal boundary, its directional derivative is also continuous due to the continuity of E_y along the z direction. From the boundary conditions provided in (2.21), E_y is everywhere continuous except along the y direction. Denote $E_{y\parallel}(\mathbf{r})$ as normal vector $\mathbf{n}(\mathbf{r}) \perp \hat{y}$ and $E_{y\perp}$ otherwise, we have

$$\begin{aligned} E_{y\parallel} &= E_{y\parallel}^l = E_{y\parallel}^r \\ E_{y\perp} &= n_l^2 E_{y\perp}^l = n_r^2 E_{y\perp}^r \\ \frac{\partial E_y}{\partial \mathbf{n}} &= \frac{\partial E_y^l}{\partial \mathbf{n}^l} = -\frac{\partial E_y^r}{\partial \mathbf{n}^r} \end{aligned} \quad (3.33)$$

Taking E_y as the field component represented by U , we have in the semi-vector formalism of the quasi-TE mode

$$\begin{aligned} \gamma^r \alpha_{TE}^r(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial \mathbf{n}_j^r} \alpha_{TE}^r(\mathbf{r}_j) U_j(\mathbf{r}_j) ds - \sum_j \int_{S_j} G_r(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j(\mathbf{r}_j)}{\partial \mathbf{n}_j} ds + SR \\ \gamma^l \alpha_{TE}^l(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial \mathbf{n}_j^l} \alpha_{TE}^l(\mathbf{r}_j) U_j(\mathbf{r}_j) ds + \sum_j \int_{S_j} G_l(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j(\mathbf{r}_j)}{\partial \mathbf{n}_j} ds + SL \end{aligned} \quad (3.34)$$

The semi-vector coefficient $\alpha_{TE}^{l,r}(\mathbf{r})$ depends on the normal vector at the boundary surface $\mathbf{n}(\mathbf{r})$ according to

$$\alpha_{TE}^{l,r}(\mathbf{r}) = \begin{cases} 1 & \mathbf{n}(\mathbf{r}) \perp \hat{y} \\ \frac{1}{n_{l,r}^2} & \mathbf{n}(\mathbf{r}) \parallel \hat{y} \end{cases} \quad (3.35)$$

3.5.2 Quasi-TM Mode

A similar analysis applies to the quasi TM mode. The directional derivative of E_x is continuous in the y, z direction at each boundary point. In the x direction, we have

$$n_l^2 E_x^l = n_r^2 E_x^r \quad (3.36)$$

The quasi-TM formalism is given by

$$\begin{aligned} \gamma \alpha_{TM}^r(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial \mathbf{n}_j^r} \alpha_{TM}^r(\mathbf{r}_j) U_j(\mathbf{r}_j) ds - \sum_j \int_{S_j} G_r(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j(\mathbf{r}_j)}{\partial \mathbf{n}_j} ds + SR \\ \gamma \alpha_{TM}^l(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial \mathbf{n}_j^l} \alpha_{TM}^l(\mathbf{r}_j) U_j(\mathbf{r}_j) ds + \sum_j \int_{S_j} G_l(\mathbf{r}_j - \mathbf{r}) \frac{\partial U_j(\mathbf{r}_j)}{\partial \mathbf{n}_j} ds + SL \end{aligned} \quad (3.37)$$

where the field U now stands for the E_x component. The Quasi-TM coefficient is given by

$$\alpha_{TM}^{l,r}(\mathbf{r}) = \begin{cases} 1 & \mathbf{n}(\mathbf{r}) \perp \hat{x} \\ \frac{1}{n_{l,r}^2} & \mathbf{n}(\mathbf{r}) \parallel \hat{x} \end{cases} \quad (3.38)$$

3.5.3 Summary for Scalar and Semi-Vector Formalism

Comparing the scalar and semi-vectorial formalism we can unify the three expressions (3.30), (3.34) and (3.37) by inducing a coefficient α_F . The resulting unified expression is

$$\begin{aligned} \gamma \alpha_F^r(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j^r} \alpha_F^r(\mathbf{r}_j) U(\mathbf{r}_j) ds - \sum_j \int_{S_j} G_r(\mathbf{r}_j - \mathbf{r}_i) \frac{\partial U(\mathbf{r}_j)}{\partial n_j} ds + SR \\ \gamma \alpha_F^l(\mathbf{r}) U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{S_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j^l} \alpha_F^l(\mathbf{r}_j) U(\mathbf{r}_j) ds + \sum_j \int_{S_j} G_l(\mathbf{r}_j - \mathbf{r}_i) \frac{\partial U(\mathbf{r}_j)}{\partial n_j} ds + SL \end{aligned} \quad (3.39)$$

Here α_F applies to α_{TM} , α_{TE} and α_{SC} . For the various choices of F we have

$$\begin{aligned} \alpha_{SC}^{l,r} &= 1 \\ \alpha_{TE}^{l,r} &= \begin{cases} 1 & \mathbf{n}(\mathbf{r}) \perp \hat{y} \\ \frac{1}{n_{l,r}^2} & \mathbf{n}(\mathbf{r}) \parallel \hat{y} \end{cases} \\ \alpha_{TM}^{l,r} &= \begin{cases} 1 & \mathbf{n}(\mathbf{r}) \perp \hat{x} \\ \frac{1}{n_{l,r}^2} & \mathbf{n}(\mathbf{r}) \parallel \hat{x} \end{cases} \end{aligned} \quad (3.40)$$

3.6 Constant Element Algorithm

3.6.1 Constant Element Approximation

The constant element Algorithm is based on the approximation that the field distribution over the element is constant, (see Figure 3.5 in which U_i is the field at the center of element i). Substituting

$$U(\mathbf{r}_i) \approx U_i \quad (3.41)$$

Figure 3.5: Constant element method approximation. Within a discretized element i , the field is approximated by a constant

into the equation (3.30) for the scalar formalism and assuming that the observation point is placed at node i , we obtain

$$\begin{aligned} \frac{1}{2}\alpha_F^r(\mathbf{r}_i)U_i &= -\sum_{j \neq i} U_j \int_{S_j} \alpha_F^r(\mathbf{r}_j) \frac{\partial G_r(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j} ds - \sum_j \frac{\partial U_j}{\partial n_j} \int_{S_j} G_r(\mathbf{r}_j - \mathbf{r}_i) ds + SR_i \\ \frac{1}{2}\alpha_F^l(\mathbf{r}_i)U_i &= -\sum_{j \neq i} U_j \int_{S_j} \alpha_F^l(\mathbf{r}_j) \frac{\partial G_l(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j} ds + \sum_j \frac{\partial U_j}{\partial n_j} \int_{S_j} G_l(\mathbf{r}_j - \mathbf{r}_i) ds + SL_i \end{aligned} \quad (3.42)$$

Here we take $\gamma = \frac{1}{2}$ since the center of element i is taken to be the observation point inside the planar element which spans a solid angle $\Omega = 2\pi$. Since $i \in \{1 \dots N\}$, there are a total of $2N$ independent linear equations of (3.42) with $2N$ unknowns $(U_1, \frac{\partial U_1}{\partial n_1}, \dots, U_N, \frac{\partial U_N}{\partial n_N})$. Defining

$$\mathbf{V} = \begin{pmatrix} U_1 \\ \frac{\partial U_1}{\partial n_1} \\ U_2 \\ \frac{\partial U_2}{\partial n_2} \\ \vdots \\ U_N \\ \frac{\partial U_N}{\partial n_N} \end{pmatrix}; \quad \mathbf{S} = \begin{pmatrix} SR_1 \\ SL_1 \\ SR_2 \\ SL_2 \\ \vdots \\ SR_N \\ SL_N \end{pmatrix} \quad (3.43)$$

we can rewrite equation (3.31) in matrix form as

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (3.44)$$

where

$$\mathbf{H} = \begin{pmatrix} \frac{1}{2}\alpha_F^r(\mathbf{r}_1) & g_{11}^r & h_{12}^r & \cdots & g_{1(N-1)}^r & h_{1N}^r & g_{1N}^r \\ \frac{1}{2}\alpha_F^l(\mathbf{r}_1) & -g_{11}^l & h_{12}^l & \cdots & -g_{1(N-1)}^l & h_{1N}^l & -g_{1N}^l \\ h_{21}^r & g_{21}^r & \frac{1}{2}\alpha_F^r(\mathbf{r}_2) & \cdots & g_{2(N-1)}^r & h_{2N}^r & g_{2N}^r \\ \vdots & & & \ddots & & & \vdots \\ h_{(N-1)1}^l & -g_{(N-1)1}^l & h_{(N-1)2}^l & \cdots & -g_{(N-1)(N-1)}^l & h_{(N-1)N}^l & -g_{(N-1)N}^l \\ h_{N1}^r & g_{N1}^r & h_{N2}^r & \cdots & g_{N(N-1)}^r & \frac{1}{2}\alpha_F^r(\mathbf{r}_N) & g_{NN}^r \\ h_{N1}^l & -g_{N1}^l & h_{N2}^l & \cdots & -g_{N(N-1)}^l & \frac{1}{2}\alpha_F^l(\mathbf{r}_N) & -g_{NN}^l \end{pmatrix} \quad (3.45)$$

is a matrix composed of four submatrices $G^{l,r}$, $H^{l,r}$ with matrix elements as

$$\begin{aligned} (G^{l,r})_{i,j} &= g_{ij}^{l,r} \\ (H^{l,r})_{i,j} &= h_{ij}^{l,r} \end{aligned} \quad (3.46)$$

This is the constant element algorithm. By solving the matrix equation (3.44), we can find the field distribution $\mathbf{V}$ on the boundary of waveguides.

3.6.2 Calculation of Matrix Elements

This subsection derives the value of the matrix elements of $G^{l,r}$, $H^{l,r}$. In our algorithm, we evaluate off-diagonal submatrices elements by Gaussian Integration and the diagonal elements by series expansion. Such arrangement is a result of the balance between efficiency and accuracy.

A) Off-diagonal Elements of $G^{l,r}$, $H^{l,r}$

As in previous contexts, the off-diagonal matrix elements in submatrix $G^{l,r}$, $H^{l,r}$ are given by

$$h_{ij}^{l,r} = \begin{cases} -\int_{S_j} \alpha_F^{l,r}(\mathbf{r}_j) \frac{1-jk\rho}{4\pi\rho^2} \exp(-jk\rho) \frac{\mathbf{n} \cdot \vec{\rho}}{n\rho} ds & \text{element } i, j \text{ in the same region} \\ 0 & \text{otherwise} \end{cases} \quad (3.47)$$

Figure 3.6: Subdivide different elements into simple triangles centered at A_0 (A). Quadrilateral subdivided as triangles T1,T2,T3,T4: (B). Triangular subdivided as T1,T2,T3

$$g_{ij}^{l,r} = \begin{cases} \int_{S_i} \frac{1}{4\pi\rho} \exp(-jk\rho) ds & \text{element } i, j \text{ in the same region} \\ 0 & \text{otherwise} \end{cases} \quad (3.48)$$

The integrals above can now be performed numerically through Gaussian quadrature.

B) Diagonal Elements

Since the diagonal matrix elements of $H^{l,r}$, $G^{l,r}$ are given by

$$h_{ii}^{l,r} = - \int_{S_i} \alpha_F^{l,r}(\mathbf{r}_j) \frac{1 + jk\rho}{4\pi\rho^2} \exp(-jk\rho) \frac{\mathbf{n} \cdot \vec{\rho}}{n\rho} ds \quad (3.49)$$

$$g_{ii}^{l,r} = \int_{S_i} \frac{1}{4\pi\rho} \exp(-jk\rho) ds \quad (3.50)$$

where $h_{ii}^{l,r} = 0$ since $\mathbf{n} \perp \vec{\rho}$ for a planar element. The series solution of $g_{ii}^{l,r}$ involves an integration over an area and therefore depends on the shape of the discretized element. It can be of either triangular or quadrilateral shape. However, we can always subdivide polygons into simple triangles as in Figure 3.6. By deriving a series solution at each triangular sub-element and summing, we obtain a series solution for $g_{ii}^{l,r}$. In the next two subsections, we will obtain the series solution to the diagonal elements for both quadrilateral and triangular elements.

Figure 3.7: Subtriangle of T1 in quadrilateral node. $\phi = \pi - \theta_1^1 - \theta$

3.6.3 Quadrilateral Elements

A quadrilateral element can be divided into 4 triangular sub-elements sharing the common vertex A_0 as in Figure 3.6. The choice of A_0 is arbitrary provided that A_0 is inside the element. In our case, we specify A_0 to be the center of element i . Then the diagonal matrix element $g_{ii}^{l,r}$ can be expressed as the sum of the 4 integrals performed on each sub-triangle. e.g.

$$\begin{aligned} g_{ii}^{l,r} &= \sum_{k=1}^4 \int_{\Delta_k} \frac{1}{4\pi\rho} \exp(-jk\rho) ds \\ &= g_1 + g_2 + g_3 + g_4 \end{aligned} \quad (3.51)$$

We evaluate (g_1, g_2, g_3, g_4) separately as in Figure 3.7

$$\begin{aligned} g_1 &= \int_{\Delta_{T1}} \frac{1}{4\pi\rho} \exp(-jk\rho) ds \\ &= \int_0^{\theta_0^1} d\theta \int_0^{\rho_0(\theta)} \frac{1}{4\pi\rho} \exp(-jk\rho) \rho d\rho \\ &= \int_0^{\theta_0^1} \frac{1 - \exp(-jk\rho_0(\theta))}{4jk\pi} d\theta \end{aligned} \quad (3.52)$$

From the geometry of the triangle, it is easy to show that

$$\frac{\rho_0(\theta)}{\sin \theta_1^1} = \frac{r_1}{\sin(\pi - \theta - \theta_1^1)} \quad (3.53)$$

where

$$\theta_1^1 = \cos^{-1} \frac{(\mathbf{r}_{A0} - \mathbf{r}_{A1}) \cdot (\mathbf{r}_{A2} - \mathbf{r}_{A1})}{|\mathbf{r}_{A0} - \mathbf{r}_{A1}| |\mathbf{r}_{A2} - \mathbf{r}_{A1}|} \quad (3.54)$$

and

$$\theta_0^1 = \cos^{-1} \frac{(\mathbf{r}_{A1} - \mathbf{r}_{A0}) \cdot (\mathbf{r}_{A2} - \mathbf{r}_{A0})}{|\mathbf{r}_{A1} - \mathbf{r}_{A0}| |\mathbf{r}_{A2} - \mathbf{r}_{A0}|} \quad (3.55)$$

Substituting the above into equation (3.52) yields

$$\begin{aligned} g_1 &= \frac{1}{4\pi jk} \int_0^{\theta_0^1} \left[1 - \sum_{n=0}^{\infty} \frac{(-jkr_0 \sin \theta)^n}{n!} \right] d\theta \\ &= -\frac{1}{4\pi jk} \sum_{n=1}^{\infty} \frac{(-jkr_1 \sin \theta_1^1)^n}{n!} \int_0^{\theta_0^1} \frac{d\theta}{\sin^n(\theta + \theta_1^1)} \\ &= -\frac{1}{4\pi jk} \sum_{n=1}^{\infty} \frac{(-jkr_1 \sin \theta_1^1)^n}{n!} p_n(\theta_1^1, \theta_0^1) \end{aligned} \quad (3.56)$$

Similarly

$$g_2 = -\frac{1}{4\pi jk} \sum_{n=1}^{\infty} \frac{(-jkr_2 \sin \theta_2^2)^n}{n!} p_n(\theta_2^2, \theta_0^2) \quad (3.57)$$

$$g_3 = -\frac{1}{4\pi jk} \sum_{n=1}^{\infty} \frac{(-jkr_3 \sin \theta_3^3)^n}{n!} p_n(\theta_3^3, \theta_0^3) \quad (3.58)$$

$$g_4 = -\frac{1}{4\pi jk} \sum_{n=1}^{\infty} \frac{(-jkr_4 \sin \theta_4^4)^n}{n!} p_n(\theta_4^4, \theta_0^4) \quad (3.59)$$

Here we have defined a new function

$$p_n(\theta_1, \theta_2) = \int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta + \theta_1)} \quad (3.60)$$

This function is calculated by a recursive algorithm as in Section 3.8. With the recursive relation, we can solve g_1 numerically. Similarly, stepping through the index i , we can solve for $g_i, i = 1, 2, 3, 4$ as well, and therefore the diagonal matrix element $g_{ii}^{l,r} = \sum_{k=0}^4 g_i$.

3.6.4 Triangular Elements

For a triangular element, the series solution found in the quadrilateral element case still applies, except that the element is subdivided into three subtriangles instead of four as shown in figure 3.6 (B). Thus for a triangular element

$$g_{ii}^{l,r} = \sum_{k=1}^3 g_k \quad (3.61)$$

where the definition of the g_k remains the same as in the previous section.

Figure 3.8: Linear Element: The field in the element is assumed to vary linearly

3.7 Linear Element Algorithm

The linear element algorithm is based on the approximation that the fields within an element varies linearly, that is

$$U(\mathbf{r}_i) \approx U_i + \nabla U(0) \cdot \mathbf{r}_i \quad (3.62)$$

as shown in Figure 3.8. This is a higher-order approximation than that leading to the constant element algorithm. In the following subsections, we will develop the linear element algorithm based on quadrilateral and triangular mesh elements.

