ABSTRACT

HONNALLI, NARENDRA V. Finite-Difference Time-Domain Simulations on Overgrown InGaN/GaN Multiple Quantum Well Light Emitting Diode. (Under the direction of Dr. Leda Lunardi.)

Light emitting diodes are emerging as compact, rugged, bright and efficient light sources making them a compelling substitute for general lighting applications. Recent breakthroughs in GaN-based blue light emitting diode device growth techniques have not only led to a substantial progress in their internal quantum efficiency but also to the improvement of their light extraction efficiency. Previous experimental data reported an enhancement of almost 3 times in the light output intensity of an InGaN/GaN multiple quantum well light emitting diode overgrown by the embedded voids approach on sapphire substrate using the metal organic chemical vapor deposition technique.

This dissertation presents the simulation results of light output for two structures emitting at $\lambda = 460nm$: with embedded voids and without them. The latter consists of a model depicting the conventional c-plane GaN-based multiple quantum well light emitting diode fabricated under similar growth conditions as that of embedded voids structure. The software tool used for device modeling implements one of the most popular numerical techniques for solving electromagnetic propagation problems known as Finite-Difference Time-Domain method. It is also used to design different configurations of models through Scheme coding interface.

Simulations to measure the light output of InGaN/GaN embedded voids light emitting diode-like structures were performed to study the simultaneous effect of light reflection, scattering, and guiding due to voids as a function of their number, relative separation, different sizes and the source amplitude. A step-by-step procedure was systematically developed to study the effect of embedded voids feature sizes on light transmission and light output efficiency. The results indicate that embedded voids contribute to a light output enhancement up to 2.88 times larger than those with conventional c-plane which is in close agreement with those reported experimentally.
Finite-Difference Time-Domain Simulations on Overgrown InGaN /GaN Multiple Quantum Well Light Emitting Diode

by

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DEDICATION

To my parents and family.
BIOGRAPHY

Narendra Honnalli was born in what was once known as the Manchester city of Karnataka State, Davangere, India in 1990. He graduated from Siddaganga Institute of Technology, Tumkur with a Bachelor’s degree in Electrical and Electronics Engineering in 2013. He was awarded two gold medals for securing the highest cumulative GPA and highest grades in Electrical Machine Design and Network Analysis courses.

He joined North Carolina State University in Fall 2013 for his Master’s degree in Electrical Engineering. Since Fall 2014, he has pursued graduate research in the area of Nanoelectronics and Photonics.
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Chapter 1

Introduction

1.1 Background

Energy efficiency improvement is the primary motivation behind the onset of emerging Group III nitride based light emitting diode (LED) technology. Solid-state lighting (SSL) based on GaN LEDs not only made a major impact on the total energy savings but also helped in a wider coverage of visible wavelengths. As a result, LEDs have dominated a broad field of applications ranging from automotive indicators to high-performance display devices and projection systems. Irrespective of the application, LED’s performance strongly depends on the subtleties of its electronic and optical properties (which includes all active and passive materials) and the interplay between them. The most powerful way to configure its optical properties is to carefully architecture the material design using novel fabrication techniques.

The successive generations of as-grown GaN LEDs come with a prerequisite of satisfying stringent color requirements and improved light output both of which are equally competitive to achieve. The former suffers from what is known as green gap, where the external quantum efficiency (EQE) of device drops significantly in the green visible spectral region. This is due to large induced piezoelectric field and strain effects on the active layers with increased indium
percentages. Over the past few years, the green gap was gradually covered by the increased external quantum efficiency of semi-polar and non-polar In$_x$Ga$_{1-x}$N based LEDs with increased indium incorporation.

When light is generated in the active layer, it is redistributed several times within the device before it ends the journey by radiating into the outer medium. However, it turns out that majority of light gets trapped within the device causing a major output intensity loss and thus low light output. Hence a basic understanding is needed on different ways of light redistribution inside the device to address the cause for low light output.

1.2 Motivation

The focus of this work is to conduct Finite-Difference Time-Domain (FDTD) simulations on the light output efficiency of InGaN/GaN multiple quantum well (MQW) LEDs overgrown on semipolar and non-polar planes with a GaN nucleation layer on sapphire substrate. Dr. Bedair’s group at North Carolina State University (NCSU) has demonstrated an InGaN/GaN MQW LED structure overgrown on semipolar and non-polar planes by using Embedded Voids Approach (EVA) that has achieved almost 3x higher light output than the conventional ones [1]. One of the unique characteristics of this structure is the presence of embedded voids that seem to contribute such a high light output.

Other researchers have followed this technique of enhancing the light extraction for GaN-based LEDs with SiO$_2$ nanorod arrays [2]. The results obtained by conducting FDTD simulations using a commercial software called FullWAVE$^\text{TM}$ demonstrated an increase of about 1.45 times in its light extraction efficiency than the c-plane LEDs [2, 3]. The enhanced light output intensity of embedded voids LED at high current injection level is the motivation for our work. We intend to examine the effect of embedded voids has on the light output efficiency of InGaN/GaN MQW light emitting diodes and compare directly with conventional c-plane
LEDs devoid of these elements. This study will investigate the effect of spacing, number and size of voids on the light output and its transmission.

1.3 Overview of Work

The aim of this work is to investigate and quantify light output of a GaN-based LED structure containing voids by conducting FDTD simulations. Chapter 2 presents a review on the LED structure, simultaneous enhancement of photon generation and reduced dislocation density in the device. Followed by a brief description about light extraction efficiency and recent developments in the research field on improving the performance of GaN-based LEDs.