3.7.1 Quadrilateral Elements

The first step in the refinement process is to perform a linear transformation from the Cartesian coordinate system (x_1, x_2, x_3) into a dimensionless system defined on a node. as shown in figure 3.9. The choice of Cartesian is arbitrary provided that the planar element is on the (x_1, x_2) plane. The transformation results in the element becoming a square element in the (η_1, η_2) coordinates with its center point at the origin. The transformation follows the relationship.

$$\mathbf{r} = \sum_{k=1}^4 \phi_k \mathbf{r}^k \quad (3.63)$$

Figure 3.9: Linear transformation from (x_1, x_2) to dimensionless (η_1, η_2) coordination

Where $\mathbf{r}^k (k = 1, \dots, 4)$ are the coordinates of the four vertices of that element in Cartesian coordinates. ϕ_k are the interpolation coefficients that satisfy

$$\begin{aligned}\phi_1 &= \frac{1}{4}(1 - \eta_1)(1 - \eta_2) \\ \phi_2 &= \frac{1}{4}(1 + \eta_1)(1 - \eta_2) \\ \phi_3 &= \frac{1}{4}(1 + \eta_1)(1 + \eta_2) \\ \phi_4 &= \frac{1}{4}(1 - \eta_1)(1 + \eta_2)\end{aligned}\quad (3.64)$$

(η_1, η_2) are varying from -1 to +1 as shown in the Figure 3.8. Correspondingly, we have

$$\frac{\partial \mathbf{r}}{\partial \bar{\eta}} = \sum_{k=1}^4 \frac{\partial \phi_k}{\partial \bar{\eta}} \mathbf{r}^k \quad (3.65)$$

The Jacobian matrix is written as

$$\begin{aligned}|\mathbf{J}(\eta_1, \eta_2)| &= \left| \frac{\partial \mathbf{r}}{\partial \bar{\eta}} \right| \\ &= \begin{vmatrix} \sum_{k=1}^4 \frac{\partial \phi_k}{\partial \eta_1} x^k & \sum_{k=1}^4 \frac{\partial \phi_k}{\partial \eta_2} x^k \\ \sum_{k=1}^4 \frac{\partial \phi_k}{\partial \eta_1} y^k & \sum_{k=1}^4 \frac{\partial \phi_k}{\partial \eta_2} y^k \end{vmatrix}\end{aligned}\quad (3.66)$$

The interpolation function of any linearly varying function $f(\eta_1, \eta_2)$ can be written as

$$f(\eta_1, \eta_2) = \phi_1 f_1 + \phi_2 f_2 + \phi_3 f_3 + \phi_4 f_4$$

$$= \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix} \quad (3.67)$$

where f_k is the value of the function f on the four vertices of the element. Due to the assumption that U and $\frac{\partial U}{\partial n}$ vary linearly, we have

$$U^e(\eta_1, \eta_2) = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \\ U_4^e \end{pmatrix} \quad (3.68)$$

$$\frac{\partial U^e(\eta_1, \eta_2)}{\partial n^e} = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{pmatrix} \begin{pmatrix} \frac{\partial U_1^e}{\partial n_1^e} \\ \frac{\partial U_2^e}{\partial n_2^e} \\ \frac{\partial U_3^e}{\partial n_3^e} \\ \frac{\partial U_4^e}{\partial n_4^e} \end{pmatrix} \quad (3.69)$$

where U_i^e is the field at the i -th vertex of the element e and $\frac{\partial U_i^e}{\partial n_i^e}$ is its directional derivative respectively. By replacing the interpolation functions of $U(\mathbf{r})$ in Equation (3.39), we

obtain the following equations for a quadrilateral element in the linear element method

$$\begin{aligned}
\gamma^r \alpha_F^r U_i &= - \sum_{e \neq i}^n \begin{pmatrix} h_1^{e,r} & h_2^{e,r} & h_3^{e,r} & h_4^{e,r} \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \\ U_4^e \end{pmatrix} \\
&\quad - \sum_{e=1}^n \begin{pmatrix} g_1^{e,r} & g_2^{e,r} & g_3^{e,r} & g_4^{e,r} \end{pmatrix} \begin{pmatrix} q_1^e \\ q_2^e \\ q_3^e \\ q_4^e \end{pmatrix} + S R_i \\
\gamma^l \alpha_F^l U_i &= - \sum_{e \neq i}^n \begin{pmatrix} h_1^{e,l} & h_2^{e,l} & h_3^{e,l} & h_4^{e,l} \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \\ U_4^e \end{pmatrix} \\
&\quad + \sum_{e=1}^n \begin{pmatrix} g_1^{e,l} & g_2^{e,l} & g_3^{e,l} & g_4^{e,l} \end{pmatrix} \begin{pmatrix} q_1^e \\ q_2^e \\ q_3^e \\ q_4^e \end{pmatrix} + S L_i
\end{aligned} \tag{3.70}$$

where U_i is the field at node i while $U_1^e, U_2^e, U_3^e, U_4^e$ are the fields of the four vertices on the element e . $q_1^e, q_2^e, q_3^e, q_4^e$ are the directional derivatives. $\gamma^{l,r}$ depends on the solid angle of node i as discussed before.

3.7.2 Matrix Representation of Green's Equation

For a system with N nodes on the boundary, each node must satisfy two boundary element equations (3.70) simultaneously, one for each region. The set of all such equations forms a linear system with $2N$ equations. Notice that each node can be shared by at most four quadrilateral elements. As shown in Figure 3.10 node j is thus shared by vertex 1 of element E_1 , vertex 2 of E_2 , vertex 3 of E_3 and vertex 4 of E_4 . We therefore

Figure 3.10: Node j is shared by four elements, as 1st node of element E1, 2nd node of E2, 3rd node of E3 and 4th of E4, respectively

obtain

$$\begin{aligned} U_1^{E_1} &= U_2^{E_2} = U_3^{E_3} = U_4^{E_4} = U_j \\ q_1^{E_1} &= q_2^{E_2} = q_3^{E_3} = q_4^{E_4} = q_j \end{aligned} \quad (3.71)$$

By rearranging the locally labeled vertex into global nodes we obtain a linear system of $2N$ equations with $2N$ unknowns. As in our exposition of the the constant element algorithm, we write the Green's equation in matrix form

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (3.72)$$

where $\mathbf{H}$ is composed of elements of submatrices $G^{l,r}, H^{l,r}$. Unlike in the case of the constant element algorithm, each matrix element is mapped into a single vertex node instead of the entire discretized element. Since each node i can be a vertex of four different elements as illustrated in Figure 3.10, each matrix element should be written as the sum of the values contributed by each of these four elements.

$$\begin{aligned} h_{ij} &= h_1^{e1} + h_2^{e2} + h_3^{e3} + h_4^{e4} \\ g_{ij} &= g_1^{e1} + g_2^{e2} + g_3^{e3} + g_4^{e4} \end{aligned} \quad (3.73)$$

3.7.3 Calculation of the Matrix Elements h_j^e, g_j^e

If node i does not belong to the same region (refer to definition in the Constant Element algorithm) as element e , we have $h_j^e = g_j^e = 0$. Otherwise, if node i is in the same region as element e but does not belong to that element, inserting the Green function (3.20) into (3.70), we obtain

$$\begin{aligned} \begin{pmatrix} h_1^e \\ h_2^e \\ h_3^e \\ h_4^e \end{pmatrix} &= \frac{1}{4\pi} \int_{S_e} \alpha_F^{l,r} \frac{-1-jk\rho}{\rho^2} \exp(-jk\rho) \cos \angle(\rho; \mathbf{n}) \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} ds \\ &= \frac{\alpha_F^{l,r}}{4\pi} \int_{-1}^{+1} \int_{-1}^{+1} \frac{-1-jk\rho}{\rho^2} \exp(-jk\rho) \cos \angle(\rho; \mathbf{n}) \begin{pmatrix} \frac{(1-\eta_1)(1-\eta_2)}{4} \\ \frac{(1+\eta_1)(1-\eta_2)}{4} \\ \frac{(1+\eta_1)(1+\eta_2)}{4} \\ \frac{(1-\eta_1)(1+\eta_2)}{4} \end{pmatrix} | \mathbf{J}(\eta_1, \eta_2) | d\eta_1 d\eta_2 \end{aligned} \quad (3.74)$$

$$\begin{aligned} \begin{pmatrix} g_1^e \\ g_2^e \\ g_3^e \\ g_4^e \end{pmatrix} &= \frac{1}{4\pi} \int_{S_e} \frac{1}{\rho} \exp(-jk\rho) \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix} ds \\ &= \frac{1}{4\pi} \int_{-1}^{+1} \int_{-1}^{+1} \frac{1}{\rho} \exp(-jk\rho) \begin{pmatrix} \frac{(1-\eta_1)(1-\eta_2)}{4} \\ \frac{(1+\eta_1)(1-\eta_2)}{4} \\ \frac{(1+\eta_1)(1+\eta_2)}{4} \\ \frac{(1-\eta_1)(1+\eta_2)}{4} \end{pmatrix} | \mathbf{J}(\eta_1, \eta_2) | d\eta_1 d\eta_2 \end{aligned} \quad (3.75)$$

in which ρ is also a function of η_1, η_2 , and satisfies the relation

$$\rho = | \mathbf{r}^e(\eta_1, \eta_2) - \mathbf{r}_i | \quad (3.76)$$

The equations (3.74) and (3.75) can now be evaluated by Gaussian quadrature.

3.7.4 Series Solution for Rectangular Elements

If node i is the j -th vertex of element e , then $h_j^e = 0$ as $\vec{\rho} \perp \mathbf{n}$ and the integrals of g_j^e have removable singularities at one of the corners. For an arbitrary quadrilateral element, the Jacobian $|\mathbf{J}(\eta_1, \eta_2)|$ is a complicated expression and it is therefore difficult to obtain a series solution for the diagonal elements. However, if the element is rectangular, the series solution is relatively simple to derive. Our discussion below thus focuses on rectangular elements only.

As shown in Figure 3.11, the transformation from (η_1, η_2) to (x_1, x_2)

$$\begin{cases} \eta_1 &= 2 * x_1 / l_1 \\ \eta_2 &= 2 * x_2 / l_2 \end{cases} \quad (3.77)$$

(l_1, l_2) is the length and width of that rectangular elements. The Jacobian $\mathbf{J}$ is given by

$$|\mathbf{J}| = \frac{l_1 l_2}{4} \quad (3.78)$$

Consider the case where node i is vertex 1 of element e . Obviously $h_1 = 0$ since $\vec{\rho}$ is perpendicular to $\mathbf{n}$. The integral in the expression for g_1^e then becomes

$$g_1^e = \frac{l_1 l_2}{16\pi} \int_{-1+\epsilon}^{+1} \int_{-1+\epsilon}^{+1} \frac{\exp(-jk\rho)}{\rho} \frac{(1-\eta_1)(1-\eta_2)}{4} d\eta_1 d\eta_2 \quad (3.79)$$

where the integration area is the rectangular region of element e . To evaluate this integral, we can subdivide the rectangular element into 2 sub-triangles see (Figure 3.11). Then the integral is the sum of the integrals over two triangular regions, which are simply performed in the polar coordinate system of Figure 3.11

$$g_1^e = g_{1,1} + g_{1,2} = \sum_{k=1}^2 g_{1,k} \quad (3.80)$$

$$g_{1,k} = \frac{1}{4\pi} \int_{\Delta_{e_k}} \frac{\exp(-jk\rho)}{\rho} \frac{(1-\eta_1)(1-\eta_2)}{4} ds \quad (3.81)$$

Here $k = 1, 2$ and T_k denotes the k -th subtriangle. The transformation into the (η_1, η_2) coordinate system is

$$\begin{cases} r \cos \theta &= (\eta_1 + 1) \frac{l_1}{2} \\ r \sin \theta &= (\eta_2 + 1) \frac{l_2}{2} \end{cases} \quad (3.82)$$

Figure 3.11: Linear transformation from (η_1, η_2) to (x_1, x_2) in a rectangular elements. the rectangular element is subdivided into two simple triangle

Substituting the above expression into equation (3.81) and changing to a polar coordinate system, we obtain for the integral

$$\begin{aligned}
g_{1,1} &= \frac{1}{4\pi} \int_0^{\Theta_1^1} d\theta \int_0^{\frac{l_1}{\cos \theta}} \frac{\exp(-jkr)}{r} \left(1 - \frac{r \cos \theta}{l_1}\right) \left(1 - \frac{r \sin \theta}{l_2}\right) r dr \\
&= \frac{1}{4\pi} \int_0^{\Theta_1^1} d\theta \int_0^{\frac{l_1}{\cos \theta}} \exp(-jkr) \left(1 - \frac{r \cos \theta}{l_1} - \frac{r \sin \theta}{l_2} + \frac{r^2 \sin \theta \cos \theta}{l_1 l_2}\right) dr \\
&= I_0(\Theta_1^1, l_1) - \frac{1}{l_1} I_1(\Theta_1^1, l_1) - \frac{1}{l_2} I_2(\Theta_1^1, l_1) + \frac{1}{l_1 l_2} I_3(\Theta_1^1, l_1)
\end{aligned} \tag{3.83}$$

Here, we define four functions I_0, I_1, I_2, I_3

$$I_0(\Theta, l_1) = \frac{1}{4\pi} \int_0^{\Theta} d\theta \int_0^{\frac{l_1}{\cos \theta}} \exp(-jkr) dr \tag{3.84}$$

$$I_1(\Theta, l_1) = \frac{1}{4\pi} \int_0^{\Theta} d\theta \int_0^{\frac{l_1}{\cos \theta}} \exp(-jkr) r \cos \theta dr \tag{3.85}$$

$$I_2(\Theta, l_1) = \frac{1}{4\pi} \int_0^{\Theta} d\theta \int_0^{\frac{l_1}{\cos \theta}} \exp(-jkr) r \sin \theta dr \tag{3.86}$$

$$I_3(\Theta, l_1) = \frac{1}{4\pi} \int_0^{\Theta} \sin \theta \cos \theta d\theta \int_0^{\frac{l_1}{\cos \theta}} \exp(-jkr) r^2 dr \tag{3.87}$$

We now further apply polar coordinate to the triangle T_2 as shown in Figure 3.11. The transformation function then becomes

$$\begin{cases} r \sin \theta &= (\eta_1 + 1) \frac{l_2}{2} \\ r \cos \theta &= (\eta_2 + 1) \frac{l_2}{2} \end{cases} \tag{3.88}$$

Therefore,

$$\begin{aligned}
g_{1,2} &= \frac{1}{4\pi} \int_0^{\Theta_1^2} d\theta \int_0^{\frac{l_2}{\cos \theta}} \frac{\exp(-jkr)}{r} \left(1 - \frac{r \sin \theta}{l_1}\right) \left(1 - \frac{r \cos \theta}{l_2}\right) r dr \\
&= \frac{1}{4\pi} \int_0^{\Theta_1^2} d\theta \int_0^{\frac{l_2}{\cos \theta}} \exp(-jkr) \left(1 - \frac{r \cos \theta}{l_2} - \frac{r \sin \theta}{l_1} + \frac{r^2 \sin \theta \cos \theta}{l_1 l_2}\right) dr \\
&= I_0(\Theta_1^2, l_2) - \frac{1}{l_2} I_2(\Theta_1^2, l_2) - \frac{1}{l_1} I_1(\Theta_1^2, l_2) + \frac{1}{l_1 l_2} I_3(\Theta_1^2, l_2)
\end{aligned} \tag{3.89}$$

Hence, if we know the series solution for I_0, I_1, I_2, I_3 , we obtain g_1 as a linear combination of this set of functions through

$$g_1^e = g_{1,1} + g_{1,2} \tag{3.90}$$

3.7.5 Solution to $I_0(\Theta, l), I_1(\Theta, l), I_2(\Theta, l), I_3(\Theta, l)$

To solve the four functions I_i defined above, first consider the integrals as follows:

$$\begin{aligned}
i_1(\theta) &= \int_0^{\frac{l}{\cos \theta}} \exp(-jkr) dr \\
&= -\frac{1}{jk} [\exp(-\frac{jkl}{\cos \theta}) - 1] \\
&= -\sum_{n=1}^{\infty} \frac{(jk)^{n-1} l^n}{n! \sin^n(\theta - \frac{\pi}{2})}
\end{aligned} \tag{3.91}$$

$$\begin{aligned}
i_2(\theta) &= \int_0^{\frac{l}{\cos \theta}} \exp(-jkr) r dr \\
&= \frac{\partial i_1(\theta)}{\partial(-jk)} \\
&= \sum_{n=2}^{\infty} \frac{(n-1)(jk)^{n-2} l^n}{n! \sin^n(\theta - \frac{\pi}{2})}
\end{aligned} \tag{3.92}$$

$$\begin{aligned}
i_3(\theta) &= \int_0^{\frac{l}{\cos \theta}} \exp(-jkr) r^2 dr \\
&= \frac{\partial i_2(\theta)}{\partial(-jk)} \\
&= -\sum_{n=3}^{\infty} \frac{(n-1)(n-2)(jk)^{n-3} l^n}{n! \sin^n(\theta - \frac{\pi}{2})}
\end{aligned} \tag{3.93}$$

From the integrals above we solve the inner integral of I_0 , I_1 , I_2 , I_3 in terms of p_n as was defined in previous subsection.

$$\begin{aligned}
I_0(\Theta, l) &= \frac{1}{4\pi} \int_0^{\Theta} i_1(\theta) d\theta \\
&= -\sum_{n=1}^{\infty} \frac{(jk)^{n-1} l^n}{4\pi n!} \int_0^{\Theta} \frac{d\theta}{\sin^n(\theta - \frac{\pi}{2})} \\
&= -\sum_{n=1}^{\infty} \frac{(jk)^{n-1} l^n}{4\pi n!} p_n(-\frac{\pi}{2}, \Theta)
\end{aligned} \tag{3.94}$$

$$\begin{aligned}
I_1(\Theta, l) &= \frac{1}{4\pi} \int_0^{\Theta} \cos \theta i_2(\theta) d\theta \\
&= -\sum_{n=2}^{\infty} \frac{(n-1)(jk)^{n-2} l^n}{4\pi n!} \int_0^{\Theta} \frac{d\theta}{\sin^{n-1}(\theta - \frac{\pi}{2})} \\
&= -\sum_{n=1}^{\infty} \frac{(n)(jk)^{n-1} l^{n+1}}{4\pi(n+1)!} p_n(-\frac{\pi}{2}, \Theta)
\end{aligned} \tag{3.95}$$

$$\begin{aligned}
I_2(\Theta, l) &= \frac{1}{4\pi} \int_0^{\Theta} \sin \theta i_2(\theta) d\theta \\
&= \sum_{n=2}^{\infty} \frac{(-1)^n (n-1)(jk)^{n-2} l^n}{4\pi n!} \int_0^{\Theta} \frac{d \cos \theta}{\cos^n \theta} \\
&= \sum_{n=2}^{\infty} \frac{(-1)^n (jk)^{n-2} l^n}{4\pi n!} \left[\frac{1}{\cos^{n-1} \Theta} - 1 \right] \\
&= \frac{1}{4\pi(jk)^2} [\cos \Theta \exp(-\frac{jkl}{\cos \Theta}) - \exp(-jkl) + 1 - \cos \Theta]
\end{aligned} \tag{3.96}$$

$$\begin{aligned}
I_3(\Theta, l) &= \frac{1}{4\pi} \int_0^{\Theta} \sin \theta \cos \theta i_3(\theta) d\theta \\
&= \sum_{n=3}^{\infty} \frac{(-1)^n (n-1)(n-2)(jk)^{n-3} l^n}{4\pi n!} \int_0^{\Theta} \frac{d \cos \theta}{\cos^{n-1} \theta} \\
&= \sum_{n=3}^{\infty} \frac{(-1)^n (n-1)(jk)^{n-3} l^n}{4\pi n!} \left[\frac{1}{\cos^{n-2} \Theta} - 1 \right]
\end{aligned} \tag{3.97}$$

The series solution for I_0 and I_1 can be obtained from the recursive solution of p_n whereas I_2 , I_3 can be determined conventionally.

3.7.6 Analysis of g_i^e

We now write g_1 in terms of four independent functions I_0, I_1, I_2, I_3 defined by

$$\begin{aligned} g_1^e &= g_{1,1} + g_{1,2} \\ &= I_0(\Theta_1^1, l_1) - \frac{1}{l_1} I_1(\Theta_1^1, l_1) - \frac{1}{l_2} I_2(\Theta_1^1, l_1) + \frac{1}{l_1 l_2} I_3(\Theta_1^1, l_1, l_2) \\ &\quad + I_0(\Theta_1^2, l_2) - \frac{1}{l_2} I_2(\Theta_1^2, l_2) - \frac{1}{l_1} I_1(\Theta_1^2, l_2) + \frac{1}{l_1 l_2} I_3(\Theta_1^2, l_2, l_1) \end{aligned} \quad (3.98)$$

where l_1, l_2, Θ_1^1 are as shown in Figure 3.11. Θ_1^1 is a function of l_1, l_2 defined by

$$\begin{aligned} \Theta_1^1 &= \tan^{-1} \frac{l_2}{l_1} \\ \Theta_1^2 &= \frac{\pi}{2} - \Theta_1^1 \end{aligned} \quad (3.99)$$

We define a new set of functions with variables l_1, l_2 only

$$I'_0(l_1, l_2) = I_0(\tan^{-1} \frac{l_2}{l_1}, l_1) + I_0(\tan^{-1} \frac{l_1}{l_2}, l_2) \quad (3.100)$$

$$I'_1(l_1, l_2) = \frac{1}{l_1} I_1(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_2} I_2(\tan^{-1} \frac{l_1}{l_2}, l_2) \quad (3.101)$$

$$I'_2(l_1, l_2) = \frac{1}{l_2} I_2(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_1} I_1(\tan^{-1} \frac{l_1}{l_2}, l_2) \quad (3.102)$$

$$I'_3(l_1, l_2) = \frac{1}{l_1 l_2} I_3(\tan^{-1} \frac{l_2}{l_1}, l_1) + \frac{1}{l_1 l_2} I_3(\tan^{-1} \frac{l_1}{l_2}, l_2) \quad (3.103)$$

We can now expand g_1 as a linear combination of the I'_i . Similarly, if node i is the second, third or fourth node in element e , it can be expressed in terms of I'_0, I'_1, I'_2 and I'_3 according to

$$\begin{pmatrix} g_1^e \\ g_2^e \\ g_3^e \\ g_4^e \end{pmatrix} = \begin{pmatrix} I'_0(l_1, l_2) - I'_1(l_1, l_2) - I'_2(l_1, l_2) + I'_3(l_1, l_2) \\ I'_1(l_1, l_2) - I'_3(l_1, l_2) \\ I'_3(l_1, l_2) \\ I'_2(l_1, l_2) - I'_3(l_1, l_2) \end{pmatrix} \quad (3.104)$$

Although quite complicated, the series solutions of I'_0, I'_1, I'_2, I'_3 can be obtained from I_0, I_1, I_2, I_3 .

3.7.7 Triangular Elements

In the case of triangular elements problem, we can apply a dimensionless set of coordinate (η_1, η_2, η_3) which satisfies

$$\mathbf{r} = \sum_{k=1}^3 \eta_k \mathbf{r}^k \quad (3.105)$$

Where $(\mathbf{r}^1, \mathbf{r}^2, \mathbf{r}^3)$ are the coordinates of the three vertices on a triangular element. (η_1, η_2, η_3) are not independent and they follow the relationship

$$\eta_1 + \eta_2 + \eta_3 = 1 \quad (3.106)$$

It should be noted that (η_1, η_2, η_3) all vary from 0 to 1. (η_1, η_2) can be chosen as independent bases and we have $\eta_3(\eta_1, \eta_2) = 1 - \eta_1 - \eta_2$

$$\begin{aligned} \frac{\partial \mathbf{r}}{\partial \eta_1} &= \mathbf{r}^1 - \mathbf{r}^3 \\ \frac{\partial \mathbf{r}}{\partial \eta_2} &= \mathbf{r}^2 - \mathbf{r}^3 \end{aligned} \quad (3.107)$$

The corresponding Jacobian matrix is

$$\begin{aligned} |\mathbf{J}(\eta_1, \eta_2)| &= \begin{vmatrix} x^1 - x^3 & y^1 - y^3 \\ x^2 - x^3 & y^2 - y^3 \end{vmatrix} \\ &= 2S_{\Delta} \end{aligned} \quad (3.108)$$

This transformation can be more clearly pictured by rearranging equation 3.105 such that

$$\mathbf{r} - \mathbf{r}^3 = \eta_1(\mathbf{r}^1 - \mathbf{r}^3) + \eta_2(\mathbf{r}^2 - \mathbf{r}^3) \quad (3.109)$$

For an arbitrary but linearly varying function f

$$f(\eta_1, \eta_2, \eta_3) = \eta_1 f_1 + \eta_2 f_2 + \eta_3 f_3 \quad (3.110)$$

Here f_1, f_2 and f_3 are the values of f at the three vertices of the triangular elements. We further assume a linear variation for the U^e and $\frac{\partial U^e}{\partial \mathbf{n}^e}$, e.g.

$$\begin{aligned} U^e &= \begin{pmatrix} \eta_1 & \eta_2 & \eta_3 \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \end{pmatrix} \\ \frac{\partial U^e}{\partial \mathbf{n}^e} &= \begin{pmatrix} \eta_1 & \eta_2 & \eta_3 \end{pmatrix} \begin{pmatrix} \frac{\partial U_1^e}{\partial \mathbf{n}_1^e} \\ \frac{\partial U_2^e}{\partial \mathbf{n}_2^e} \\ \frac{\partial U_3^e}{\partial \mathbf{n}_3^e} \end{pmatrix} \end{aligned} \quad (3.111)$$

Figure 3.12: Triangular elements

The Green's function can now be written as

$$\begin{aligned}
\gamma^r \alpha_F^r U_i &= -\sum_{e \neq i}^n \begin{pmatrix} h_1^{e,r} & h_2^{e,r} & h_3^{e,r} \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \end{pmatrix} \\
&\quad - \sum_{e=1}^n \begin{pmatrix} g_1^{e,r} & g_2^{e,r} & g_3^{e,r} \end{pmatrix} \begin{pmatrix} \frac{\partial U_1^e}{\partial n} \\ \frac{\partial U_2^e}{\partial n} \\ \frac{\partial U_3^e}{\partial n} \end{pmatrix} + S R_i \\
\gamma^l \alpha_F^l U_i &= -\sum_{e \neq i}^n \begin{pmatrix} h_1^{e,l} & h_2^{e,l} & h_3^{e,l} \end{pmatrix} \begin{pmatrix} U_1^e \\ U_2^e \\ U_3^e \end{pmatrix} \\
&\quad + \sum_{e=1}^n \begin{pmatrix} g_1^{e,l} & g_2^{e,l} & g_3^{e,l} \end{pmatrix} \begin{pmatrix} \frac{\partial U_1^e}{\partial n} \\ \frac{\partial U_2^e}{\partial n} \\ \frac{\partial U_3^e}{\partial n} \end{pmatrix} + S L_i
\end{aligned} \tag{3.112}$$

The value of $\gamma^{l,r}$ depends on the position of node i . Furthermore, $\gamma^{l,r} = \frac{\Omega_i}{4\pi}$ depends on the value of the solid angle it spans. The coefficients $h_1^e, h_2^e, h_3^e, g_1^e, g_2^e$ and g_3^e can be calculated as

$$\begin{pmatrix} h_1^e \\ h_2^e \\ h_3^e \end{pmatrix} = \frac{\alpha_F}{4\pi} \int_{\Delta_e} \frac{-1 - jk\rho}{\rho^2} \exp(-jk\rho) \cos \angle(\rho, \mathbf{n}) \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix} ds \tag{3.113}$$

$$\begin{pmatrix} g_1^e \\ g_2^e \\ g_3^e \end{pmatrix} = \frac{1}{4\pi} \int_{\Delta_e} \frac{1}{\rho} \exp(-jk\rho) \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix} ds \tag{3.114}$$

Again, the value of ρ satisfies the relationship

$$\rho = | \mathbf{r}^e(\eta_1, \eta_2, \eta_3) - \mathbf{r}_i | \tag{3.115}$$

As for quadrilateral elements, the Green's formulation can be expressed in a matrix form as

$$\mathbf{H}\mathbf{V} = \mathbf{S} \tag{3.116}$$

where $\mathbf{H}$ is composed of four submatrices $H^{l,r}, G^{l,r}$ as discussed before and each submatrix element satisfies

$$\begin{aligned}(H^{l,r})_{ij} &= \sum_{k=1}^K h_{vk}^{ek} \\ (G^{l,r})_{ij} &= \sum_{k=1}^K g_{vk}^{ek}\end{aligned}\tag{3.117}$$

Here we assume that node j is the vertex vk of element ek . ($vk = 1, 2, 3$).

Calculation of Matrix Elements

If node i is not a vertex of element e , the integrals in the expressions for h_k^e, g_k^e are not singular and thus these quantities can be computed numerically by, for example, Gaussian quadrature. If node i is a corner node of element j , then the integral is singular and can be performed through a Taylor series expansion. Without loss of generality, it will be assumed that node i is vertex 3 of the element e . In (η_1, η_2, η_3) coordinate system, $r^i = (0, 0, 1)^T$. The value of ρ as obtained from equation (3.109) is (c.f. figure 3.12)

$$\begin{aligned}\rho &= |\mathbf{r} - \mathbf{r}^i| \\ &= \sqrt{l_1^2 \eta_1^2 + l_2^2 \eta_2^2 - 2\mathbf{l}_1 \cdot \mathbf{l}_2 \eta_1 \eta_2}\end{aligned}\tag{3.118}$$

Since ρ is perpendicular to $\mathbf{n}$, ie. $\cos(\angle \rho, \mathbf{n}) = 0$, then

$$\begin{pmatrix} h_1^e \\ h_2^e \\ h_3^e \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\tag{3.119}$$

Substituting (3.118) into equation (3.114), and expanding the exponential term into Taylor series, we obtain

$$\begin{aligned}g_{1,2}^e &= \frac{1}{4\pi} \int_{\Delta_e} \frac{1}{\rho} \exp(-jk\rho) \eta_{1,2} ds \\ &= \frac{1}{4\pi} \int_{\Delta_e} \frac{\sum_{n=0}^{\infty} \frac{(-jk\rho)^n}{n!}}{\rho} \eta_{1,2} ds \\ &= \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{(-jk)^n}{n!} \int_{\Delta_e} \rho^{n-1} \eta_{1,2} ds\end{aligned}\tag{3.120}$$

Furthermore, g_3^e can be expressed as a function of g_1^e, g_2^e according to

$$\begin{aligned} g_3^e &= \frac{1}{4\pi} \int_{\Delta_e} \frac{\exp(-jk\rho)}{\rho} \eta_3 ds \\ &= \frac{1}{4\pi} \int_{\Delta_e} \frac{\exp(-jk\rho)}{\rho} (1 - \eta_1 - \eta_2) ds \\ &= g_0^e - g_1^e - g_2^e \end{aligned} \quad (3.121)$$

where

$$\begin{aligned} g_0^e &= \frac{1}{4\pi} \int_{\Delta_e} \frac{\exp(-jk\rho)}{\rho} ds \\ &= \frac{\Theta_3}{4jk\pi} + \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{(-jk)^{n-1}}{n!} (l_1 \sin \Theta_1)^n \int_0^{\Theta_3} \frac{d\theta}{\sin^n(\Theta_1 + \theta)} \\ &= \frac{\Theta_3}{4jk\pi} + \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{(-jk)^{n-1} (l_1 \sin \Theta_1)^n}{n!} p_n(\Theta_1, \Theta_3) \end{aligned} \quad (3.122)$$

The quantity $p_n(\Theta_1, \Theta_3) = \int_0^{\Theta_3} \frac{d\theta}{\sin^n(\theta + \Theta_1)}$ can then be obtained recursively as described in Section 3.8. Notice that the relationship between (η_1, η_2) and the polar coordinates is

$$\frac{\eta_1 l_1}{\sin(\Theta_3 - \theta)} = \frac{\rho}{\sin(\pi - \Theta_3)} \quad (3.123)$$

That is

$$\eta_1 = \frac{\rho \sin(\Theta_3 - \theta)}{l_1 \sin \Theta_3} \quad (3.124)$$

so that the integral of g_1^e becomes

$$\begin{aligned} g_1^e &= \frac{1}{4\pi} \int_{\Delta_e} \frac{\exp(-jk\rho)}{\rho} \eta_1 ds \\ &= \frac{1}{4\pi} \int_0^{\Theta_3} d\theta \int_0^{\frac{l_1 \sin \Theta_1}{\sin(\Theta_1 + \theta)}} \frac{\exp(-jk\rho)}{\rho} \frac{\rho \sin(\Theta_3 - \theta)}{l_1 \sin \Theta_3} \rho d\rho \end{aligned} \quad (3.125)$$

We can obtain a series solution for g_1^e as

$$\begin{aligned} g_1^e &= \frac{1}{4\pi l_1 \sin \Theta_3} \left\{ \frac{\sin \Theta_2}{(-jk)^2} [\sin \Theta_1 \exp(-jkl_1) - \sin \Theta_2 \exp(-\frac{jkl_1 \sin \Theta_1}{\sin \Theta_2})] \right. \\ &\quad + \frac{\cos \Theta_2}{(-jk)^2} [-\cos \Theta_1 - \cos \Theta_2 + \sum_{n=0}^{\infty} \frac{n(-jkl_1 \sin \Theta_1)^{n+1}}{(n+1)!} p_n] \} \\ &\quad + \frac{\tan \frac{\Theta_1}{2}}{4\pi l_1 (-jk)^2} \end{aligned} \quad (3.126)$$

By symmetry, g_2^e is identical to g_1^e except for the interchanging the (Θ_1, Θ_2) and (l_1, l_2) , so that

$$\begin{aligned} g_2^e &= \frac{1}{4\pi l_2 \sin \Theta_3} \left\{ \frac{\sin \Theta_1}{(-jk)^2} [\sin \Theta_2 \exp(-jkl_2) - \sin \Theta_1 \exp(-\frac{jkl_2 \sin \Theta_2}{\sin \Theta_1})] \right. \\ &\quad + \frac{\cos \Theta_1}{(-jk)^2} [-\cos \Theta_1 - \cos \Theta_2 + \sum_{n=0}^{\infty} \frac{n(-jkl_2 \sin \Theta_2)^{n+1}}{(n+1)!} p_n(\Theta_2, \Theta_3)] \} \\ &\quad + \frac{\tan \frac{\Theta_2}{2}}{4\pi l_2 (-jk)^2} \end{aligned} \quad (3.127)$$

and

$$g_3^e = g_0^e - g_1^e - g_2^e \quad (3.128)$$

Similarly, we can obtain the series solution of g_k^e by choosing (η_1, η_3) as independent bases if node i is vertex 2 of element e . choosing (η_2, η_3) if node i is vertex 3 of element e . The form of solutions should be similar to previous solutions except interchange subscripts. The consequent solution is:

- If node i is vertex 1 of element e

$$\begin{aligned} g_0^e &= \frac{\Theta_1}{4jk\pi} + \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{(-jk)^{n-1} (l_2 \sin \Theta_2)^n}{n!} p_n(\Theta_2, \Theta_1) \\ g_2^e &= \frac{1}{4\pi l_2 \sin \Theta_1} \left\{ \frac{\sin \Theta_1}{(-jk)^2} [\sin \Theta_2 \exp(-jkl_2) - \sin \Theta_3 \exp(-\frac{jkl_2 \sin \Theta_2}{\sin \Theta_3})] \right. \\ &\quad + \frac{\cos \Theta_1}{(-jk)^2} [-\cos \Theta_2 - \cos \Theta_3 + \sum_{n=0}^{\infty} \frac{n(-jkl_2 \sin \Theta_2)^{n+1}}{(n+1)!} p_n] \} \\ &\quad + \frac{\tan \frac{\Theta_1}{2}}{4\pi l_2 (-jk)^2} \\ g_3^e &= \frac{1}{4\pi l_3 \sin \Theta_1} \left\{ \frac{\sin \Theta_2}{(-jk)^2} [\sin \Theta_3 \exp(-jkl_3) - \sin \Theta_2 \exp(-\frac{jkl_3 \sin \Theta_3}{\sin \Theta_2})] \right. \\ &\quad + \frac{\cos \Theta_2}{(-jk)^2} [-\cos \Theta_2 - \cos \Theta_3 + \sum_{n=0}^{\infty} \frac{n(-jkl_3 \sin \Theta_3)^{n+1}}{(n+1)!} p_n(\Theta_3, \Theta_1)] \} \\ &\quad + \frac{\tan \frac{\Theta_1}{2}}{4\pi l_3 (-jk)^2} \\ g_1^e &= g_0^e - g_2^e - g_3^e \end{aligned} \quad (3.129)$$

- If node i is vertex 2 of element e

$$\begin{aligned} g_0^e &= \frac{\Theta_2}{4jk\pi} + \frac{1}{4\pi} \sum_{n=0}^{\infty} \frac{(-jk)^{n-1} (l_3 \sin \Theta_3)^n}{n!} p_n(\Theta_3, \Theta_2) \\ g_3^e &= \frac{1}{4\pi l_3 \sin \Theta_1} \left\{ \frac{\sin \Theta_1}{(-jk)^2} [\sin \Theta_3 \exp(-jkl_3) - \sin \Theta_1 \exp(-\frac{jkl_3 \sin \Theta_3}{\sin \Theta_1})] \right. \\ &\quad + \frac{\cos \Theta_1}{(-jk)^2} [-\cos \Theta_3 - \cos \Theta_1 + \sum_{n=0}^{\infty} \frac{n(-jkl_3 \sin \Theta_3)^{n+1}}{(n+1)!} p_n] \} \\ &\quad + \frac{\tan \frac{\Theta_2}{2}}{4\pi l_3 (-jk)^2} \\ g_1^e &= \frac{1}{4\pi l_1 \sin \Theta_2} \left\{ \frac{\sin \Theta_3}{(-jk)^2} [\sin \Theta_1 \exp(-jkl_1) - \sin \Theta_3 \exp(-\frac{jkl_1 \sin \Theta_1}{\sin \Theta_3})] \right. \\ &\quad + \frac{\cos \Theta_3}{(-jk)^2} [-\cos \Theta_3 - \cos \Theta_1 + \sum_{n=0}^{\infty} \frac{n(-jkl_3 \sin \Theta_1)^{n+1}}{(n+1)!} p_n(\Theta_1, \Theta_2)] \} \\ &\quad + \frac{\tan \frac{\Theta_2}{2}}{4\pi l_1 (-jk)^2} \\ g_2^e &= g_0^e - g_3^e - g_1^e \end{aligned} \quad (3.130)$$

3.8 Recursive Evaluation of $p_n(\theta_1, \theta_2)$

We now present a recursive formula for the set of functions $p_n(\theta_1, \theta_2)$ defined by

$$p_n(\theta_1, \theta_2) = \int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta + \theta_1)} \quad (3.131)$$

that have appeared frequently in previous sections. The p_n have been generally used to construct the function $f(x)$ according to

$$f(x) = \sum_{n=0}^{\infty} c_n(x) p_n(\theta_1, \theta_2) \quad (3.132)$$

In terms of f the sum of the infinite series in equation (3.132) can then be expressed as dot product of the two vectors infinite dimensional vectors $\mathbf{C}, \mathbf{P}$

$$f(x) = \mathbf{C} \cdot \mathbf{P} \quad (3.133)$$

given by

$$\mathbf{C} = \begin{pmatrix} c_0(x) \\ c_1(x) \\ \vdots \\ c_{\infty}(x) \end{pmatrix}; \quad \mathbf{P} = \begin{pmatrix} p_0(\theta_1, \theta_2) \\ p_1(\theta_1, \theta_2) \\ \vdots \\ p_{\infty}(\theta_1, \theta_2) \end{pmatrix} \quad (3.134)$$

For all elements discussed in this chapter, the series representation of function $f(x)$ is absolutely convergent, so that we can evaluate the series. Since we encounter this type of series numerous times throughout this chapter, it's tedious to prove the convergence case by case. However, notice that all the series solution we involved have the form $f(x) = \sum_n \frac{n^k (cx)^n}{n!} p_n(\theta_1, \theta_2)$ where k is non-negative integer, $0 < \theta_1 + \theta_2 < \pi$, c is some constant and x is length or width of the discretized element. It can be proved in the next subsection that such series converge absolutely. We can thus take the first N components of the vectors $\mathbf{C}, \mathbf{P}$ to form new vectors $\mathbf{C}_N, \mathbf{P}_N$ in N dimensional subspace such that $f(x)$ is equal to

$$f(x) = \mathbf{C}_N(x) \cdot \mathbf{P}_N + O(x^{N+1}) \quad (3.135)$$

where N is a sufficiently large number. Practically the series converges rapidly and for $N = 20$ the relative error will typically be less than 10^{-5} . The manner in which $\mathbf{C}_N$ is

evaluated is problem dependent and usually can be evaluated recursively. This quantity can be obtained either directly or recursively in all the problems in this thesis. However, constructing P_N is somewhat time-consuming since the integral

$$p_n(\theta_1, \theta_2) = \int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta + \theta_1)} \quad (3.136)$$

does not have a simple analytic expression when n gets larger than 3. The following recursive approach, that has been developed by the author, allow the p_n in terms of p_{n-1} and p_{n-2} . Since the quantities p_0, p_1 are easily obtained, this recursive algorithm is computationally efficient and requires little computer memory. The steps of the algorithm are

- Evaluate the base case. ($n=0,1$)

To evaluate p_0 and p_1 , observe that

$$p_0(\theta_1, \theta_2) = \int_0^{\theta_2} d\theta = \theta_2 \quad (3.137)$$

$$p_1(\theta_1, \theta_2) = \int_0^{\theta_2} \frac{d\theta}{\sin(\theta + \theta_1)} = \ln \tan \frac{\theta_1 + \theta_2}{2} - \ln \tan \frac{\theta_1}{2} \quad (3.138)$$

- $n=2,3, \dots$

Thus p_n can be found recursively as

$$\begin{aligned} p_n(\theta_1, \theta_2) &= \int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta + \theta_1)} \\ &= \frac{\cos \theta_1}{(n-1)q_{n-1}(\theta_1)} - \frac{\cos(\theta_1 + \theta_2)}{(n-1)q_{n-1}(\theta_1 + \theta_2)} + \frac{n-2}{n-1} p_{n-2}(\theta_1, \theta_2) \end{aligned} \quad (3.139)$$

where

$$q_n(\theta) = \sin^n \theta = \sin \theta q_{n-1}(\theta) \quad (3.140)$$

can be evaluated recursively as well.