In Chapter 3, we start with Maxwell’s equations in differential form and then discuss a widely acclaimed numerical solution to its curl equations called FDTD method through Yee’s algorithm [27]. Stability criterion required to avoid numerical instability in the results is elucidated. Further, we hover on implementation of the Yee’s algorithm using free software package with an example.

A two dimension simulation model featuring the linear material parameters of the fabricated LED sample is designed in chapter 4. Considerations and assumptions used for building the complete model are validated numerically. Dielectric profile output and source behavior in the software are illustrated to verify the correctness of our design.

The measurement of light output as a function of number of voids, their relative separation, sizes and the source amplitude is presented in chapter 5. Step-by-step execution procedures are duly gone through to obtain the transmission spectrum and the light output efficiency for a finite grid resolution. The effect of variations in spacing and height of voids on them is investigated with the assistance of field profiles and plots.

Chapter 6 briefly summarizes the work and results obtained in course of iterative simulations. It also suggests some topics in the area that can be pursued for further study.
Chapter 2

Literature Review

This chapter introduces the figures of merit used in scaling the LED’s performance. A brief review is provided on fabrication steps involved in the formation of embedded voids in an In$_x$Ga$_{1-x}$N/GaN MQW LED during the crystal growth and factors contributing to its increased internal quantum efficiency. It also explains some recent research approaches on boosting the overall performance of GaN-based LEDs.

2.1 External Quantum Efficiency

The external quantum efficiency, $\eta_{EQE}$, of an LED is defined as the ratio of external light emitted to the electrically injected electron-hole pairs into the device [4]. It can be expressed as:

$$\eta_{EQE} = \eta_{IQE} \cdot C_{ext}$$

(2.1)

where $\eta_{IQE}$ is the internal quantum efficiency (IQE) which is the fraction of electron-hole pairs injected into the active region that radiatively recombine to generate photons and

$C_{ext}$ is the light extraction efficiency which is the fraction of photons generated in the active region that is obtained as external light.
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The $\eta_{IQE}$ in the equation above implicitly involves the injection efficiency $\eta_{inj}$ which takes into account the fraction of injected electrons captured within the active region.

2.2 An Overgrown Light Emitting Diode Structure

In the past few years, there has been an increasing trend to build blue LEDs based on GaN (wurtzite) nanostructures because the facets of GaN nanostructures expose their semi-polar and non-polar planes for the active layer growth. Specifically, InGaN/GaN multiple quantum wells are widely used as active layers because of its tunable band gap with indium concentration. As a result, this helps in eliminating the effects like Quantum Confined Stark Effect (QCSE) in the active layers and enhances the radiative recombination rate in them. One such approach was successfully demonstrated by Dr. Hosalli et al. in Dr. Bedair’s group at NCSU by conformally overgrowing $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}$ MQWs and planarized p-type GaN on GaN nanowires (NWs) [1].

Growing Group III nitrides in a single-crystal form is quite challenging due to the large dissociation pressure at high temperatures of crystal growth [5]. That is why these materials are deposited on foreign substrates such as sapphire or silicon carbide. Although GaN has large lattice mismatch of approximately 32% with sapphire substrate, it is still used because of its excellent electrical insulating properties and transparency in the visible wavelength range. The conformal overgrowth of the LED structure on GaN NWs was carried out using EVA [6]. It starts with the growth of a low-temperature GaN buffer layer of 100nm thick on a c-plane sapphire substrate. After annealing, bulk GaN:Si (n-type) film of $\approx 2.5\mu\text{m}$ thickness is grown by metal organic chemical vapor deposition (MOCVD) technique. Then to form an array of GaN NWs, the n-GaN film is preferentially etched at dislocations using maskless inductively coupled plasma-reactive ion etching (ICP-RIE) technique. The tips of these NWs orient themselves in semi-polar and non-polar planes as illustrated in Fig. 2.1.
On these semi-polar and non-polar planes, five $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ quantum well/barriers are overgrown followed by the growth of 20nm Mg-doped $\text{Al}_{0.2}\text{Ga}_{0.8}\text{N}$ layer which acts as the electron blocking layer for the injected electron-hole pairs. After the initiation of overgrowth, voids were formed in between the coalesced NWs as shown in Fig. 2.2(a) due to high lateral growth rate on semi-polar planes compared to that on non-planar planes. Finally, a top planar magnesium doped $\text{p-GaN}$ is grown for a thickness of $\sim 300\text{ nm}$. For comparison, a schematic of the conventional $\text{c-plane InGaN/GaN MQW LED structure}$ fabricated under similar growth conditions as that of embedded voids is illustrated in Fig. 2.3.
(a) Cross-sectional transmission electron micrograph of the light emitting diode structure overgrown on nanowires showing the embedded voids (V1, V2 and V3), multiple quantum wells and the top p-GaN layer.

Figure 2.2 InGaN/GaN multiple quantum well light emitting diode structure fabricated using embedded voids approach (Reprinted with the permission from [7]).