3.9 Convergence of Series Solution

In this section, we will prove the series of the type $f(x) = \sum_n \frac{n^k (cx)^n}{n!} p_n(\theta_1, \theta_2)$ converges absolutely provided k is non-negative integer, $0 < \theta_1 + \theta_2 < \pi$, c is a constant and x is small enough.

First we can prove for $0 < \theta_1 + \theta_2 < \pi$, $|p_n(\theta_1, \theta_2)|$ bounded. It is obvious since

$$\begin{aligned}
 |p_n(\theta_1, \theta_2)| &= \left| \int_0^{\theta_2} \frac{d\theta}{\sin^n(\theta + \theta_1)} \right| \\
 &< \int_0^{\theta_2} \frac{d\theta}{|\sin(\theta + \theta_1)|^n} \\
 &< \int_0^{\theta_2} \frac{d\theta}{C_{min}^n} \\
 &= \frac{\theta_2}{C_{min}^n}
 \end{aligned} \tag{3.141}$$

C_{min} is a finite value that satisfies

$$C_{min} = \text{Min}\left(\frac{1}{|\sin(\theta + \theta_1)|}, 0 < \theta < \theta_2\right) \tag{3.142}$$

According to Cauchy convergence criterion, the series $g(x) = \sum_n g_n = \sum_n \frac{n^k |cx|^n}{n! C_{min}^n} \frac{\theta_2}{C_{min}^n}$ converges absolutely since

$$\lim_{n \rightarrow \infty} \frac{g_n}{g_{n-1}} = \lim_{n \rightarrow \infty} \frac{|cx|}{nC_{min}} \left(1 + \frac{1}{n-1}\right)^k = 0 \tag{3.143}$$

Further $|f(x)| < g(x)$, implying that $f(x)$ converges absolutely.

3.10 Conclusion

In this chapter we have developed a three dimensional boundary element algorithm. Specifically, we found that in a piecewise homogeneous medium the scalar potential of an electromagnetic field can be expressed as the surface integral on the boundary given by

$$\gamma U(r) + \int_{S-S_e} U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'} ds' = \int_{S-S_e} G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'} ds' \tag{3.144}$$

Here $\gamma = \frac{\Omega_0}{4\pi}$ depends on the shape of the waveguide. As a result, we have

$$\gamma = \begin{cases} 1 & \text{inside region} \\ \frac{1}{2} & \text{on the smooth boundary} \\ \frac{\Delta\Omega_0}{4\pi} & \text{on sharp corner of boundary} \end{cases} \tag{3.145}$$

The Green's function $G(\mathbf{r}', \mathbf{r})$ appearing in the above equations, in three dimensional space, has the form

$$\begin{cases} G(\rho) &= \frac{1}{4\pi\rho} \exp(-jk\rho) \\ \frac{\partial G(\rho)}{\partial n} &= -\frac{1-jk\rho}{4\pi\rho^2} \exp(-jk\rho) \end{cases} \tag{3.146}$$

For a single boundary node, we can always find two equations corresponding to the regions on the both sides of the node. Thus if we discretize the waveguide boundary into N cells, there are $2N$ equations and $2N$ unknowns. Expressing these linear equations in matrix form yields

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (3.147)$$

By solving this linear system, we obtain the field distribution on the waveguide boundary and the field inside the waveguide. Within each cell, the scalar potential is expressed by the Taylor expansion

$$U(\mathbf{r}') = U(0) + \nabla' U(\mathbf{r}') \cdot \mathbf{r} + O(|\mathbf{r}'|^2) \quad (3.148)$$

Retaining only the first term in this series yields the constant element algorithm while including as well the second term generates the linear element algorithm.

The computation of the matrix element in $\mathbf{H}$ will be finally discussed in Section 3.31 and Section 3.7.

Chapter 4

Two Dimensional Boundary Element Method

4.1 Introduction

This chapter presents the theory of the two dimensional boundary element method (BEM). While not immediately applicable to most realistic waveguide structures, the two-dimensional formalism is relatively simple compared to the three-dimensional discussion of Chapter 3. In Section 4.3 we will discuss the scalar and vector formulation of the problem. The constant element formulation and the linear element formulation are studied in the last two sections respectively.

4.2 2-D Green's Theorem

Consider a two-dimensional waveguide in which the dimensionality of the Helmholtz Equation (3.8) is reduced by one

$$\nabla_{\perp}^2 U(x, z) + n(x, z)^2 k_0^2 U(x, z) = 0 \quad (4.1)$$

so that $\nabla_{\perp}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}$ is now a two dimensional operator. We can find a two-dimensional Green's function then satisfies.

$$\nabla_{\perp}^2 G(\mathbf{r}', \mathbf{r}) + k^2 G(\mathbf{r}', \mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}) \quad (4.2)$$

which is solved by a zeroth order Hankel function of the second kind

$$G(\mathbf{r}', \mathbf{r}) = G(\rho) = \frac{1}{4j} H_0^{(2)}(k\rho) \quad (4.3)$$

The directional derivative of G is given as

$$\begin{aligned} \frac{\partial G(\rho)}{\partial n} &= \frac{\partial G(\rho)}{\partial \rho} \cos \angle(\rho, \mathbf{n}) \\ &= \frac{jk}{4} H_1^{(2)}(k\rho) \cos \angle(\rho, \mathbf{n}) \end{aligned} \quad (4.4)$$

As a special case of the three dimensional problem, all the derivations given in our discussion of the three dimensional BEM formulation are valid in two dimensions if the boundary surface is treated as infinite along the y direction (Figure 4.1). If the length of boundary surface is written as L where L is sufficiently large, the volume and boundary surface integral described in Chapter 3 become

$$\begin{aligned} \int_V \phi d\tau &= L \int_{s_{\perp}} \phi d\sigma \\ \oint_S \phi ds &= L \int_{\Gamma} \phi dl \end{aligned} \quad (4.5)$$

where ϕ can be any function that is invariant along the y direction. $d\tau$ is the volume integral over infinite region V , $d\sigma$ is the area integral cross section $s_{\perp}$ on x, z plan. In the second equation, ds is the area integral over V 's boundary surface S and dl is the line integral over $s_{\perp}$'s boundary. Hence the three dimensional divergence theorem reduces to

$$\int_{s_{\perp}} \nabla_{\perp} \cdot \mathbf{A} d\sigma = \oint_l \mathbf{A} \cdot \mathbf{n} dl \quad (4.6)$$

By applying Green's formula and following the three-dimensional derivation we obtain the two dimensional Green's equation analogous to Equation (3.12)

$$-\int_{\Gamma_c} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] dl' = \int_{\Gamma} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] dl' \quad (4.7)$$

Figure 4.1: Two dimension problem as a special case of a three dimension problem in which the boundary surface is infinite in y direction

In the above equation Γ_ϵ is an infinitely small circle that encloses the observation point $\mathbf{r}'$. As the radius of the circle approaches zero, we have

$$-\frac{\partial U(\mathbf{r})}{\partial n} \int_{\Gamma_\epsilon} G(\mathbf{r}', \mathbf{r}) dl' + U(\mathbf{r}) \int_{\Gamma_\epsilon} \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'} dl' = \int_{\Gamma} [G(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial n'} - U(\mathbf{r}') \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'}] dl' \quad (4.8)$$

The evaluation of the two integrals on the left of (4.8) is then rather simple, as

$$\begin{aligned} \int_{\Gamma_\epsilon} G(\mathbf{r}', \mathbf{r}) dl' &= \lim_{\rho_\epsilon \rightarrow 0} \int_0^{2\pi} \frac{1}{4j} H_0^{(2)}(k\rho) \rho d\theta \\ &= 0 \end{aligned} \quad (4.9)$$

$$\begin{aligned} \int_{\Gamma_\epsilon} \frac{\partial G(\mathbf{r}', \mathbf{r})}{\partial n'} dl' &= \lim_{\rho_\epsilon \rightarrow 0} \int_0^{2\pi} \frac{ik}{4} H_1^{(2)}(k\rho) \rho d\theta \\ &= \frac{\delta\theta}{2\pi} \end{aligned} \quad (4.10)$$

This leads to the following 2-D Green's equation which is analogous to Equation (3.24)

$$\gamma U(\mathbf{r}) + \int_{\Gamma} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}', \mathbf{r})}{\partial \mathbf{n}'} dl' = \int_{\Gamma} G^{(i)}(\mathbf{r}', \mathbf{r}) \frac{\partial U(\mathbf{r}')}{\partial \mathbf{n}'} dl' \quad (4.11)$$

Figure 4.2: Angle spans by field point

The γ coefficient depends on both the position of the observation point and the waveguide geometry (Figure 4.2)..

$$\gamma = \begin{cases} 1 & \text{inside region} \\ \frac{1}{2} & \text{on the smooth boundary} \\ \frac{\delta\theta}{2\pi} & \text{on sharp corner of boundary} \end{cases} \quad (4.12)$$

The discrete integral (4.11) is given as

$$U(\mathbf{r}) + \sum_{j=1}^N \int_{\Gamma_j} U(\mathbf{r}') \frac{\partial G^{(i)}(\mathbf{r}_j, \mathbf{r})}{\partial \mathbf{n}_j} dl = \sum_{j=1}^N \int_{\Gamma_j} G^{(i)}(\mathbf{r}_j, \mathbf{r}) \frac{\partial U(\mathbf{r}_j)}{\partial \mathbf{n}_j} dl \quad (4.13)$$

Where $\mathbf{r}$ is inside the waveguide, for the case $\mathbf{r}$ on the boundary, we obtain

$$\gamma U(\mathbf{r}) + \sum_{j \neq i_0}^N \int_{\Gamma_j} U(\mathbf{r}_j) \frac{\partial G^{(i)}(\mathbf{r}_j, \mathbf{r})}{\partial \mathbf{n}_j} dl = \sum_{j=1}^N \int_{\Gamma_j} G^{(i)}(\mathbf{r}_j, \mathbf{r}) \frac{\partial U(\mathbf{r}_j)}{\partial \mathbf{n}_j} dl \quad (4.14)$$

Here we discretize the boundary into N segments and $\mathbf{r}$ lies on the i_0 -th element.

4.3 Scalar Formalism

As discussed in Chapter 3, the scalar formalism can be applied to general three dimensional waveguides if the difference in refractive index across boundary is small as all the field components and their directional derivatives are then nearly continuous across each

boundary between media with different refractive indices. In 2-D, besides, scalar formalism is exact solution to E_y . If the input field is TE, only the (H_x, E_y, H_z) components are nonzero. From the Maxwell's Equations, we have

$$\begin{aligned}\frac{\partial E_y}{\partial x} &= j\omega\mu H_z \\ \frac{\partial E_y}{\partial z} &= -j\omega\mu H_x\end{aligned}\quad (4.15)$$

The fields H_x, H_z are continuous across the waveguide boundaries, insuring the continuity the directional derivative of E_y . The continuity E_y across boundaries is further guaranteed by the boundary conditions discussed in Chapter 2. The scalar approximation is thus exact on E_y component of the TE mode. Once we obtain the E_y field distribution, we can solve for H_x, H_z by rearranging the equations (4.15)

$$\begin{aligned}H_z &= \frac{1}{j\omega\mu} \frac{\partial E_y}{\partial x} \\ H_x &= \frac{j}{\omega\mu} \frac{\partial E_y}{\partial z}\end{aligned}\quad (4.16)$$

As in 3-D case, the nodes on waveguide boundary will satisfy Helmholtz equations in both the left and right regions adjacent to the node, thus

$$\begin{aligned}\gamma^r U^r(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial n_j^r} U^r(\mathbf{r}_j) dl + \sum_j \int_{\Gamma_j} G_r(\mathbf{r}_j - \mathbf{r}) \frac{\partial U^r(\mathbf{r}_j)}{\partial n_j^r} dl + SR \\ \gamma^l U^l(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial n_j^l} U^l(\mathbf{r}_j) dl + \sum_j \int_{\Gamma_j} G_l(\mathbf{r}_j - \mathbf{r}) \frac{\partial U^l(\mathbf{r}_j)}{\partial n_j^l} dl + SL\end{aligned}\quad (4.17)$$

All the definitions of U, n, SR, SL are similar to the 3-D case. However, we can drop the superscript l, r by noticing that

$$\begin{aligned}U(\mathbf{r}) &= U^l(\mathbf{r}) = U^r(\mathbf{r}) \\ \frac{\partial U(\mathbf{r})}{\partial n} &= \frac{\partial U^l(\mathbf{r})}{\partial n^l} = -\frac{\partial U^r(\mathbf{r})}{\partial n^r}\end{aligned}\quad (4.18)$$

Equation (3.30) then becomes

$$\begin{aligned}\gamma^r U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial n_j^r} U(\mathbf{r}_j) dl - \sum_j \int_{\Gamma_j} G_r(\mathbf{r}_j - \mathbf{r}) \frac{\partial U(\mathbf{r}_j)}{\partial n_j^r} dl + SR \\ \gamma^l U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial n_j^l} U(\mathbf{r}_j) dl + \sum_j \int_{\Gamma_j} G_l(\mathbf{r}_j - \mathbf{r}) \frac{\partial U(\mathbf{r}_j)}{\partial n_j^l} dl + SL\end{aligned}\quad (4.19)$$

4.4 Semi-Vector Formalism

For a TM input field, the only nonzero field components are (H_y, E_x, E_z) . H_y is continuous since it is transverse to any boundary. On the other hand,

$$\begin{aligned}\frac{\partial H_y}{\partial x} &= -j\omega\epsilon E_z \\ \frac{\partial H_y}{\partial z} &= j\omega\epsilon E_x\end{aligned}\tag{4.20}$$

Since E_z, E_x are continuous along the x, z directions respectively, the directional derivative of H_y induces a discontinuity and

$$\begin{aligned}\frac{1}{\epsilon_1} \frac{\partial H_{y1}}{\partial x} &= \frac{1}{\epsilon_2} \frac{\partial H_{y2}}{\partial x} \\ \frac{1}{\epsilon_1} \frac{\partial H_{y1}}{\partial z} &= \frac{1}{\epsilon_2} \frac{\partial H_{y2}}{\partial z}\end{aligned}\tag{4.21}$$

Taking H_y as the wave component U to be calculated, we have

$$\begin{aligned}U &= H_y^l = H_y^r \\ \frac{\partial U}{\partial n} &= \frac{1}{n_l^2} \frac{\partial H_y^l}{\partial n^l} = -\frac{1}{n_r^2} \frac{\partial H_y^r}{\partial n^r}\end{aligned}\tag{4.22}$$

The semi-vector formalism for the TM mode can now be written as

$$\begin{aligned}\gamma^r U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial n_j^r} U_j(\mathbf{r}_j) dl - \sum_j \int_{\Gamma_j} G_r(\mathbf{r}_j - \mathbf{r}) \alpha_{TM}^r \frac{\partial U_j(\mathbf{r}_j)}{\partial n_j} dl + SR \\ \gamma^l U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial n_j^l} U_j(\mathbf{r}_j) dl + \sum_j \int_{\Gamma_j} G_l(\mathbf{r}_j - \mathbf{r}) \alpha_{TM}^l \frac{\partial U_j(\mathbf{r}_j)}{\partial n_j} dl + SL\end{aligned}\tag{4.23}$$

where the TM coefficient $\alpha_{TM}^{l,r}$ satisfies

$$\alpha_{TM}^{l,r} = n_{l,r}^2\tag{4.24}$$

To be consistent with 3-D case, we can introduce a global coefficient α_F where F can be TM or TE , for TE mode, $\alpha_{TE} = 1$, thus we can unify scalar, TE and semi-vector TM formalism as

$$\begin{aligned}\gamma^r U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r})}{\partial n_j^r} U_j(\mathbf{r}_j) dl - \sum_j \int_{\Gamma_j} G_r(\mathbf{r}_j - \mathbf{r}) \alpha_F^r \frac{\partial U_j(\mathbf{r}_j)}{\partial n_j} dl + SR \\ \gamma^l U(\mathbf{r}) &= -\sum_{j \neq i_0} \int_{\Gamma_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r})}{\partial n_j^l} U_j(\mathbf{r}_j) dl + \sum_j \int_{\Gamma_j} G_l(\mathbf{r}_j - \mathbf{r}) \alpha_F^l \frac{\partial U_j(\mathbf{r}_j)}{\partial n_j} dl + SL\end{aligned}\tag{4.25}$$

Figure 4.3: Field distribution in (A) Constant Element (B) Linear Element

4.5 Constant Element Algorithm

The basic idea of the constant element algorithm is the same as that discussed in 3-D case. We assume a uniform field distribution within each boundary element. For a certain boundary element i with node i at center of that element, if we assume that the field distribution is approximately equal to a constant value U_i ,

$$U(\mathbf{r}_i) = U_i + O(\delta l) \quad (4.26)$$

Discretizing the waveguide, and assuming constant U over a single element, we obtain the constant element formalism, (Figure 4.4)

$$\begin{aligned} \frac{1}{2}U_i^r &= -\sum_{j \neq i} U_j^r \int_{\Gamma_j} \frac{\partial G_r(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j^r} dl + \sum_j \frac{\partial U_j^r}{\partial n_j^r} \alpha_F^r \int_{\Gamma_j} G_r(\mathbf{r}_j - \mathbf{r}_i) dl + S R_i \\ \frac{1}{2}U_i^l &= -\sum_{j \neq i} U_j^l \int_{\Gamma_j} \frac{\partial G_l(\mathbf{r}_j - \mathbf{r}_i)}{\partial n_j^l} dl + \sum_j \frac{\partial U_j^l}{\partial n_j^l} \alpha_F^l \int_{\Gamma_j} G_l(\mathbf{r}_j - \mathbf{r}_i) dl + S L_i \end{aligned} \quad (4.27)$$

Again, as in the three dimensional case, the above equation can be rewritten in matrix form as

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (4.28)$$

The definitions of $\mathbf{H}$, $\mathbf{V}$, $\mathbf{S}$ are the same as in the three dimensional constant element algorithm. The matrix $\mathbf{H}$ is composed of submatrices $G^{l,r}$, $H^{l,r}$ where the matrix elements

Figure 4.4: Configuration of 2 dimension structure

are line integrals and the distance between two elements is given by (Figure 4.4)

$$\vec{\rho} = \mathbf{r}_j - \mathbf{r}_i = \mathbf{r}_{ij}^0 + \vec{\xi} \quad (4.29)$$

- Off-diagonal elements

If element $i \neq j$, introducing the dimensionless coordinate ξ which varies from -1 to +1 on element j , the matrix element of the submatrices $G^{l,r}$, $H^{l,r}$ is given by

$$\begin{aligned} h_{ij}^{l,r} &= \int_{\Delta l} \frac{\partial G^{l,r}(\mathbf{r}_i, \mathbf{r}_j)}{\partial \mathbf{n}_j} dl \\ &= \int_{-1}^{+1} \frac{1}{4} j k H_1^{(2)}(k\rho) \cos \angle(\rho, \mathbf{n}) d\xi \frac{l_j}{2} \end{aligned} \quad (4.30)$$

$$\begin{aligned} g_{ij}^{l,r} &= \alpha_F^{l,r} \int_{\Delta l} G(\mathbf{r}_i, \mathbf{r}_j) dl \\ &= \int_{-1}^{+1} \frac{1}{4j} H_0^{(2)}(k\rho) d\xi \frac{l_j}{2} \end{aligned} \quad (4.31)$$

As the integrals above do not involve in singular integration, we can evaluate them by Gaussian Quadrature.