(b) Schematic of the light emitting diode structure grown on n-GaN nanowires template.
2.3 Enhanced Internal Quantum Efficiency

The internal quantum efficiency is improved when majority of the recombination events are radiative in nature and emission wavelength corresponds to the designed wavelength. The processing steps used to fabricate the structure in Fig. 2.2 led to the enhancement of its internal quantum efficiency. Some of the main reasons for the improvement of its $\eta_{IQE}$ are listed as follows:

1. The formation of NWs due to preferential etching at the dislocations in n-GaN layer resulted in reduction of dislocation density and thus decreasing the rate of non-radiative recombination. The embedded voids act as dislocation sinks for the threading dislocations propagating from GaN-sapphire interface thereby reducing the compressive strain on the
MQWs [6].

2. The minimized impact of induced polarization field due to overgrowth of MQWs on semi-polar and non-polar planes reducing the effect of QCSE.

3. The geometrical orientation of conformal MQWs on the hexagonal tips of NWs provided an increase in the effective area of emission compared to the planar MQWs in a conventional c-plane LED.

2.4 Light Extraction Efficiency

The efforts put in for efficient generation of photons in the active region will go in vain if the generated photons are not protected from loss mechanisms occurring inside the device. Ideally when all the generated photons escape from the LED die, unity extraction efficiency is said to be achieved. However, in a real device, not all photons emitted from the active region will escape into free space and majority of them get trapped in the semiconductor itself [4]. Some of the mechanisms responsible for that are: light incident on the metallic contacts gets reflected into the device, emitted light gets absorbed by the template and substrate and the inevitable phenomenon of total internal reflection mitigates the escape of light from the semiconductor. Hence the light extraction efficiency can be defined as:

\[
\eta_{\text{extraction}} = \frac{\text{number of photons emitted into free space per second}}{\text{number of photons emitted from active region per second}} = \frac{\left( \frac{P}{\hbar \nu} \right)}{\left( \frac{P_{\text{int}}}{\hbar \nu} \right)}
\]  

(2.2)

where \( P \) is the optical power emitted into free space and \( P_{\text{int}} \) is the optical power emitted from the active region.

A significant amount of light gets trapped within the device owing to the large refractive
index of the semiconductor \((n_{\text{semi}} \approx 2 - 3)\) compared to that of air \((n_{\text{air}} = 1)\). When a light ray traveling in a high refractive index material is incident on a low refractive index interface at an angle greater than the critical angle \(\theta_c\), it suffers total internal reflection as illustrated in Fig. 2.4.

\[ n_1 > n_2 \]

\[ \theta_i > \theta_c \]

\[ \theta_i < \theta_c \]

\[ \theta_r \]

\[ \theta_c \]

\[ \theta_i \]

\[ n_1 \sin \theta_i = n_2 \sin \theta_r \] \hspace{1cm} (2.3)

**Figure 2.4** Refraction of the light ray for angles of incidence, \(\theta_i < \theta_c\) and total internal reflection for \(\theta_i \geq \theta_c\).
The boundary condition at which total internal reflection starts to occur is when \( \theta_i = \theta_c \) and \( \theta_r = 90^\circ \). Hence critical angle can be written as:

\[
\theta_c = \arcsin \left( \frac{n_2}{n_1} \right)
\] (2.4)

The critical angle calculated from Eq. 2.4 determines the light escape cone of the semiconductor-dielectric interface. The dielectric can either be air or the substrate (in this case sapphire). The refractive index of GaN in the visible wavelength range is about 2.4 and that of sapphire substrate is 1.7. Therefore, the critical angle for GaN-sapphire interface would be:

\[
(\theta_c)_{\text{GaN–saph}} = \arcsin \left( \frac{1.7}{2.4} \right) = 45.09^\circ
\] (2.5)

and the critical angle for GaN-air interface would be,

\[
(\theta_c)_{\text{GaN–air}} = \arcsin \left( \frac{1}{2.4} \right) = 24.62^\circ
\] (2.6)

Given these conditions, significant amount of light generated from MQWs of the LED suffers total internal reflection at GaN-sapphire and GaN-air interfaces. Fig. 2.5 shows the schematic of narrow light escape cone for the GaN-air interface.

However, light escaping within the cone suffer Fresnel reflections at the interface depending on its polarization. The fraction of light reflected at the interface is given by Fresnel equations for transverse electric (TE) and transverse magnetic (TM) polarizations.

\[
\rho_{TE} = \frac{n_1 \cos \theta - \sqrt{n_2^2 - n_1^2 \sin^2 \theta}}{n_1 \cos \theta + \sqrt{n_2^2 - n_1^2 \sin^2 \theta}} \quad \text{and} \quad R_{TE} = |\rho_{TE}|^2
\] (2.7)
Figure 2.5 Schematic of the light escape cone for the GaN-air interface.

\[ \rho_{TM} = \frac{-n_2^2 \cos \theta + n_1 \sqrt{n_2^2 - n_1^2 \sin^2 \theta}}{n_2^2 \cos \theta + n_1 \sqrt{n_2^2 - n_1^2 \sin^2 \theta}} \quad \text{and} \quad R_{TM} = |\rho_{TM}|^2 \quad (2.8) \]

where \( R_{TE} \) and \( R_{TM} \) are the reflectances of s-polarized (TE) and p-polarized (TM) light respectively, \( \theta \) is the angle of incidence and \( n_1, n_2 \) are the refractive indices of the media. The plot of Eqs. 2.7 and 2.8 for GaN-air interface and GaN-sapphire interface as a function of incident angles are shown in Figs. 2.6 and 2.7 respectively. It can be observed that greater the difference between refractive indices of the two media, narrower is the light escape cone and hence more total internal reflection. The cascaded effect of multiple Fresnel reflections at GaN-sapphire and GaN-air interfaces results in more trapping of light inside GaN. If \( P_{in} \) is the light power from a point-like source inside the semiconductor of refractive index \( n_s \) then the amount of power
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Figure 2.6 Fresnel reflectance as function of incident angle for the GaN-sapphire interface. The critical angle occurs at 45°.