- Diagonal Matrix Elements

If the element i and j are identical, the integrals above become singular and are given by

$$h_{ii}^{l,r} = \int_{-1}^{0-} \frac{1}{4} j k H_1^{(2)}(k\rho) \cos \angle(\rho, \mathbf{n}) d\xi \frac{l_i}{2} + \int_{0+}^{+1} \frac{1}{4} j k H_1^{(2)}(k\rho) \cos \angle(\rho, \mathbf{n}) d\xi \frac{l_i}{2} \quad (4.32)$$

$$\begin{aligned} g_{ii}^{l,r} &= \int_{-1}^{0-} \frac{1}{4j} H_0^{(2)}(-\frac{k l_i}{2} \xi) d\xi \frac{l_i}{2} + \int_{0+}^{+1} \frac{1}{4j} H_0^{(2)}(\frac{k l_i}{2} \xi) d\xi \frac{l_i}{2} \\ &= 2 \int_{0+}^{+1} \frac{1}{4j} H_0^{(2)}(\frac{k l_i}{2} \xi) d\xi \frac{l_i}{2} \end{aligned} \quad (4.33)$$

The variable ρ can now be written as

$$\rho = \frac{l_i}{2} |\xi| \quad (4.34)$$

The evaluation of h_{ii} is similar to the three dimensional case. However, since $\vec{\rho}$ is perpendicular to $\mathbf{n}$ e.g. $\cos \angle(\vec{\rho}, \mathbf{n}) = 0$, we have

$$h_{ii} = 0 \quad (4.35)$$

An analytic form for g_{ii} is difficult to obtain since it involves an integral of the zeroth order Hankel function. However a series form is constructed by expanding

the Hankel function. The series expansion of 0th order Hankel Function of the second kind is

$$H_0^{(2)}(z) = \sum_{k=1}^{\infty} \frac{(-1)^k}{(k!)^2} \left(\frac{z}{2}\right)^{2k} \left[1 - i\frac{2}{\pi}(\ln \frac{z}{2} + \gamma) + \frac{2i}{\pi} \sum_{m=1}^k \frac{1}{m}\right] + [1 - i\frac{2}{\pi}(\ln \frac{z}{2} + \gamma)] \quad (4.36)$$

Where $\gamma^E = 0.5772157$ is the Euler Constant. Substitute the series expansion of the zero order Hankel function (4.36) into the integral (4.33). To integrate the resulting series, we apply the formula

$$\begin{aligned} \int \ln z z^{2k} dz &= \frac{1}{2k+1} \int \ln z dz^{2k+1} \\ &= \frac{1}{2k+1} z^{2k+1} (\ln z - \frac{1}{2k+1}) \end{aligned} \quad (4.37)$$

This yields

$$\begin{aligned} \int H_0^{(2)}(z) dz &= \int \left\{ \sum_{k=1}^{\infty} \frac{(-1)^k}{(k!)^2} \left(\frac{z}{2}\right)^{2k} \left[1 - i\frac{2}{\pi}(\ln \frac{z}{2} + \gamma) + \frac{2i}{\pi} \sum_{m=1}^k \frac{1}{m}\right] \right. \\ &\quad \left. + [1 - i\frac{2}{\pi}(\ln \frac{z}{2} + \gamma)] \right\} dz \\ &= \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+1)2^{2k}(k!)^2} z^{2k+1} \left[1 - i\frac{2}{\pi}(\ln \frac{z}{2} + \gamma - \frac{1}{2k+1}) + \frac{2i}{\pi} \sum_{m=1}^k \frac{1}{m}\right] \\ &\quad + [1 - i\frac{2}{\pi}(\ln \frac{z}{2} - 1 + \gamma)] z \end{aligned} \quad (4.38)$$

Our series expansion for g_{ii} is finally

$$\begin{aligned} g_{ii} &= \int_{\Delta l} \frac{1}{4j} H_0^{(2)}(k\rho) dl \\ &= \int_{-1}^{+1} \frac{1}{4j} H_0^{(2)}\left(\frac{kl_z}{2}\xi\right) d\xi \frac{l_z}{2} \\ &= \frac{1}{2jk} \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+1)2^{2k}(k!)^2} \left(\frac{kl_z}{2}\right)^{2k+1} \left[1 - i\frac{2}{\pi}(\ln \frac{kl_z}{4} + \gamma - \frac{1}{2k+1} - \sum_{m=1}^k \frac{1}{m})\right] \\ &\quad + [1 - i\frac{2}{\pi}(\ln \frac{kl_z}{4} - 1 + \gamma)] \frac{kl_z}{2} \end{aligned} \quad (4.39)$$

This series converges absolutely.

4.5.1 Summary of Constant Element Algorithm

In this section we have expressed the constant element algorithm as

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (4.40)$$

with matrix elements for $i \neq j$

$$g_{ij}^{l,r} = \begin{cases} \int_{-1}^{+1} \frac{1}{4j} H_0^{(2)}(k\rho) d\xi \frac{l_z}{2} & (j \text{ in left/right region of } i) \\ 0 & (j \text{ not in left/right region of } i) \end{cases} \quad (4.41)$$

$$h_{ij}^{l,r} = \begin{cases} \int_{-1}^{+1} \frac{jk}{4} H_1^{(2)}(k\rho) \cos \angle(\vec{\rho}, \mathbf{n}) d\xi \frac{l_e}{2} & (j \text{ in left/right region of } i) \\ 0 & (j \text{ not in left/right region of } i) \end{cases} \quad (4.42)$$

We can calculate matrix element $h_{ij}^{l,r}$ and $g_{ij}^{l,r}$ using Gaussian quadrature. If $i = j$, we obtain, from the fact $\vec{\rho}$ is perpendicular to the normal vector to the boundary $\mathbf{n}$ that

$$h_{ii}^{l,r} = 0 \quad (4.43)$$

while $g_{ii}^{l,r}$ has the series form

$$g_{ii}^{l,r} = \frac{1}{2jk} \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+1)2^{2k}(k!)^2} \left(\frac{kl_e}{2}\right)^{2k+1} \left[1 - i\frac{2}{\pi} \left(\ln \frac{kl_e}{4} + \gamma - \frac{1}{2k+1} - \sum_{m=1}^k \frac{1}{m}\right)\right] + \left[1 - i\frac{2}{\pi} \left(\ln \frac{kl_e}{4} - 1 + \gamma\right)\right] \frac{kl_e}{2} \quad (4.44)$$

4.6 Linear Element Algorithm

In the linear element algorithm as shown in Figure 4.3, we assume the field varies linearly within each discrete element. Writing the field at the both ends of the element as U_1 and U_2 , the field $U(\xi)$ within the element can be expressed as

$$U(\xi) = \frac{1-\xi}{2} U_1 + \frac{1+\xi}{2} U_2 \quad (4.45)$$

and the Green's function can be written as

$$\gamma U_i + \sum_{e=1}^n \begin{bmatrix} h_1^e & h_2^e \end{bmatrix} \begin{bmatrix} U_1^e \\ U_2^e \end{bmatrix} = \sum_{e=1}^n \begin{bmatrix} g_1^e & g_2^e \end{bmatrix} \begin{bmatrix} \frac{\partial U_1^e}{\partial n} \\ \frac{\partial U_2^e}{\partial n} \end{bmatrix} \quad (4.46)$$

where U_i is the field at node i . In matrix form the above equation is

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (4.47)$$

The definitions of $\mathbf{H}$, $\mathbf{V}$, $\mathbf{S}$ are the same as in the three dimensional linear element algorithm. The matrix elements are evaluated as below.

- Off-diagonal elements

If node i does not belong to element e , the matrix elements can be obtained by Gaussian Quadrature

$$\left. \begin{matrix} h_1 \\ h_2 \end{matrix} \right\} = \int_{-1}^1 \frac{1}{2} (1 \pm \xi) \frac{jk}{4} H_1^{(2)}(k\rho) \cos \angle(\vec{\rho}, \mathbf{n}) d\xi \frac{l_e}{2} \quad (4.48)$$

$$\left. \begin{matrix} g_1 \\ g_2 \end{matrix} \right\} = \int_{-1}^1 \frac{1}{2} (1 \pm \xi) \frac{1}{4j} H_0^{(2)}(k\rho) d\xi \frac{l_e}{2} \quad (4.49)$$

• Diagonal elements

In two cases the integration above is singular.

(a) if node i is vertex 1 of element e ,

(b) if node i is vertex 2 of element e .

First we consider case (a) for which

$$\rho = \frac{l_e}{2}(\xi + 1) \quad (4.50)$$

$$h_1 = h_2 = 0 \quad (4.51)$$

The series expressions for g_1 and g_2 can be obtained as before. First, considering g_1 , notice that there is a singularity at $\xi = -1$. This singularity is removable as a result of the properties of Hankel's function $\lim_{z \rightarrow 0} H_0^{(2)} = -i \frac{2}{\pi} \ln z$, so that $\lim_{z \rightarrow 0} z H_0^{(2)} = -i \frac{2}{\pi} \lim_{z \rightarrow 0} z \ln z = 0$. Further, for a sufficiently small ϵ , integral

$$\begin{aligned} \int_{0+}^{\epsilon} H_0^{(2)}(z) dz &\approx -i \frac{2}{\pi} \int_{0+}^{\epsilon} \ln z dz \\ &= -i \frac{2}{\pi} [z \ln z \Big|_{0+}^{\epsilon} - z \Big|_{0+}^{\epsilon}] \\ &\rightarrow 0 \end{aligned} \quad (4.52)$$

Thus g_1, g_2 are integrable. We can therefore write the integral as

$$\begin{aligned} g_1 &= \int_{-1+\epsilon}^1 \frac{1}{2} (1 - \xi) \frac{1}{4j} H_0^{(2)}\left(\frac{kl_e}{2}(\xi + 1)\right) d\xi \frac{l_e}{2} \\ &= \int_{-1+\epsilon}^1 \frac{1}{2} [2 - (1 + \xi)] \frac{1}{4j} H_0^{(2)}\left(\frac{kl_e}{2}(\xi + 1)\right) d\xi \frac{l_e}{2} \\ &= \int_{z=0+}^{kl_e} \frac{1}{4kj} H_0^{(2)}(z) dz - \int_{z=0+}^{kl_e} \frac{z}{4kj} H_0^{(2)}(z) dz \end{aligned} \quad (4.53)$$

The expression for g_1 now contains two integrations over the Hankel functions $\int H_0^{(2)}(z) dz$ and $\int z H_0^{(2)}(z) dz$. We derived the series solution of the first integration in our discussion of the constant element algorithm while the second integration is

$$\begin{aligned} \int_{0+}^{kl_e} z H_0^{(2)}(z) dz &= z H_1^{(2)}(z) \Big|_{0+}^{kl_e} \\ &= kl_e H_1^{(2)}(kl_e) - \frac{2j}{\pi} \end{aligned} \quad (4.54)$$

Thus the series solution of g_1 is

$$g_1 = \sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+1)2^{2k}(k!)^2} (kl_e)^{2k+1} \left[1 - i \frac{2}{\pi} \left(\ln \frac{kl_e}{2} + \gamma - \frac{1}{2k+1} \right) + \frac{2i}{\pi} \sum_{m=1}^k \frac{1}{m} \right] \\ + \left[1 - i \frac{2}{\pi} \left(\ln \frac{kl_e}{2} - 1 + \gamma \right) \right] z - \frac{kl_e}{4kj} H_1^{(2)}(kl_e) + \frac{1}{2k\pi} \quad (4.55)$$

Similarly, we obtain the solution for g_2 as

$$g_2 = \int_{-1+\epsilon}^1 \frac{1}{2} (1 + \xi) \frac{1}{4j} H_0^{(2)} \left(\frac{kl_e}{2} (\xi + 1) \right) d\xi \frac{l_e}{2} \\ = \frac{1}{4kj} H_1^{(2)}(kl_e) - \frac{1}{2k^2 l_e \pi} \quad (4.56)$$

which is the series solution for g_1, g_2 in the case (a). For case (b), to solve g'_1, g'_2 we simply interchange the values of g_1, g_2 we obtained in case (a), which is valid since

$$\rho' = (1 - \xi) \frac{l_e}{2} \quad (4.57)$$

$$g'_1 = \int_{-1+\epsilon}^{1-\epsilon} \frac{1}{2} (1 - \xi) \frac{1}{4j} H_0^{(2)} \left(\frac{kl_e}{2} (1 - \xi) \right) d\xi \frac{l_e}{2} \\ = \int_{-1+\epsilon}^1 \frac{1}{2} (1 + \xi') \frac{1}{4j} H_0^{(2)} \left(\frac{kl_e}{2} (1 + \xi') \right) d\xi' \frac{l_e}{2} \\ = g_2 \quad (4.58)$$

where $\xi' = -\xi$ and similarly

$$g'_2 = g_1 \quad (4.59)$$

4.7 Mode Calculation

Although the 2-D BEM can be used to calculate the reflectivity of two dimensional dielectric waveguide facets, it is more frequently employed to calculate the modes of three dimensional waveguides. From basic waveguide theory, any field component, $U(x, y, z)$, of a normal mode can be written as

$$U(x, y, z) = U(x, y) \exp(j\beta z) \quad (4.60)$$

The second derivative of $U(x, y, z)$ is given by

$$\frac{\partial^2 U(x, y, z)}{\partial x^2} = \frac{\partial^2 U(x, y)}{\partial x^2} \exp(j\beta z) \\ \frac{\partial^2 U(x, y, z)}{\partial y^2} = \frac{\partial^2 U(x, y)}{\partial y^2} \exp(j\beta z) \\ \frac{\partial^2 U(x, y, z)}{\partial z^2} = -\beta^2 U(x, y) \exp(j\beta z) \quad (4.61)$$

Substituting into the Helmholtz equation, we obtain the Fresnel equation

$$\frac{\partial^2 U(x, y)}{\partial x^2} + \frac{\partial^2 U(x, y)}{\partial y^2} + (n(x, y)^2 k_0^2 - \beta^2) U(x, y) = 0 \quad (4.62)$$

by defining a new wave-vector $k'^2 = n(x, y)^2 k_0^2 - \beta^2$. We can obtain the field distribution on the incident plane using 2-D BEM method. For each explicit value of β , we determine the field distribution satisfies Helmholtz Equation (4.62) by discretizing the boundary at incident plane and solving the linear system (4.63)

$$\mathbf{H}(\beta) \mathbf{V} = 0 \quad (4.63)$$

Notice that for the normal mode corresponding to a resonant solution of $\mathbf{V}$ in the absence of exiting source the right side of (4.63) should be zero. Also since (4.63) is a homogeneous linear equation system as $\mathbf{V}$ is non-zero only if the determinant of $\mathbf{H}$ equals to zero. Thus by finding a set of β values which will result $|\mathbf{H}| = 0$ we can locate the corresponding modes of the waveguide while the eigenvectors are the field distributions on the boundary. The largest value of β is then the propagation constant of the fundamental mode. Applying the 2-DBEM second time with the β and boundary field distributions known, we can thus compute the field distribution everywhere on that plane.

4.8 Singularity of the Nodes at a Sharp Corner

In linear element method, the nodes are at the edge of each boundary element. This leads to a singularity when the two adjacent elements are not flat and the node at the intersection therefore doesn't have a well-defined directional derivative. c.f. 4.5 (a), element 1 and element 2 are interconnected at node k and their normal vector $\mathbf{N1} \perp \mathbf{N2}$. So at node k , it's directional derivative is not defined since if we approach node k from element 1 or element 2 will give us two different values of directional derivative, $\frac{\partial U_k}{\partial N1} \neq \frac{\partial U_k}{\partial N2}$. In such a case, the assumption that the directional derivative is well defined and single valued everywhere in the problem region is not valid, leading

■ Corner node with undefined directional derivative

Figure 4.5: Solution to the singularity at corner node. (a) original element with corner node has undefined directional derivative; (b) Split corner elements; (c) Plus detach two elements slightly; (d) Add smooth boundary at corner

to numerical errors. There are several ways to minimize the impact of this error on our computation as shown in figure 4.5 and discussed below:

- Decreasing the corner element size

By splitting the origin element on the corner of boundary into smaller elements we can minimize the contribution of the corner node to the system. Since at node k

we have an inaccurate value of $\frac{\partial U_k}{\partial n_k}$, but the element it belongs to is so small that it has much lower contribution than other elements do. This reduces the impact of the singularity of the nodes on the entire boundary field distribution. Usually, it's desirable to take $\frac{\partial U_k}{\partial n_k} = \frac{\frac{\partial U_k}{\partial y_1} + \frac{\partial U_k}{\partial y_2}}{2}$ to improve the accuracy.

- Move the two corner elements a short distance away from node k

In this method, we split the corner node into two distinct nodes, or from another point of view, we remove the two small pieces of corner elements from consideration. The field distribution and the directional derivative of all the nodes in our problem are then well defined so that the singularity vanishes. However the error of the field at nodes close to the corner increases due to the absence of the corner elements and this error will propagate to the nodes away from the corner.

- Smooth the sharp corner

This is done by connecting the two corner elements with a stream of smoothly turning fine elements. This generates a more physical solution for the singular problem. However, adding such elements is more complex than the previous two methods.

In 2-D Linear element calculation, the author applied improvement (b) split the corner element by two and (c) moved all the boundary $0.01 * discretizationlength$ from the intersection and obtain the improvement of modal reflectivity as good as around 1 dB for single AR coating waveguide.

Chapter 5

Implementation of BEM

In this chapter the numerical implementation of the BEM will be discussed. We have coded the 2-D BEM in matlab while the 3-D BEM is written in C++. Both solvers consist mainly of four modules: the Element Generator, the Mode Generator, the BEM solver and the Mode Extractor. In addition, the 3-D BEM uses SparseLib++ to analyze the complex sparse matrix problem[95],[96]. The block diagrams are as shown in Figure 5.1 and 5.2. It should be noted that while the Linear Element and Constant Element algorithms are coded slightly differently, their purpose and functionality is identical. Observe also that as a result of the programming language details, the vector and matrix indices start from 1 in the 2-D BEM and 0 in the 3-D BEM. To avoid confusion, we assume that all the indices start from 1 in the implementation of the pseudo code.

We now discuss each of the program modules in turn.

5.1 The Element Generator

The task of the Element Generator is to discretize the boundary of a given waveguide into finite elements and then assign a distinct unsigned integer number, **Element_Id**, to each element. In the constant element algorithm, each element is further associated with a node distinguished by **Node_Id**. In the two dimensional case, the node is the middle point of the element and in the three dimensional case, it is the center of mass

Figure 5.1: Block Diagram of 2-D BEM code

Figure 5.2: Block Diagram of 3-D BEM code

point of that element. In the linear element algorithm, the nodes refer to the vertices of that element, and thus a node can belong to more than one element.

The configuration of the waveguide is specified by a set of variables. Assume that the waveguide under consideration is formed by K boundaries with L boundary intersections, which are also called boundary vertices. Those boundaries divide the waveguide into M regions. The following variables describe the geometry.

- **Vertex** ($L \times 3$) double type matrix

It specifies the coordinates of each boundary vertex. Each row i stores the (x, y, z) coordinates value of vertex i .

- **Boundary** ($K \times 2$) unsigned integer type matrix

It stores the vertex id of the vertices at a given boundary. The coordinates of these 2 vertices can be further retrieved from **Vertex**. Although it is easy to extend our program to curved boundaries, in our context, we assume that all boundaries are uncurved.

- **Region** ($M \times K$) integer type matrix

Each row stores the list of boundaries which enclose a region. A region is defined as a volume with a homogeneous refractive index in a waveguide. If the region is at the left side of a boundary, the boundary is stored as $-boundary_id$. If fewer than K boundaries which enclose that region, the rest of the row elements are filled with 0.

- **n** M ary refractive index type vector Stores the refractive index of each region.

Once the waveguide information is provided, the Element Generator module generates boundary elements on a boundary-by-boundary basis. These can be placed in uniform or in non-uniform positions. Especially in the linear element implementation, it is desirable to reduce the spatial extent of elements which are close to the corners to achieve higher accuracy.

Assuming that the waveguide boundaries are discretized into N_e elements with N_n nodes, and that each element has K_e nodes as vertices. For the constant element algorithm, $N_e = N_n$, the output variables in the module are.

- **Node** ($N_n \times 3$) A double type matrix. Stores coordinates of each node.
- **Element** ($N_e \times K_e$) An unsigned integer type matrix. Stores the nodes id of the vertices of that element. The coordinates of each node can be further retrieved from **Node**.
- **Area** N_e dimensional double type vector. Used in 3-D only. Each vector element corresponds to the area of a single element.
- **Length** N_e dimensional double type vector. Used in 2-D only. Each element corresponds to the length of a single element.

Additional information is accessible by other modules through procedure calls. This information includes the **Normal_Vector** of each element, the regions to which a given element belongs and the refractive index of each region.

A separate module reserves storage for various components of the BEM solver which are:

- **H** A ($2N_n \times 2N_n$) complex double type sparse matrix as described in the previous chapters.
- **V** A $2N_n$ dimensional complex double type Vector with each vector element corresponding to the field distribution or its the directional derivative of each node. (See definition in previous chapters).
- **S** A $2N_n$ dimensional complex double type Vector representation of the source function. (See definition in previous chapters).

The mode generator subsystem employs the finite difference method to construct different modes that serve as input to the field solver. In 3-D, the input mode is generated

by 2-D semi-vector BEM as discussed in chapter 4. Usually the input field coincides with the fundamental mode. However, our routine automatically provides the propagation constant of all modes. The incident field distribution is then stored as a vector **Source** where

$$\mathbf{Source} = \begin{pmatrix} U_{n1} \\ \frac{\partial U_{n1}}{\partial n} \\ \vdots \\ U_{nk} \\ \frac{\partial U_{nk}}{\partial n} \end{pmatrix} \quad (5.1)$$

and $(n1, n2, \dots, nk)$ are the nodes of elements where the incident light is launched.

5.2 The BEM solver

The BEM solver module is used to construct the matrices required to implement the BEM equation:

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (5.2)$$

It then calculates the matrix and the vector elements of $\mathbf{H}, \mathbf{S}$ and evaluates the field distribution $\mathbf{V}$ by solving the linear system

$$\mathbf{V} = \mathbf{H}^{-1}\mathbf{S} \quad (5.3)$$

where $\mathbf{H}^{-1}$ is the inverse matrix of $\mathbf{H}$. The construction of $\mathbf{H}, \mathbf{S}$, however, is different from Linear and Constant Element algorithm. We will accordingly discuss them separately.

Both the 2-D and 3-D constant element algorithms share the following c-like pseudo-code.

The driving (main) program is

```
main()
```

```
{
```

```
Execute the Element Generator;
```

Execute the Mode Generator:

Reserve the storage for **S**, **V** and **H**:

for each region in the waveguide

```
{
  for each node_i in that region
  {
    for each element_j in that region
      //This procedure differs in Constant and Linear Element
      Process_H_S(this_region.node_i.element_j);
    };
  };
};
V = H-1S;
};
```

Execute the Mode Extractor to calculate reflectivity and plot graphs:

● Constant Element

The pseudo code for the constant element is. (node_i is the central node of element_i):

```
Procedure Process_H_S(this_region.node_i.element_j);
{
  col=2*element_j-1;
  case region on
  right side of element_i:
    row=2*node_i-1;
  left side of element_i:
    row=2*node_i;
  endcase;
```

case region on

right side of element.j:

if node.i belongs to element.j

{

$$H(row, col) = 0.5;$$

$$H(row, col + 1) = g_{node.i, node.i}^r;$$

}

elseif $\angle \tilde{\rho}_{ij}, \mathbf{n}_j \neq 0$

{

$$H(row, col) = h_{node.i, node.j}^r;$$

$$H(row, col + 1) = g_{node.i, node.j}^r;$$

}

left side of element.j:

if node.i belongs element.j

{

$$H(row, col) = 0.5;$$

$$H(row, col + 1) = -g_{node.i, node.i}^l;$$

}

elseif $\angle \tilde{\rho}_{ij}, \mathbf{n}_j \neq 0$

{

$$H(row, col) = h_{node.i, node.j}^l;$$

$$H(row, col + 1) = -g_{node.i, node.j}^l;$$

};

endcase;

if element.j is on the source boundary

$$S(row)+ = (H(row, col) - j\beta H(row, col + 1))Source(row);$$

}

The definition and calculation of $g_{ij}^{l,r}, h_{ij}^{l,r}$ for the 2-D and 3-D cases is described separately in Chapter 3 and 4.

- **2-D Linear Element Algorithm**

The pseudo code for Linear Element Algorithm is slightly more complicated in that the node can simultaneously be the vertex of more than one elements.

Procedure Process **H.S**

```
{
  for m=1,Max_No_Of_Node_Per_Element
    col_(mj)=2*node_(mj)-1;
  case region on
  right side of node_i:
    row=2*node_i-1;
  left side of element_i:
    row=2*node_i;
  endcase;

  case region on
  right side of element_j:
    for m=1,Max_No_Of_Node_Per_Element
      {
        if node_i==node_(mj)
          {
             $H(row, col_(mj)) + = \gamma_{node\_i}^r$ ;
             $H(row, col_(mj) + 1) + = g_{(node\_i, node\_i), (mj)}^r$ ;
          }
        elseif  $\angle \vec{\rho}_{ij}, n_j \neq 0$ 
```

```

{
     $H(row, col\_ (mj)) + = h_{(node\_innode\_j), (mj)}^r;$ 
     $H(row, col\_ (mj) + 1) + = g_{(node\_innode\_j), (mj)}^r;$ 
}
}

```

left side of element_j:

```

for m=1, Max_No_Of_Node_Per_Element
{
    if node_i==node_(mj)
    {
         $H(row, col\_ (mj)) + = \gamma_{node\_i}^r;$ 
         $H(row, col\_ (mj) + 1) - = g_{(node\_innode\_i), (mj)}^l;$ 
    }
    elseif  $\angle \vec{\rho}_{ij}, n_j \neq 0$ 
    {
         $H(row, col\_ (mj)) + = h_{(node\_innode\_j), (mj)}^l;$ 
         $H(row, col\_ (mj) + 1) - = g_{(node\_innode\_j), (mj)}^l;$ 
    };
}

```

endcase;

if element_j is on the source boundary

```

{
    for m=1, Max_No_Of_Node_Per_Element
         $S(row) + = (H(row, col\_ (mj)) - j\beta H(row, col\_ (mj) + 1)) Source(col\_ (mj));$ 
    }
}

```

5.3 The Mode Extractor

This module calculates the modal reflectivity of Equation (2.40). The vector **Source** stores the normalized incident modal field distribution along the boundary along which the field is launched while the vector **Ref** is the reflected field distribution on the same boundary. The modal reflectivity is then expressed as in section 2.40 through the expression

$$\begin{aligned} R &= \langle Ref | Source \rangle \\ &= \sum_k Ref_k Source_k Area_k \end{aligned} \tag{5.4}$$

Chapter 6

2-D Boundary Element Method Simulation Result and Error Analysis

6.1 Introduction

This chapter applies the Two Dimensional Boundary Element Method to

- (a) waveguides without an anti-reflection coating;
- (b) waveguides with a single AR coating layer;
- (c) waveguides with a double coating layer at the end facet.

In Section 6.2, we will further simulate the wave propagation in the symmetric slab waveguide. We seek in particular to minimize the modal reflection by varying the thickness of coating and tilting the facet angle. In later sections, we apply the BEM method to wide angle structures. We simulate the wave propagation in an L-type reflector and a T-splitter. The results of our simulations are shown to be close to those of other methods such as FD-TD method with the PML absorbing boundary condition [46].

(A)

(B)

Figure 6.1: Symmetric slab wave guide

6.2 Symmetric Slab Waveguide

We will consider the symmetric slab waveguide as shown in Figure 6.1 in which the guiding region is surrounded by cladding regions with equal refractive indices N_c . In this first section, we study the reflection of the fundamental TE_0 mode of this slab waveguide at both a coated and an uncoated facet.

6.2.1 Modal Reflectivity for Slab Waveguide without Coating

Consider first the symmetric slab waveguide of Fig. 6.1 (A) without an antireflection coating on the end facet. The refractive index of the guiding region (N_g) and cladding region (N_c) are chosen to be $N_g = 3.6$ and $N_c = 3.564$. the incident wavelength is $\lambda = 1.55\mu m$ and the waveguide width $D = 1.46\mu m$. Our matlab program discretizes the waveguide structure into boundary elements in its Element Generator module. The fundamental mode is produced by the FD method in the Mode Generator module and mapped to the input boundary elements to serve as incident field. The 2-D BEM solver then computes the field distribution on all the boundary elements. The results are then analyzed by the mode extractor module, which calculates the modal reflectivity and generates graphs of the field distribution in the waveguide. Figure 6.2 shows the total field distribution, and in Figure 6.3 we extract the reflected wave from the incident wave using $E_y(x, y, z) = E_{total} - E_{in} = E_{total} - E_{TE0} \exp(j\beta z)$. In these figures, $|E_y|$ is the magnitude of E_y , which is in turn also normalized such that the maximum value of E_y in the incident field is unity. A modal reflectivity of 0.58 is achieved in this calculation.

6.2.2 Minimization of Reflectivity by Varying the Thickness of Single Layer Coating

As we have found in the above section, our slab wave guide displays substantial reflection loss at an uncoated waveguide/air interface. To minimize the modal reflection at the facet, an anti-reflection coating can be placed on the interface. The fabrication process of the AR coating is as discussed in Chapter 1 . In our example the refractive index of

Figure 6.2: Total field distribution of waveguide without coating for a wave incident at $z = 0 \mu m$ and reflected by an air interface at $z = 0.4 \mu m$

Figure 6.3: Field distribution of the waveguide without coating. Inside the waveguide, incident field is absent.

Figure 6.4: Single-layer AR coated slab waveguides: (A) End facet perpendicular to propagation axis; (B) End facet tilted with respect to the propagation axis.

the coating is chosen to be $N_{AC} = \sqrt{N_{Eff}} = 1.8938$, where N_{Eff} is the effective index of the waveguide. This coating thickness is chosen so that destructive interference may occur at the front end of the coating since $L \approx \frac{\lambda_0}{4N_{AC}}$, where the λ_0 is the wavelength in free space. The true optimum coating thickness can then be calculated by our BEM simulation. Figure 6.5 shows the coating thickness vs. the power reflectivity. At coating thickness $L = 0.206\mu m$, we find the lowest power reflectivity of $-43.34dB$, which is in close agreement with published result. [46].

Figure 6.6 shows the field distribution of the waveguide with optimized single layer of AR coating with a thickness of $0.208\mu m$. The AR coating is deposited at $z = 0.4\mu m$. As we can see from the figure, the standing wave ratio is reduced significantly compared to the case without anti reflection coating. Figure 6.7 shows the same field distribution as Figure 6.6 except that the incident field is extracted from the total field. Both figures show that the waveguide with a single layer coating has low reflectivity. Observe that in Figure 6.6, the field distribution drops abruptly very close to air/coating interface ($z = 0.608\mu m$), which is unphysical. This behavior is present in all calculations if the grid point at which the field distribution is computed is too close to the boundary element (typically the problem becomes visible for $\rho < 0.002\mu m$). The source of the error is as expected that the Gaussian Quadrature formula employed to calculate the matrix element becomes inaccurate if the integrand in $g_{ij} = \int_{-1}^{+1} \frac{1}{4j} H_0^{(2)}(k\rho) d\xi \frac{l}{2}$ in equation (4.41) becomes singular for $\rho \rightarrow 0$. To avoid this difficulty, the more accurate series solution can be employed for the relevant nodes. Although an optimized single layer coating can reduce the reflectivity to lower than $-43dB$, the dynamic range of this type of waveguide is quite narrow. That is, if the input wavelength deviates from the center wavelength $1.55\mu m$, the reflectivity increases sharply. Figure 6.13 (a) shows the manner in which the modal reflectivity varies when the wavelength is changed. Again, this result agrees with published results [46].

From our figures we find that the reflectivity increases more than $10dB$ when the wavelength is $0.05\mu m$ off the center wavelength. The dynamic range can however be increased by applying a multiple coating as discussed in a later section.

Figure 6.5: Modal reflection vs. coating thickness for a single-layer AR coated slab waveguide as calculated with both the BEM and the FD-TD method incorporating the PML boundary condition

Figure 6.6: Total field distribution in the a waveguide coated with a single layer, $0.208\mu\text{m}$ thick AR coating.

Figure 6.7: The field distribution in the waveguide with a single layer $0.208\mu m$ thick AR coating

Figure 6.8: The power reflectivity versus tilt angle for a single-layer AR coated waveguide

6.2.3 Minimize Reflectivity by Tilting Facet Angle

By angling the end facet of the waveguide, the reflected fields can be directed into a higher-order, generally unbound mode, so that less energy will be reversely coupled into the fundamental mode, a process called mode conversion. Figure 6.8 shows the decrease in the reflected modal power obtainable by adjusting the tilt angle. The reflectivity

minimum is obtained at tilt angle of 7° . At this angle, the reflected modal power is 10 dB less than at 0° .

Although the reflectivity can be decreased in this manner compared to the perpendicular facet, the dynamic range however shows no improvement as indicated in Figure 6.9. To increase the dynamic range, we have to apply a double layer coating as calculated in the next section. Figure 6.9 also shows the reflectivity minimum at $\lambda_{a0} = 1.55\mu m$. In Figure 6.10 we display the field distribution in the waveguide while Figure 6.11 shows the same result, but after subtracting the input field excitation. The field strength in the waveguide was calculated using the Green's formulation discussed in Chapter 4.

6.2.4 Double Layer Coating Structure

As seen above, the modal reflectivity can be reduced to -43 dB with a perpendicular single layer coating. But the dynamic range for such a structure is quite small. In practice a wider dynamic range is often required. This can be achieved by a double layer coating structure as shown in Figure 6.12.

In Figure 6.12, the reflective indices of the two coating layers are chosen that $N_{AC1} = N_{AC2}\sqrt{N_E} \approx 2.76494$, $N_{AC2} = 1.46$, $L_1 = \frac{\lambda}{4N_{AC1}} = 0.138\mu m$, $L_2 = \frac{\lambda}{4N_{AC2}} = 0.266\mu m$. The propagating field is shown in Figure 6.14 while Figure 6.15 shows the reflected field. Figure 6.13 clearly demonstrates the enhancement of the dynamic range and the minimum modal reflectivity minimum in comparison to the single layer AR coating. The results are in excellent agreement with published FD-TD with PML results [46].

The modal reflectivity can again be further reduced by tilting the output facet as discussed previously. Figure 6.16 shows that at an angle of 8° , the modal reflectivity reaches a minimum.

6.3 Wide Angle Reflection Structures

In this section, we simulate wave propagation in wide angle reflection structures, which is difficult to simulate using the standard Beam Propagation Method (BPM) as discussed

Figure 6.9: Power reflectivity vs. wavelength for a 7° end facet tilt for a single layer AR-coated waveguide

Figure 6.10: The field distribution for a single-layer AR coated waveguide and a 7° end-facet tilt

Figure 6.11: Field distribution at degree=7. reflection field extracted

Figure 6.12: Double AR-coated slab waveguides (A) Tilted end facet (B) Untilted end facet

Figure 6.13: Modal reflectivity vs. wavelength for a single-layer and double-layer AR coated slab waveguide as calculated with both the BEM and the FD-TD method with the PML boundary condition.

Figure 6.14: Total field distribution in the double-coated waveguide

Figure 6.15: Total field in double-coated waveguide, reflection field extracted

Figure 6.16: Reflection minimization by tilting the output facet for a waveguide with double AR coating

Figure 6.17: 90° Reflector

in Chapter 2. The optical structures studied here include a 90° reflector and a T-splitter.