\[ n_1 = 2.4(\text{GaN}), \quad n_2 = 1.7(\text{Sapphire}) \]

\[ C_{ext} = \frac{P_{out}}{P_{in}} \approx \frac{n_{air}}{4(n_s)^2} \]  

From Eq. 2.9, \( C_{ext} \) for GaN-air interface would be 4.3% which indicates that only a small percentage of generated light can escape the device. This means that an improvement in \( C_{ext} \) is essential to take advantage of high internal quantum efficiency LEDs.

2.5 Recent Research

There have been several advancements in augmenting the internal quantum efficiency and light extraction efficiency of an LED. Some of them are discussed below:
1. Majority of the areas on GaN-based LED exploration is concentrated on obtaining the right emission wavelength by achieving high quality of the epitaxial layers. Some of the experimentation involved mitigating the strain effects arising from threading dislocations at GaN-sapphire substrate. Recent advances show that vertically aligned and large density GaN-nanowires can be grown by having a sub-monolayer thickness (<1nm) of Ni on the sapphire substrate which helps in strain relaxation. The thin Ni film leads to the formation of very small and dense Ni islands on the substrate resulting in high degree of vertical alignment. This fabrication technique also helps in facilitating device integration with other optical and electronic devices [8].

2. The performance of InGaN-based light emitting diodes in the green spectral region is hindered by the effects of high indium percentage on the active layers. The higher stability
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of InN on N-polar GaN surface enables increased indium percentage with a major disadvantage of impurity incorporation owing to its rough hexagonal surface. Thus achieving a good p-type on this surface is quite challenging.

An alternative approach is to invert the N-polar surfaces to Ga-polar surfaces prior to p-type growth. This was realized using an MOCVD growth technique of depositing a thin heavy Mg doped GaN layer on top of the active layers [9]. Thus an LED structure with the advantages of high indium incorporation for the active layers on N-polar surface and an improved p-type film on inverted Ga-polar surface can be fabricated to achieve low turn-on voltage.

3. The InGaN/GaN MQW structures are known to behave differently even under similar growth conditions due to their physical and electronic variations which in turn affect the emission wavelength of LEDs. This is mainly due to strain in the underlying GaN template layer induced from lattice mismatch with the substrate (typically sapphire). One of the ways to relax the strain is to grow a 15µm thick GaN template layer which makes it virtually unstrained compared to a 5µm thick template layer [5]. With this relaxation, not only a red-shift in the emission output can be attained but also high indium incorporation and growth rates can be gained.

4. Another practice is to grow In$_x$Ga$_{1-x}$N/GaN “strain-balanced” multiple quantum wells on thick In$_y$Ga$_{1-y}$N templates for $x > y$ using MOCVD technique [10]. These strain-balanced layers consist of alternating layers of In$_x$Ga$_{1-x}$N wells and GaN barriers under compressive and tensile stresses respectively which have been lattice matched to a thick In$_y$Ga$_{1-y}$N template ($\approx 180$ nm). When compared to conventional In$_x$Ga$_{1-x}$N/GaN MQWs grown on GaN templates, the strain-balanced structures showed a comparatively high redshift and increased intensity in the emission wavelength. This tactic can be utilized for fabricating LEDs with higher emission wavelength with less indium percentage and more periods of
5. When GaN film is grown on foreign substrates such as sapphire, the interface leads to the formation of threading dislocations which ultimately influences the performance of the device. To uniformly reduce dislocations over a large area of the substrate, the embedded voids approach was implemented [6]. This is based on overgrowth of GaN on GaN nanowires created by a mask-less etching technique. The overgrowth was made possible due to the inception of network of voids which acted as pools for dislocations propagating from the GaN/sapphire interface.

6. One of the early designs to improve light extraction was to encapsulate an LED with a dome-shaped epoxy of high refractive index ($n > 1.5$). As a result of encapsulation, the critical angle for semiconductor-resin interface would increase thereby increasing the light escape cone. The efficiency of LED increased by 2-3 times when refractive index of the dome was matched with that of the semiconductor [11]. One may suspect the effect of total internal reflection at the resin-air interface due their refractive index difference. But it can be seen in Fig. 2.8 the light will be incident at an angle equal to 90° due to the hemispherical geometry of the dome. Besides improving the extraction efficiency of the LED, the encapsulant also helps in obtaining a directed light emission pattern by acting as a lens.

7. Light extraction can also be improved by using the remaining five facets of the LED chip besides the emission facet [12]. Since the lateral dimensions of the chip are comparatively large, much of the light traveling laterally will be absorbed by the semiconductor as it hits the facets at a constant angle due to their rectangular cross section which may be greater than its critical angle causing total internal reflection. A slight tilting of the facets will aid the light to be incident within its escape cone at least after multiple reflections along with the use of transparent substrates and window layers. However, this kind of
setup implies a volume-emitting LED with side emission. This increases the expense of resources on packaging to obtain a directed light extraction.