6.3.1 Two Dimensional Reflector

In this subsection, we consider a reflector constructed from the waveguide with the profile given above, c.f. Fig. 6.17. The waveguide has refractive index of $N_g = 3.6$ in the guiding region and $N_c = 3.564$ in cladding region. The fundamental mode is launched from the input arm and is reflected by a bending structure into an output arm. The input waveguide and output waveguide have the same structure so that no mode conversion between input mode and output mode occur at reflection. The reflector is fabricated by etching through the guiding layer. Fig. 6.18 shows the wave propagating

Figure 6.18: Wave propagation in reflector

in the waveguide. This example yields a transmission loss of -1.698 dB and reflectivity as low as -37 dB.

6.3.2 Two Dimensional Splitter

Next, we examine the T-splitter shown in Fig. 6.19. The output waveguide has half the width of the input waveguide, so that the input and output waveguides have different sets of normal modes. This structure has a much larger transmission loss mainly due to the off-center field profile in the output arms. Figure 6.20 demonstrates the field

Figure 6.19: T-Splitter

distribution in the T-splitter.

6.4 Error Performance

This section presents an error analysis for the 2-D BEM method. In the constant element algorithm, the computational error results mainly from two factors: the size of the discrete finite element and the size of the computational window. In the linear element algorithm, an additional factor contributes to the error: the singularity of the nodes at the sharp corners of the waveguide.

In this section, we studied the error performance of BEM constant element, linear element with uniform and non-uniform mesh scheme on the rectangular waveguide with single layer of AR coating. Figure 6.21 and Figure 6.22 shows the modal reflectivity vs. different discretization lengths along the x and y directions. Figure 6.23 and Figure 6.24 show the modal reflectivity variation with respect to different computation windows at transversal direction with and without an end angle tilt. When the end facet is tilted more than 7° , more reflection power reaches the edge of the computational window, the

Figure 6.20: Wave propagation in T-Splitter

Figure 6.21: Discretization error: power reflectivity vs. grid point spacing dx

reflectivity calculation is less accurate for such titled angles in flat angle employing the same computation window.

Figure 6.22: Discretization error: power reflectivity vs. grid point spacing dz

Figure 6.23: The reflected power vs. computational window size for the waveguide with a single-layer AR coating and an untilted end facet.

Figure 6.24: power reflectivity vs. computational window size for a single-layer AR coated waveguide with an end facet tilt of 7° with respect to the propagation axis.

Chapter 7

3-D BEM Simulation Result and Error Analysis

In this chapter, we simulate the wave propagation in three dimensional structures. In Section 7.1 we study the modal reflectivity of rectangular waveguides with or without an AR-coating. We then study the mode conversion produced by tilting the angle of the output facet.

7.1 Rectangular Waveguides

Our rectangular waveguide model is shown in Fig. 7.1. In this model, the guiding region has a rectangular profile with a guiding refractive index $N_g = 3.52$ embedded in a cladding region with $N_c = 3.20$ while the width and thickness of the four waveguides considered are given by $(0.4\mu m \times 0.4\mu m)$, $(0.4\mu m \times 1.5\mu m)$, $(0.15\mu m \times 1.5\mu m)$ and $(0.15\mu m \times 3.0\mu m)$ respectively. The modal reflectivity with and without AR coating is studied. We will examine the effect of tilting the end facet angle.

7.1.1 Normal Modes of Rectangular Waveguides

We first compute the normal modes that will be used to excite the input of the three dimensional waveguide with our Mode Generator module. This program employs the FD

Figure 7.1: (A) Uncoated and (B) single-layer AR coated rectangular waveguides

Table 7.1: Effective refractive index in the different modes

(Height, Width) μm	Mode	n_{eff}
(0.4,0.4)	TE_{00}	3.2774
	TM_{00}	3.2774
(0.4,1.5)	TE_{00}	3.3775
	TM_{00}	3.3647
(0.15,1.5)	TE_{00}	3.2528
(0.15,3.0)	TE_{00}	3.2637
	TE_{01}	0.2479

method to compute the fundamental mode used in the scalar formalism. Alternatively, it can employ a more accurate semi-vector 2-D BEM to compute the modes required by our semi-vector formalism. The effective indices of the individual modes are computed and listed in Table 7.1.1. We found that the reflective indices of the TE_{00} and TM_{00} mode are identical for a square waveguide as expected due to the waveguide symmetry. With increasing the waveguide width, the difference of the effective refractive indices between the TE , TM modes increases. These refractive index differences can cause substantial variations in the modal reflectivity. It is found that the waveguide with a $(0.15, 3.0)\mu m$ cross section geometry can support higher order modes such as TE_{01} and TM_{01} . Figure 7.2 illustrates the TE_{01} mode of the waveguide with a geometry of $(0.15\mu m \times 3.0\mu m)$ computed by 2-D semi-vector BEM. The effective refractive index of TE_{01} mode is found to be $n_{eff} = 3.2479$. As will be discussed in more detail later, the presence of the higher-order modes may result in an enhanced degree of mode conversion.

7.1.2 Scalar Formalism

As discussed in Chapter 3, the scalar formalism ignores the discontinuity of the field component across the refractive index discontinuities. Hence the scalar result is generally only accurate when difference in the refractive index is small such that the TE

Figure 7.2: TE_{01} mode of rectangular waveguides ($0.15\mu m \times 3.0\mu m$), using semi-vectorial 2-D BEM

and TM modes are indistinguishable. However, the scalar approximation leads to considerable simplifications and is thus of practical use for three dimensional waveguides. We will study the square-shaped dielectric waveguide below, and will later demonstrate good agreement with the semi-vectorial results.

- Rectangular waveguide without anti-reflection coating

Consider the single-mode ($0.4\mu m \times 0.4\mu m$) square waveguide excited by its fundamental mode. Figure 7.3 shows the reflected field $0.05\mu m$ away from the air/waveguide interface while Fig. 7.4 depicts the transmitted field. The size of the discretized element is ($0.1\mu m \times 0.1\mu m$). The computational window is set to be ($2\mu m \times 2\mu m$) in order to insure that most reflected power is inside the window. The modal reflectivity of 0.46308 is recorded in this case. It is in close agreement with the value of 0.4 ± 0.2 which are given in [12].

- Single Layer AR coating

Adding a single layer AR coating at the output end of the waveguide as discussed in the previous section decreases the modal reflectivity substantially. Figure 7.5 displays the reflected field profile obtained after propagating the field back from the guide/coating interface. The refractive index of the AR coating and its thickness are determined with the EIM method to be 1.81 and $0.208\mu m$ respectively. The reflectivity is calculated to be 0.013739. In comparison with the waveguide without an AR coating (c.f. Figure 7.3), we find that while the reflectivity of the uncoated waveguide is significant, it can be greatly reduced by adding an AR coating layer.

- Optimal AR coating profile

Since the EIM is not an exact method for three dimensional waveguides so that the calculations of the preceeding chapter may only be heuristic in nature for the 3 dimensional waveguides considered here, the AR coating parameters for realistic waveguides must still be optimized. Figure 7.6 shows the coating thickness vs. power reflectivity with refractive index of an AR coating given by 1.81 and 2.0399

Figure 7.3: Reflected field at $z = 0$ of an uncoated ($0.4\mu m \times 0.4\mu m$) rectangular waveguide. The air/waveguide interface is located at $z = 0.05\mu m$

Figure 7.4: Transmitted field at $z = 0.05\mu m$ of a $(0.4\mu m \times 0.4\mu m)$ uncoated rectangular waveguide. The air/waveguide interface is located at $z = 0.05\mu m$

Figure 7.5: The reflected wave at $z = 0$ of a rectangular waveguide with a single layer AR coating at $z = 0.1\mu m$. The AR coating has a thickness of $0.208\mu m$

respectively. Although the value of the optimum refractive index predicted by the EIM is $n_{ac} = \sqrt{n_{eff}} = 1.81$, this figure shows that a lower reflectivity is obtained for $n_{ac} = 2.0399$. For this n_{ac} , the optimum coating thickness resulting in the lowest power reflectivity is $0.18\mu m$ and the calculated reflectivity is 0.69×10^{-3} which is within the range for the minimum reflectivity predicted by [12]. The AR coating for the minimum reflectivity is thinner when $n_{ac} = 2.0399$ than $n_{ac} = 1.81$. That is reasonable, since the destructive interference at the AR coating end requires the light travel a distance $\frac{\lambda}{2}$. That is $2n_{ac}t_c = \frac{\lambda_0}{2}$, where t_c is the coating thickness and λ_0 is the wavelength of light in vacuum. So for the higher value of n_{ac} , the coating thickness should be thinner. Figure 7.7 displays the reflected field profile for the optimum refractive index and the coating thickness. The reflected power is suppressed substantially compared to the minimum reflection configuration predicted by the EIM.

7.1.3 Semi-Vector Formalism

Although the scalar formalism behaves well for two dimensional waveguide structures, it generally produces less satisfactory results for three dimensional profiles such as the rectangular waveguides studied here if the refractive indices differ considerably between the cladding and guiding regions. In such a case, the computed reflection is highly dependent on the polarization of the propagating electric field. Far more accurate results can then be obtained from the semi-vector algorithm of Chapter 3. Thus we next present a calculation which is based on this semi-vectorial formalism.

7.1.4 Waveguides with Single-layer Coating

In this subsection we study the reflectivity of a $(0.4 \times 0.4\mu m)$ and a $(0.4 \times 1.5\mu m)$ rectangular waveguide with a single-layer AR coated output facet in the semi-vectorial approximation. We will examine both the TE_{00} and TM_{00} waveguide modes. Figure 7.8 shows the modal reflectivity vs coating thickness for the $(0.4\mu m \times 0.4\mu m)$ and $(0.4\mu m \times 1.5\mu m)$ waveguide geometries, respectively. The refractive index of the AR coating

Figure 7.6: Reflected power vs coating thickness for single-layer AR coated rectangular waveguides

reflected field

Figure 7.7: The reflected field at $z = 0$ of a rectangular waveguide with a single AR coating at $z = 0.05\mu m$

has been set to $n_{ac} = 1.92$. The TE_{00} and TM_{00} modal reflectivities are identical in the square case, as expected from the symmetry of the profile. The $(0.4 \times 1.5\mu m)$ waveguide on the other hand shows well a separated coating thickness/reflectivity curve between the TE and TM modes, again in close agreement with [12]. Our AR coating layer parameters for both waveguide configurations, as displayed in Figure 7.9 yield reflectivities as low as 10^{-3} which again is close to previously published values. The optimized AR coating refractive index for $(0.4\mu m \times 1.5\mu m)$ is 1.85 for the TM mode and 1.94 for the TE mode. Figure 7.10 shows the reflected field distribution in the $(0.4\mu m \times 0.4\mu m)$ waveguide excited by its TE_{00} mode. A power reflectivity of 6.6×10^{-4} is recorded in this calculation, which is identical with the observed modal reflectivity of the TM_{00} mode.

7.1.5 Angled Facets without Coating

Tilting the facet angle causes the reflected power to shift from the center of the waveguide, thus decreasing the overlap between the input and reflected fields[12]. Figure 7.11 shows the resulting decrease in reflectivity with increasing tilt angle. The magnitude of the reduction generally increases with increased guide width. This decrease is of special interest for the $(0.15 \times 3.0\mu m)$ waveguide since reflectivity minima exist at tilt angles of around 7° and 10° , as previously noted in [18]. Figure 7.12 displays as well the mode conversion which is caused by the tilted output facet to the higher (TE_{10}, TM_{10}) modes that our previous mode calculations have shown to exist in the waveguide.

7.1.6 Error Analysis

The sources of computational error associated with the 3-D BEM are essentially identical to those encountered in the 2-D BEM. For example, Figure 7.13 shows the power reflectivity vs. computational window size for a square waveguide $(0.4\mu m \times 0.4\mu m)$ with a single layer AR coating ($n_{ac} = 1.81$). Using the value of the reflected power at the largest computational window size as a reference value, we observe that for a window size of $(1.8\mu m \times 1.8\mu m)$ the relative error in the power reflectivity is still less than 4%.

Figure 7.8: Power reflectivity vs. coating thickness in the rectangular and square waveguides

Figure 7.9: Optimization of modal reflectivities.

Figure 7.10: Reflected field in rectangular waveguide ($0.4\mu m \times 0.4\mu m$) $n_{ac} = 1.92$, using the semi-vectorial formalism.

Figure 7.11: Power reflectivity vs. tilt angle

Figure 7.12: Modal reflectivity spectrum of a $0.15 \times 3.0\mu m$ waveguide (TE mode)

Figure 7.13: Power reflectivity vs. computational window size for a $(0.4\mu m \times 0.4\mu m)$ square waveguide with a single AR coating layer ($n_{ac} = 1.81$).

Chapter 8

Conclusions

This thesis has focused on electromagnetic field reflection at coated and uncoated optical waveguide facets. In particular, numerical techniques employing the boundary element method have been developed to simulate the reflected electric field at and away from the facet.

We have introduced a matrix procedure for obtaining the reflection coefficient in the framework of the BEM. In both the two dimensional and three dimensional method the matrix equation can be represented as

$$\mathbf{H}\mathbf{V} = \mathbf{S} \quad (8.1)$$

where $\mathbf{H}$ is a highly banded sparse matrix. We also provided a procedure for evaluating the matrix elements $\mathbf{H}$ and the source function $\mathbf{S}$ using Gaussian integration. To enhance the accuracy of the method, an efficient series solution of the diagonal elements in the matrix $\mathbf{H}$ has been developed in both the two dimensional and three dimensional case. We then studied the scalar and semi-vector formalism in depth and developed constant and linear element algorithms for each case.

The BEM method was then tested for several representative waveguide reflection problems. In the two dimensional case, the method was applied to the reflection of slab waveguide with coated and uncoated waveguide facets. For a representative waveguide, in the case of uncoated facets a modal reflection coefficient of 0.58 was recorded. With a

single layer coating waveguide, a modal reflection coefficient of -43 dB was achieved, while -56 dB was obtained after tilting the facet by an angle of 7° . We further investigated a double layer waveguide coating and found a modal reflectivity of -50 dB with a reflectivity of -51 dB was found at a tilting angle of 8° .

We then examined some two dimensional structures that exhibited wide angle scattering. We simulated field propagation in an L-type Reflector and recorded a transmission loss of -1.7 dB and a reflectivity of -37 dB. In the three dimensional case, we investigated rectangular waveguides with and without coating. We studied the reflectivity of a representative square waveguide without coating and recorded a modal reflectivity of 0.46. We then studied the waveguide with a single layer coating and obtained a modal reflectivity less than 10^{-3} in an optimal configuration. With the semivectorial formalism, we then examined the modal reflectivity for single layer coating with different refractive index profiles and observed the expected difference between the TM and TE modal reflectivities. The lowest reflectivity recorded in these calculations was close to 10^{-4} . We subsequently investigated the mode conversion that results when the end facet of the waveguide is tilted. Finally, we performed an error analysis to categorize the precision of our method. We found a first order error with respect to the element size for the constant element algorithm and a second order error for the linear element algorithm.

8.1 Suggestions for future work

We have found that BEM is an accurate, efficient and versatile method for simulating wave propagation problems in dielectric waveguides consisting of a few homogeneous layers. However, this method is difficult to implement for continuously varying refractive index distributions. Thus the method would be more powerful and versatile if integrated with other methods such as the FD-TD, FEM, BPM methods. Further, although the linear element algorithm was implemented in this thesis, higher order algorithms would be desirable in future studies. The BEM method can also be extended to the four dimensional case in which the time evolution of wave propagation is described. The

possibility of developing a full vectorial formalism is also worthy of future investigation.

Bibliography

- [1] M.A. Jaswon, *Integral equation methods in potential theory I*, Proc. Roy. Soc. Ser. A 275, 1963, pp. 23-32.
- [2] G.T. Symm, *Integral equation methods in potential theory II*, Proc. Roy. Soc. Ser. A 275, 1963, pp. 33-46.
- [3] C.A. Brebbia, J. C. F. Telles and L. C. Wrobel, *Boundary Element Techniques: Theory and Applications in Engineering*, New York. Springer-Verlag, 1984.
- [4] S. Washisu and I. Fukai, "The Electromagnetic Field Analysis by Boundary Element Method", pp. 123-132.
- [5] K. Tanaka and M. Tanaka. "Guided mode extracted integral equations: a new method for CAD of open waveguide circuits", *Mathematical Methods in Electromagnetic Theory, IEEE MMET Conference Proceedings*, Piscataway, NJ, USA, 1996, pp. 55-58.
- [6] A.G. Failla, G.P. Bava and I. Montrosset. "Structural Design Criteria for Polarization Insensitive Semiconductor Optical Amplifiers", *Journal of Lightwave Technology*, Vol. 8, No. 3, March 1990, pp. 302-308.
- [7] P.W A. Mcilroy, M.S. Stern and P.C. Kendall, "Spectral Index Method for Polarized Modes in Semiconductor Rib Waveguides", *Journal of Lightwave Technology*, Vol. 8, No. 1, January 1990, pp. 113-117.

- [8] G.A. Vawter, R.E. Smith, B. Fuchs, J.R. Wendt, M. Hafich and G.R. Hadley, "A Rib Optical Waveguide with Cutoff Mesa Isolation", *Journal of Lightwave Technology*, Vol. 14, No. 2, Feb. 1996, pp. 169-172.
- [9] R. Moosburger and K. Petermann, " 4×4 Digital Optical Matrix Switch Using Polymeric Oversized Rib Waveguides", *IEEE Photonics Technology Letters*, Vol. 10, No. 5, May 1998, pp. 684-686.
- [10] M.R. Paiam and R.I. MacDonald, "A 12-Channel Phased-Array Wavelength Multiplexer with Multimode Interference Couplers", *IEEE Photonics Technology Letters*, Vol. 10, No. 2, February 1998, pp. 241-243.
- [11] B. Hermansson and D.O. Yevick, "Generalized Propagation Techniques—Application to Semiconductor Rib Waveguide Y-Junctions", *IEEE Photonics Technology Letters*, Vol. 2, No. 10, October 1990, pp. 738-740.
- [12] P.A. Besse, J.S. Gu, and H. Melchior, "Reflectivity Minimization of Semiconductor Laser Amplifiers with Coated and Angled Facets Considering Two-Dimensional Beam Profiles", *IEEE Journal of Quantum Electronics*, Vol. 27, No. 6, June 1991 pp. 1830-1836.
- [13] C. Vassallo, "Reflectivity of multielectric coatings deposited on the end facet of a weakly guiding dielectric slab waveguide", *J. Opt. Soc. Am A*, Vol. 5, No. 11, November 1988, pp. 1918-1928.
- [14] Ilan Dan-Gur, *Modal Reflectivity Measurements of AR coated and angled-facet InGaAsP/InP Devices: Comparison with theoretical Predictions*, M.Sc. Thesis, Queen's University, 1995.
- [15] K.C. Hwang, A R. Reisinger, K.H.G. Duh, M.Y. Kao, P.C. Chao, P. Ho and A.W. Swanson, "A Reliable ECR Passivation Technique on the $0.1\mu\text{m}$ InAlAs/InGaAs HEMT Device", pp. 624-627.

- [16] J. E. Sauvageau, C. J. Burroughs, P. A. A. Booii, M. W. Cromar, S. P. Benz and J. A. Koch, "Superconducting Integrated Circuit Fabrication With Low Temperature ECR-Based PECVD SiO_2 Dielectric Films", *IEEE Transactions on Applied Superconductivity*, Vol. 5, No. 2, June 1995, pp. 2303-2309.
- [17] S. Simhony, E. Kapon, e. Colas, R. Bhat, N. G. Stoffel, and D. M. Hwang, "Double Quantum Wire GaAs/AlGaAs Diode Lasers Grown by Organometallic Chemical Vapor Deposition on Grooved Substrates", *IEEE Photonics Technology Letters*, Vol. 2, No. 5, May 1990, pp. 305-306.
- [18] D. Marcuse, "Reflection Loss of Laser Mode From Tilted End", *Journal of Lightwave Technology*, Vol. 7, No. 2, February 1989, pp. 336-339.
- [19] D. Marcuse, "Tilt, Offset, and End-Separation Loss of Lowest-Order Slab Waveguide Mode", *Journal of Lightwave Technology*, Vol. LT-4, No. 11, November 1996, pp. 1647-1650.
- [20] J. Xu, *Studies of Electromagnetic Field Reflection at Coated and Uncoated Optical Waveguide Interfaces*, Ph. D Thesis, Queen's University, Mar. 1996.
- [21] HP8504A precision reflectometer user's guide, Hewlett-Packard company, 1992.
- [22] E. Kapon and R. Bhat, "Low-loss single mode GaAs/AlGaAs optical waveguides grown by organometallic vapor phase epitaxy", *Appl. Phys. Lett.*, Vol. 50, 1987, pp. 1628-1630.
- [23] R.G. Walker, "Simple and accurate loss measurement technique for semiconductor optical waveguides", *Electron. Lett.*, Vol. 23, 1989, pp. 25-27.
- [24] R. Rousina-Webb, "Low reflectivity facet coating for modulators using single layer ECR oxynitride", *Bell-Northern Research internal report*, Ottawa, Ontario, Canada, 1995.

- [25] T. Feuchter and C. Thirstrup, "High Precision Planar Waveguide Propagation Loss Measurement Technique Using a Fabry-Perot Cavity". *IEEE Photonics Technology Letters*, Vol. 6, No. 10, October 1994, pp. 1244-1247.
- [26] J.D. Jackson. *Classical Electrodynamics*, second edition, New York. Willey, 1975. pp. 223-227.
- [27] D. Yevick. "A Guide to Electric Field Propagation Techniques for Guided-wave Optics", *Optical and Quantum Electronics*, Vol. 26, 1994. pp. S185-S197.
- [28] S.M. Saad, "Review of Numerical Methods for the Analysis of Arbitrarily-Shaped Microwave and Optical Dielectric Waveguides". *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-33, No. 10, October 1985. pp. 894-899.
- [29] C.L. Yu, D. Yevick, "Application of the Bidirectional Parabolic Equation Method to Optical Waveguide Facets". *Journal of the Optical Society of America A Optics Image Science and Vision*, Vol. 14, No. 7, July 1997, pp. 1448-1450.
- [30] B. Hermansson, D.O. Yevick, W. Bardyszewski and M. Glasner, "A Comparison of Lanczos Electric Field Propagation Methods", *Journal of Lightwave Technology*, Vol. 10, No. 6, June 1992, pp. 772-776.
- [31] D. Yevick, J. Yu, F. Schmidt, "Analytic Studies of Absorbing and Impedance Matched Boundary Layers", *IEEE Photonics Technology Letters*, Vol. 9, No. 1, Jan. 1997, pp. 73-75.
- [32] M.G. Daly, P.E. Jessop, and D. Yevick. "Intersecting Rib Waveguide Structures with Reduced Crosstalk". *Can. J. Phys.*, (Suppl.), Vol. 74, 1996, pp. S39-S42.
- [33] W. Bardyszewski, D. Yevick, Y.Liu, C. Rolland and S. Bradshaw, "Theoretical and Experimental Analysis of Mach-Zehnder Quantum-well modulators", *J. Appl. Phys.*, Vol. 80, No. 2, July 1996, pp. 1136-1141.
- [34] M. Glasner, D. Yevick, B. Hermansson, "Sixth-Order Generalised Propagation Techniques", *Electronics Letters*. Vol. 27, No. 5, Feb. 1991, pp. 475-478.

- [35] D. Yevick and B. Hermansson, "Efficient Beam Propagation Techniques". *IEEE Journal of Quantum Electronics*. Vol. 26, No. 1, Jan. 1990, pp. 109-112.
- [36] D. Yevick, B. Hermansson and M. Glasner, "Fresnel studies of reflected beams". *Photonics Technol. Lett.*, Vol. 2, 1990, pp. 490-492.
- [37] B. Hermansson and D. Yevick, "Generalised propagation techniques-application to semiconductor rib waveguide Y-junctions", *Photonics Technol. Lett.*, Vol. 2, 1990, pp. 738-740.
- [38] C. Rolland, G. Mak, K.E. Fox, D.M. Adams, A.J. Springthorpe, "Fresnel Equation Studies of Longitudinally Varying Semiconductor Rib Waveguides: Reference Wavevector Dependence". *Electronics Letters*. Vol. 25, No. 18, Aug. 1989, pp. 1254-1256.
- [39] C. Rolland, G. Mak, K. E. Fox, D. M. Adams, A. J. Springthorpe, D. Yevick and B. Hermansson, "Analysis of Strongly Guiding Rib Waveguide S-bends: Theory and Experiment", *ibid*, Vol. 25, 1989, pp. 1256-1257.
- [40] D. Yevick and M. Glasner, "Analysis of Forward Wide-angle Light Propagation in Semiconductor Rib Waveguides and Integrated-Optic Structures". *Electronics Letters*, Vol. 25, No. 23, Nov. 1989, pp. 1611-1613.
- [41] D. Yevick and B. Hermansson, "Split-Step Finite Difference Analysis of Rib Waveguides". *Electronics Letters*, Vol. 25, No. 7, Mar. 1989, pp. 461-462.
- [42] D. Yevick and B. Hermansson, "New Formulations of the Matrix Beam Propagation Method: Application to Rib Waveguides", *IEEE J. Quantum Electron.*, Vol. QE-25, 1989, pp. 221-229.
- [43] B. Hermansson, D. Yevick and J. Sajonmaa, "A propagating beam analysis of two dimensional microlenses and three dimensional taper structures", *J. Opt. Soc. Am. A*, Vo. 1, 1984, pp. 663-671.

- [44] J. Yu. *The Beam Propagation Method and Its Application to the Design of Semiconductor Modulators*. Ph. D Thesis. Queen's University, Sep. 1994.
- [45] N.J.P. Frenette. *Modelling and Optimization of Integrated Y-Branch Optical Waveguides*, Ph. D Thesis. Queen's University, June 1987.
- [46] J. Yamauchi. M. Mita. S. Aoki and H. Nakano, "Analysis of Antireflection Coatings Using the FD-TD Method with the PML Absorbing Boundary Condition", *IEEE Photonics Technology Letters*. Vol. 8, No. 2, Feb. 1996, pp. 239-241.
- [47] T. Kashiwa. T. Onishi and I. Fukai, "Analysis of Microstrip Antennas on a Curved Surface Using the Conformal Grids FD-TD Method". *IEEE Transactions on Antennas and Propagation*. Vol. 42, No. 3, March 1994, pp. 423-427.
- [48] E.E. Kriezis and A.G. Papagiannakis, "A Joint Finite-Difference and FFT Full Vectorial Beam Propagation Scheme". *Journal of Lightwave Technology*, Vol. 13, No. 4, April 1995, pp. 692-698.
- [49] R. Luebbers. D. Steich and K. Kunz, "FDTD Calculation of Scattering from Frequency-Dependent Materials", *IEEE Transactions on Antennas and Propagation*, Vol. 41, No. 9, September 1993, pp. 1249-1257.
- [50] C.D. Nallo. F. Frezza. and A. Galli, "Full-Wave Modal Analysis of Arbitrarily-Shaped Dielectric Waveguides Through an Efficient Boundary-Element-Method Formulation", *IEEE Transactions on Microwave Theory and Techniques*. Vol. 43, No. 12, December 1995, pp. 2982-2989.
- [51] S. Maeda, T. Kashiwa and I. Fukai, "Full Wave Analysis of Propagation Characteristics of a Through Hole Using the Finite-Difference Time-Domain Method". *IEEE Transactions on Microwave Theory and Techniques*. Vol. 39, No. 12, December 1991, pp. 2154-2157.
- [52] K. Naishadham and X.P. Lin, "Minimization of Reflection Error Caused by Absorbing Boundary Condition in the FDTD Simulation of Planar Transmission Lines",

IEEE Transaction on Microwave Theory and Techniques. Vol. 44. No. 1, January 1996, pp. 41-46.

- [53] G. Mur. "Absorbing Boundary Conditions for the Finite-Difference Approximation of the Time-Domain Electromagnetic-Field Equations", *IEEE Transactions on Electromagnetic Compatibility*, Vol. EMC-22, No. 4, November 1981, pp. 377-383.
- [54] T. Okoshi and T. Miyoshi. "The planar Circuit-An Approach to Microwave Integrated Circuitry", *IEEE Transactions on Microwave Theory and Techniques*, April 1972, pp. 245-252.
- [55] F.J.C. Meyer and D.B. Davidson. "Time Domain Scattering from Arbitrary 2D Scatterers Obtained from Frequency Domain Data Generated Numerically". *IEEE*, 1993, pp. 1692-1695.
- [56] J. C. Grant, *Finite Element Analysis of the Rib Arrow Leaky Optical Waveguide*. M. Sc. Thesis, Queen's University, Sep. 1990.
- [57] B.H. McDonald and A. Wexler, "Finite-Element Solution of Unbounded Field Problems". *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-20, No. 12, December 1972, pp. 841-847.
- [58] M. Hano. "Finite-Element Analysis of Dielectric-Loaded Waveguides", *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-32, No. 10, October 1984, pp. 1275-1279.
- [59] M.N.O. Sadiku, "A Simple Introduction to Finite Element Analysis of Electromagnetic Problems", *IEEE Transactions on Education*, Vol. 32, No. 2, May 1989, pp. 89-94.
- [60] Y. Kagawa, Y.H. Sun, Z. Mahmood, "Regular Boundary Integral Formulation for the Analysis of Open Dielectric Optical Waveguides", *IEEE-Transactions On Microwave Theory and Techniques*, Vol. 44, No. 8, Aug. 1996, pp. 1441-1450.

- [61] M. Tanaka and K. Tanaka. "Boundary Integral Equations for Computer Aided Design of Near-field Optics". *Electronics and Communication in Japan. Part II: Electronics*. Vol. 79, No. 11, Nov. 1996. pp. 10-18.
- [62] T.L. Wu, H.C. Chang, "Vectorial Analysis of Fiber-core Effects in Weakly Fused Couplers", *IEEE Photonics Technology Letters*. Vol. 9, No. 2, Feb. 1997. pp. 218-219.
- [63] G.G. Gentili, S. Mazzetto, G. Vaninetti, "Simple Formulation of the Boundary Integral Method for the Analysis of Arbitrarily Shaped Dielectric Waveguides". *Microwave and Optical Technology Letters*. Vol. 10, No. 1, Sep. 1995. pp. 41-45.
- [64] K. Hirayama, M. Koshiba. "Rigorous Analysis of Coupling Between Laser and Passive Waveguide in Multilayer Slab Waveguide". *Journal of Lightwave Technology*, Vol. 11, No. 8, Aug. 1993, pp. 1353-1359.
- [65] K. Minami, J. Yamakita and S. Sawa, "Analysis of Lossy Dielectric Gratings Using Pseudo-periodic Green's Function", *Electronics and Communications in Japan, Part II: Electronics*, Vol. 76, No. 3, Mar. 1993, pp. 10-19.
- [66] N.N. Zernov, "Higher Order Mode Theory of Three Dimensional Irregular Waveguides", *Radio Science*. Vol. 28, No. 3, May-June 1993. pp. 339-350.
- [67] Y. Rong, "Bandwidth Characteristics of Ridged Circular Waveguides", *Microwave Opt. Technol. Lett.*, Vol. 3, No. 10, Oct. 1990. pp. 347-350.
- [68] G. Hadjicostas, K.J. Butler, G.A. Evans, N.W. Carlson, R. Amantea. "Numerical Investigation of Wave Interactions in Dielectric Waveguides with Periodic Surface Corrugations", *IEEE Journal of Quantum Electronics*. Vol. 26, No. 5, May 1990. pp. 893-902.
- [69] J.G. Ma, "Full Modes Analysis of Rectangular Optical Waveguide using New Boundary Element Method", *International Journal of Infrared and Millimeter Waves*, Vol. 11, No. 3, Mar. 1990. pp. 425-433.

- [70] M. Matsuhara, I. Toyoda, H. Shirae, "Analysis of a Bending Dielectric Slab Waveguide by Integral Equation Formulation", *Electronics and Communications in Japan Part II: Electronics*, Vol. 72, No. 5, May 1989, pp. 97-103.
- [71] F. Olyslager, D.D. Zutter, and K. Blomme, "Rigorous Analysis of the Propagation Characteristics of General Lossless and Lossy Multiconductor Transmission Lines in Multilayered Media", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 41, No. 1, Jan. 1993, pp. 79-88.
- [72] F. Olyslager and D.D. Zutter, "Rigorous Boundary Integral Equation Solution for General Isotropic and Uniaxial Anisotropic Dielectric Waveguides in Multilayered Media Including Losses, Gain and Leakage", *IEEE Transaction on Microwave Theory and Techniques*, Vol. 41, No. 8, Aug, 1993, pp. 1385-1392.
- [73] K. Tanaka and M. Tanaka, "Computer-aided Design of Dielectric Optical Waveguide Bends by the Boundary-element Method Based on Guided-mode Extracted Integral Equations", *J. Opt. Soc. Am. A*, Vol. 13, No. 7, July 1996, pp. 1362-1368.
- [74] S. Kagami and I. Fukai, "Application of Boundary-Element Method to Electromagnetic Field Problems", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 32, No. 4, April 1994, pp. 455-461.
- [75] N. Kishi and T. Okoshi, "Proposal for a Boundary-Integral Method without Using Green's Function", *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-35, No. 10, October 1987, pp. 887-892.
- [76] N. Morita, "A Method Extending the Boundary Condition for Analyzing Guided Modes of Dielectric Waveguides of Arbitrary Cross-Sectional Shape", *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-30, No. 1, January 1982, pp. 6-11.
- [77] N. Morita, "Surface Integral Representations for Electromagnetic Scattering from Dielectric Cylinders", *IEEE Transactions on Antennas and Propagation*, Vol. AP-26, No. 2, March 1978, pp. 261-266.

- [78] S.W. Lee, M.S. Sheshadri, V. Jamnejad and R. Mittra, "Refraction at a Curved Dielectric Interface: Geometrical Optics Solution", *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-30, No. 1, January 1982, pp. 12-13.
- [79] C.C. Su, "A Surface Integral Equations Method for Homogeneous Optical Fibers and Coupled Image Lines of Arbitrary Cross Sections", *IEEE Transactions on Microwave Theory and Techniques*, Vol. MTT-33, No. 11, November 1985, pp. 1114-1119.
- [80] S. Qi and Q. Yang, "Spline Boundary Element Method For Coplanar Waveguides", *Proc. IEEE Intl. Symposium Digest of Antennas and Propagation Society*, Ann Arbor, MI, USA, Vol. 3, 1993, pp. 1704-1707.
- [81] K. Miyata, "Radiation Pattern Analysis of Planar Dielectric Antennas with Metallic Strips by Boundary Element Method, *Proc. IEEE Intl. Symposium of Antennas and Propagation Society*, Vol. 3, 1993, pp. 1696-1699.
- [82] W. Sun and C.A. Balanis, "Analysis of Double- or Quadruple-Ridged Waveguides by a Magnetic Surface Integral Equation Approach", *Proc. IEEE Intl. Symposium Digest of Antennas and Propagation Society*, Vol. 1, 1993, pp. 181-184.
- [83] W. Sun and C.A. Balanis, "Analysis and Design of Quadruple-Ridged Waveguides", *IEEE Trans. Microwave Theory and Techniques*, Vol. 42, No. 12, Dec. 1994, pp. 2201-2207.
- [84] E.W. Lucas and T.P. Fontans, "A 3D Vector Variational Hybrid Finite-Element/Boundary Element Formulation for the Scattering Analysis of Arbitrary Infinite Doubly Periodic Arrays", *IEEE*, 1991, pp. 1212-1215.
- [85] A. Barka, B. Fromentin, G. Mortchelevitch and B. Veron, "A Numerical Method for the Computation of Reflection and Transmission in Slowly Evolutive Waveguides", *Proc. IEEE Intl. Symposium Digest of Antennas and Propagation Society*, Vol. 2, 1993, pp. 876-878.

- [86] E. Schlemmer, W.M. Rucker and K.R. Richter, "Boundary Element Computations of 3D Transient Scattering from Lossy Dielectric Objects", *IEEE Transactions on Magnetics*, Vol. 29, No. 2, Mar. 1993, pp. 1524-1527.
- [87] T.F. Eibert and V. Hansen, "Full-Wave 3D-Modeling of Ground-Penetrating Radars by a Finite Element/Boundary Element-Hybrid Technique", *Proc. IEEE Intl. Geoscience and Remote Sensing Symposium (IGARSS'97)*, Vol. 1, 1997, pp. 227-229.
- [88] Y. Kagawa, Y. Sun and Z. Mahmood, "Regular Boundary Integral Formulation for the Analysis of Open Dielectric/Optical Waveguides", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 44, No. 8, Aug. 1996, pp. 1441-1450.
- [89] J. Charles, H. Baudrand and D. Bajon, "A Full-Wave Analysis of an Arbitrarily Shaped Dielectric Waveguide Using Green's Scalar Identity", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 39, No. 6, June 1991, pp. 1029-1032.
- [90] J.K. Butler, W.E. Ferguson, Jr., G.A. Evans, P.J. Stabile and A. Rosen, "A Boundary Element Technique applied to the Analysis of Waveguides with Periodic Surface Corrugations", *IEEE Journal of Quantum Electronics*, Vol. 28, No. 7, July 1992, pp. 1701-1709.
- [91] R. Courant, "Variational Methods for the Solution of Problems of Equilibrium and Vibrations", *Bull. Am. Math. Soc.*, 1943.
- [92] P.V. O'Neil, *Advanced Engineering Mathematics*, 4th edition.
- [93] R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Interscience, New York, 1953.
- [94] H. Noro and T. Nakayama, "A New Approach to Scalar and Semivector Mode Analysis of Optical Waveguides", *Journal of Lightwave Technology*, Vol. 14, No. 6, June 1996, pp. 1546-1556.

- [95] J. Dongarra, A. Lumsdaine, R. Pozo and K. Remington, "A Sparse Matrix Library in C++ for High Performance Architectures". *Proceedings of the Second Object Oriented Numerics Conference*, 1994, pp. 214-218.
- [96] R. Pozo, K. Remington, A. Lumsdaine, *SparseLib++ Sparse Matrix Class Library, User's Guide*, <http://math.nist.gov/sparselib++/>

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