8. The past few years have witnessed the increase in light extraction of GaN-based LEDs with intense surface texturing. When the lack of c-plane etchability of GaN was overcome by wet chemical etching of a- and m-planes, substantial amount of surface texturing was created by pyramid-like crystalline structures [12]. The textured feature acts as sites for one or several scattering and reflection events which are sufficient to out-couple the light from the semiconductor.

Some of the efforts include nano-roughened p-GaN surface using a self-assembled Nickel metal cluster as the laser etching mask [13]. This not only increased the light extraction efficiency by $\approx 1.55$ times compared to conventional LEDs without roughened surface but
also reduced its forward voltage at the expense of non-planar top p-layer.

9. The current advanced chip designing approach adopted by some of the leading solid-state lighting industries is *thin-film flip-chip* LEDs [14]. This design technique has been applied to InGaN-based LEDs which employs several aspects in one chip to enhance light extraction. A classic device fabrication includes flip-chip mounting of the LED followed by removal of the substrate. In addition, n-GaN surface is textured and a low-loss reflective p-contact is used underneath the epi-layers resulting in a light extraction efficiency of $\sim 80\%$.

There is a technique known as *surface plasmon enhancement* which strives for improving both the light extraction and the internal quantum efficiency in visible wavelength range. It works on the principle of bypassing radiative recombination in the quantum well region and transferring high energy to surface plasmon modes in a neighboring metal surface coating [14].

10. The deposition of SiO$_2$ microspheres on the top of p-layer proved to improve the light extraction efficiency of III-nitride LEDs by a maximum of $\sim 2.2$ times with their diameter equal to a emission wavelength of 500nm and refractive index equal to that of GaN [15]. These spheres were deposited in the form of hexagonal packed structure via rapid convective deposition method, a low-cost technique for deposition of large area of spheres. Similar improvements were demonstrated using transmission gratings on top of p-GaN layer based on FDTD simulations [16].

Enhancement of light extraction was also reported by conducting FDTD simulations on an array of nanomaterials placed on top of n-GaN layer [17]. The reference used for comparison was a structure with thin Polyethylene glycol (PEG) film on top of n-GaN layer.
Photonic crystals (PCs) have attracted majority of crystal growers to implement them as a solution to overcome the low extraction efficiency of as-grown LEDs [18–26]. PCs are a periodically modulated dielectric materials which are placed close to the active region (near InGaN/GaN quantum well structures). In a conventional GaN-based LED structure with thickness of GaN template layer in few 2 – 3µms, several higher order modes are guided in course of lateral propagation of light. Since the low order modes carry most of the light, embedded PCs have been successful in their extraction due to better overlap of these modes with the crystals.

Embedded PCs involve intricate fabrication processes to obtain short periodicity of their dielectric modulation. Additional low-index cladding layers such as AlGaN can be incorporated below the active region to confine most of the low order modes.
Chapter 3

Finite-Difference Time-Domain Method

“We can scarcely avoid the conclusion that light consists in the transverse undulations of the same medium which is the cause of electric and magnetic phenomena”-

Sir James Clerk Maxwell.

The electromagnetic behavior of light explained by Sir James Clerk Maxwell are governed by a set of four partial differential equations. They are collectively known as “Maxwell’s equations”. This chapter begins with a brief review of Maxwell’s equations, deals with an effective numerical solution technique known as the FDTD method and its implementation using a software package.

3.1 Maxwell’s Equations

Maxwell’s equations describe the time and spatial dependency between the vector electric field $\mathbf{E}$ and the pseudo vector magnetic field $\mathbf{B}$. The differential form of these equations for time-
varying fields are given by Eqs. 3.1.

\[ \nabla \cdot D(x,t) = \rho(x,t) \quad \text{[Gauss' law]} \tag{3.1a} \]
\[ \nabla \times E(x,t) = -\frac{\partial B(x,t)}{\partial t} \quad \text{[Faraday's law]} \tag{3.1b} \]
\[ \nabla \cdot B(x,t) = 0 \quad \text{[Gauss' law]} \tag{3.1c} \]
\[ \nabla \times H(x,t) = J(x,t) + \frac{\partial D(r,t)}{\partial t} \quad \text{[Ampere's law]} \tag{3.1d} \]

where \( D(x,t) \) is the electric flux density in \( (C/m^2) \),
\( E(x,t) \) is the electric field intensity in \( (V/m) \),
\( B(x,t) \) is the magnetic flux density in \( (Wb/m^2) \),
\( H(x,t) \) is the magnetic field intensity in \( (A/m) \),
\( \rho(x,t) \) is the volume charge density in \( (C/m^3) \), and
\( J(x,t) \) is the electric current density in \( (A/m^2) \).

Further the relation between \( D, E, B \) and \( H \) can be inferred from what are known as constitutive relations. These conditions establish the physical properties of a medium of interest and how fields interact with it: the permeability \( \mu \) and permittivity \( \epsilon \) of the medium. For linear, isotropic and non-dispersive materials, constitutive relations are:

\[ D(x,t) = \epsilon(x)E(x,t) \tag{3.2} \]
\[ B(x,t) = \mu(x)H(x,t) \tag{3.3} \]

where \( \epsilon(x) \) and \( \mu(x) \) can be expressed in terms of dielectric constant \( \epsilon_r \) and relative permeability \( \mu_r \) of the material respectively. In order to have more closer physical meaning in terms of how electromagnetic waves propagate, a meaningful quantity called the refractive index is defined.
as in Eq. 3.4.

\[ n = \sqrt{\mu_r \epsilon_r} \]  

(3.4)

Most semiconductor materials exhibit a negligible magnetic response and hence above equation can be rewritten as:

\[ n^2 = \epsilon_r \]  

(3.5)

3.2 The Yee’s Algorithm

In 1966, Yee originated a set of finite-difference equations for the system of partial differential equations mentioned in Eq. 3.1. It was proved to be an efficient algorithm for achieving numerical solutions to a scattering problem in which the characteristic linear dimension of the object is comparatively larger than the operating wavelength [27]. The finite-difference expressions solve for both electric and magnetic fields in time and space which are second-order accurate rather than solving for electric field alone (or the magnetic field alone) with a wave equation [28, 29]. Maxwell’s curl equations (Ampere’s law and Faraday’s law) in rectangular Cartesian coordinate
CHAPTER 3. FINITE-DIFFERENCE TIME-DOMAIN METHOD

system can be written as the following six partial differential equations:

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right) \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right) \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right) \\
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \left( \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - \sigma E_x \right) \\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon} \left( \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - \sigma E_y \right) \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z \right)
\end{align*}
\]

(3.6a)  (3.6b)  (3.6c)  (3.6d)  (3.6e)  (3.6f)

It can be observed from the set of equations in Eq. 3.6 that the temporal derivatives of the magnetic field are expressed in terms of the spatial derivatives of the electric field. Conversely, the temporal derivatives of the electric field are expressed in terms of the spatial derivatives of the magnetic field. Using this relation, the partial differential equations are discretized as follows:

1. In order to discretize space and time, a Yee’s cube was introduced as illustrated in Fig. 3.1 where a grid point in space can be expressed as,

\[(i, j, k) = (i \Delta x, j \Delta y, k \Delta z)\]  (3.7)

and any function of space and time can be denoted as,

\[F(i \Delta x, j \Delta y, k \Delta z, q \Delta t) = F^q(i \Delta x, j \Delta y, k \Delta z)\]  (3.8)
where $\Delta_x, \Delta_y$ and $\Delta_z$ are the spatial offsets between sample points and $\Delta_t$ is the temporal offset with a temporal step $q$.

**Figure 3.1** Discrete positions of electric and magnetic fields in a Yee cube.

2. With the help of discretization, a set of finite-difference equations for the electric and magnetic fields can be written. For Eq. 3.6a we have,

$$
\frac{H_{x}^{q+0.5}(i, j, k) - H_{x}^{q-0.5}(i, j, k)}{\Delta t} = \frac{1}{\mu_{i, j, k}} \left( \frac{E_{y}^{q}(i, j, k + 0.5) - E_{y}^{q}(i, j, k - 0.5)}{\Delta z} \right)
$$

$$
- \frac{E_{z}^{q}(i, j + 0.5, k) - E_{z}^{q}(i, j - 0.5, k)}{\Delta y} \right)
$$

On solving for $H_{x}^{q+0.5}(i, j, k)$ in Eq. 3.9 the update equation for $H_x$ field can be obtained. It shows that the future value of $H_x$ depends on only its previous value and the neighboring
electric fields. In a similar manner, finite-difference expressions for the $H_y$ and $H_z$ field can be derived.

With the same analogy, finite-difference expressions for the $E_x$, $E_y$ and $E_z$ fields can be written. For Eq. 3.6f we have,

$$\frac{E_z^{q+1}(i, j, k) - E_z^q(i, j, k)}{\Delta t} = \frac{1}{\epsilon_{i,j,k}} \left( \frac{H_y^{q+0.5}(i + 0.5, j, k) - H_y^{q+0.5}(i - 0.5, j, k)}{\Delta x} - \frac{H_x^{q+0.5}(i, j + 0.5, k) - H_x^{q+0.5}(i, j - 0.5, k)}{\Delta y} \right)$$

(3.10)

Similar to the magnetic field update equation, the future value of $E_z$ depends on only its previous value and the value of its neighboring magnetic fields.

3. After obtaining the “update equations”, the electric fields are evaluated during each time-step and the magnetic fields are evaluated at every half time-step based on the electric field values evaluated half time-step before. This *leapfrog* time-stepping process iterates until the fields are evaluated for the desired duration and helps in avoiding the need to solve simultaneous equations from Eq. 3.6.

### 3.3 Stability Criterion

One of the most important things to consider while designing the FDTD solution is its numerical stability. The space grid size must be such that the electromagnetic field should not change significantly over one time-step increment. Otherwise, they would produce results which spuriously increase with time. Hence the explicit time-stepping, $\Delta t$ has a constraint that is often represented as the ratio of temporal step and spatial step. Since the maximum travel speed of electromagnetic energy is the speed of light $c$ in free space, the maximum distance that energy can travel in one time-step is $c\Delta t$. The ratio $c\Delta t/\Delta x$ is called the Courant factor.
Further in the FDTD algorithm, each node only affects its nearest neighbors. In one complete cycle of updating the fields, the furthest the electromagnetic field could propagate is one spatial step. So, the optimum ratio for Courant factor is also the maximum ratio allowed to get stable results [29]. Consequently, the upper limit of time-stepping in 2D is given by:

$$c_{\text{max}} \Delta t \leq \sqrt{(\Delta x)^2 + (\Delta y)^2}$$

(3.11)

where $c_{\text{max}}$ is the maximum light velocity in medium. Hence the chosen spatial resolution puts a restriction on time-stepping application of the algorithm.

### 3.4 Software Implementation

We took the advantage of MEEP which officially stands for Massachusetts Institute of Technology’s Electromagnetic Equation Propagation, a free FDTD simulation software package under GNU General Public License (GPL) developed to model electromagnetic systems [30]. MEEP uses the standard Yee grid discretization discussed above to stagger the electric and magnetic fields in space and time. Each field component is sampled at different spatial locations offset by half a pixel, allowing space and time derivatives to be expressed as finite-difference approximations. In two dimensions, the $k^{th}$ component of $E$ is stored for the locations $(i, j) + 0.5\hat{e}_k \Delta x$ and the $k^{th}$ component of $H$ is stored for the locations $(i + 0.5, j + 0.5) - 0.5\hat{e}_k \Delta x$ as shown in the Fig. 3.2.

In addition to Yee discretization, the grids are divided into chunks which help in providing the illusion of continuity in the specification of materials, sources and output fields. Material characteristics represented in Maxwell’s curl equations and their dependency on position, frequency (material dispersion) and the incident fields (non-linearity) are supported by this software. MEEP also supports different types of material modeling like Lorentz-Drude models.
and conductivities which are widely used in modeling photonic crystal light emitters.

This software typically simulates Maxwell’s curl equations by providing as much versatility as possible in terms of material and source properties. It solves the initial-value problem where the fields and currents are zero for $t < 0$, and then non-zero values evolve in response to some currents $\mathbf{J}(x, t)$ and surrounding material parameters. It also emphasizes the use of dimensionless units where the constants like $\epsilon_0$, $\mu_0$ and $c$ are unity by exploiting the scale invariance property of Maxwell’s equations. A clear understanding of units in MEEP is explained in Appendix-A.

Since FDTD simulations are performed in a finite region of computational space, the solutions should be successfully terminated with appropriate boundary conditions. This software package provides three basic types: Perfectly Matched Layer (PML) absorbing conditions, metallic walls and Bloch-periodic boundaries which help in circumventing the problem of high

Figure 3.2 2D Yee lattice for transverse electric polarization.
computational requirements. MEEP also includes some unusual features ranging from calculating the eigen-mode frequencies for a periodic structure to advanced signal processing techniques for analyzing the resonant modes of a system. The usage of MEEP revolves around the control file known as “ctl” file and peripheral utility programs required for post-processing of the output files. The ctl file contains the code specifying the environment required for the problem like geometries, current sources, flux regions etc. written in a scripting language called Scheme (see Appendix-B). This file is implemented on top of “libctl” library which simplifies the communication between Scheme and the software.

Perhaps one of the frequent tasks performed using this software package is to compute the transmission or scattering spectra from a finite arbitrary structure in response to some stimulus as a function of input frequency. Fig. 3.3 depicts the dielectric profile of a bent waveguide whose transmission spectra and field patterns are computed at the end of the waveguide. The first step would be writing a control file to define the computational region and dielectric properties of the bent waveguide. A base unit is chosen based on the problem which may be the units of length (it may be 1\(\mu\)m, 1nm or 1nm) and every simulation parameter is defined in terms of that. A 2D computational cell of 16 meep units \(\times\) 16 meep units is defined with its origin at the center. All materials will be centered at the origin unless specified exclusively and if no material is defined then the default material will have a refractive index of 1 i.e. air. The waveguide structures are specified as blocks of size 12 meep units \(\times\) 1 meep unit with a dielectric constant (non-dispersive) 12 centered at \(C_1\) and \(C_2\) respectively.

In order to efficiently couple the modes corresponding to the waveguide, a Gaussian line source is placed inside it near the left end with its width equal to that of the waveguide. With the help of a preliminary experimental data, this source is characterized by a center frequency of 0.15 meep units, a pulse-width of 0.1 meep units and its electric field component in the z-direction i.e. normal to the computational plane. PMLs of thickness 1\(\mu\)m are used as boundary conditions to minimize successive reflections when the electric field hits the end of
for discretizing the waveguide structures in space and time, an optimum resolution of 10 is set which satisfies the spatial and time-stepping stability criteria. Resolution is the number of pixels per unit base length equivalent to number of Yee-cells per unit base length. In general, at least 8-10 pixels per unit base length in the highest dielectric material is needed for higher accuracy in the simulation results. Finally, a region known as the flux region which can be a plane, line or volume is defined at the bottom of $C_2$ waveguide where the flux spectra as a function of frequency is computed. Flux regions should not be defined within the absorbing
PML regions which result in erroneous results.

After setting up all structures, sources and flux regions, the simulation is run until the Gaussian source has turned off. MEEP accumulates the Fourier transforms of the field at every point in the flux line as the simulation progresses. To ensure the convergence of the Fourier transforms, the simulation is run for some additional time to allow the pulse, reflections or any resonant modes to decay away in the cell. After the source is turned off, the program keeps running for an additional 50 time units until the component $|E_z|^2$ at the center of the flux line has decayed by $1/1000$ from its previous peak value. As far as outputs are concerned, the software generates the dielectric profile, fields and fluxes in terms of Hierarchical Data Format (HDF) files. These output files can be analyzed using tools like MATLAB\textsuperscript{TM}, HDFView and h5utils. One of the best ways is to visualize the propagation of electric or magnetic fields as color mapped images which is done by using a peripheral program h5utils. The steady-state $E_z$ profile of the bent waveguide structure is as shown in Fig. 3.4.

From the Fig. 3.4, conclusions are drawn that the electric field is suffering reflections and leakage loss around the bend. The complex part in getting the transmission spectra is to eliminate the effects of reflection, scattering and other phenomena which are also measured by the flux lines. In order to achieve that, a normalization simulation run is performed without the scattering structure which in this case would be only the waveguide centered at $C_2$. For normalization run, a flux line is defined at the right end of $C_1$ waveguide with all other features of the cell unchanged. At the end of simulation, the flux values are displayed as a comma-delimited data which can be easily imported into a spreadsheet or to any plotting program. Transmitted power through the bent waveguide is obtained by taking the ratio of flux values of bent waveguide and its normalization run. Thus by measuring the response to a short pulse, one can get scattering amplitudes over a range of frequencies.

Apart from transmission spectra, a wide variety of numerical experiments can be done using MEEP. Some of them are:
1. Similar to transmission spectra, reflection spectra can also be obtained by measuring the response of complex structures in the computational cell to a short gaussian pulse.

2. By analyzing the response of a system to a short pulse one can excite the harmonic modes of a system, measure their decay rates and corresponding frequencies.

3. Field patterns can be visualized in response to a continuous wave source (fixed frequency) or a short pulse-width gaussian source which can be combined with other computations such as photonic band diagram calculation.

In spite of handful of commercial FDTD software packages like FDTD solutions by Lumerical\textsuperscript{TM} inc. and XFtdt EM simulation software, MEEP stands out in satisfying the needs of research by providing free access to the source code. With this kind of flexibility, one can quickly experiment
with novel photonic structures to investigate their interactions with electric and magnetic fields. The minimalistic interface of MEEP and its simplicity in implementing the FDTD algorithm complements other elaborated software packages.
Chapter 4

Simulation Model

The FDTD algorithm and its implementation using MEEP, described in chapter 3 is applied for modeling the InGaN/GaN embedded voids LED structure. This chapter presents the description of the simulation model, assumptions behind it and how material parameters are incorporated using the software package.

4.1 Computational Domain

The experimental results indicated that light output intensity of In$_{0.2}$Ga$_{0.8}$N/GaN MQW LED with embedded voids was approximately 3x higher than the conventional c-plane one fabricated under similar growth conditions at a current injection level of 150mA as illustrated in Fig. 4.1. The measurement was performed by coupling the light emitted from transparent sapphire substrate to a silicon photo detector placed 2 cm below it using an optical fiber. To understand the cause of increased light output, there has to be a quantitative distinction between its IQE and light output efficiency. The IQE has been greatly improved because of the increased quality of GaN NWs template, growth of MQWs on semi-polar and non-polar planes and increased emission surface area due to their geometric orientation. But there still exists a large difference
between the refractive indices of GaN ($n = 2.4$) and air ($n = 1$).

The investigation on the light output efficiency and the light transmission was carried out by performing FDTD simulations on this LED structure. For all the calculations used in MEEP, a base unit of $1 \mu m$ is set which means that length scales and their related quantities are expressed in terms of the base unit. A schematic of 2D computational domain and the epitaxial layers of NWs LED are illustrated in the Fig. 4.2. The simulation environment is coded in Scheme scripting language in a control file. The basic features of the model are discussed below:

1. The outer bold black line demarcates the physical region within which the entire simulation takes place. The experimental LED samples were fabricated into mesas of dimensions $400 \mu m \times 400 \mu m$ which are computationally expensive to model. Since we are interested in embedded voids feature, the dimensions of our computational domain is $25 \mu m \times 33 \mu m$. 

---

**Figure 4.1** Measured light output intensity of the c-plane and nanowires light emitting diode structures as a function of applied current (Reprinted with the permission from [7]).
Figure 4.2 2D schematic of the computational domain depicting epilayers of light emitting diode structure surrounded by air.

All numerical data used to define these in the scheme code are in “meep units”. This is the computational cell which is discretized into standard Yee grids and the electric and magnetic fields are evolved at every point in the cell.

2. The inner gray region indicates the PML, an artificial absorbing medium commonly used to truncate computational grids in FDTD simulations for higher accuracy. This technique was proposed by Berenger in 1994 which absorbs plane waves of any incidence, polarization and frequency at the boundary by slowly turning on its absorption. The PML was introduced as a split-field formulation of Maxwell’s equations where each six vector field components in 3D is split into two orthogonal components and losses are introduced in it through electrical and magnetic conductivities [32, 33].

MEEP implements a version of the PML as an effective dispersive layer with anisotropic
material properties. In our simulation model we used a PML of thickness 1\(\mu m\) which is thick enough to absorb the incident field thereby avoiding the measurement of irrelevant reflections from the boundaries. Moreover, defining thinner PML increases the numerical reflections due to grid discretization. The strength of the PML is described in terms of the amplitude of light passing through it, reflecting off the edge of the computational cell and propagating back. It is a number that multiplies the PML absorption coefficient and is set to the default value of 1 in our model. Increasing the strength of PML may decrease its reflection coefficient, but will also increase numerical reflections before the incident field is absorbed.

3. The main material of LED structure, GaN is defined with a refractive index of 2.4 and a thickness of 3.3\(\mu m\). This region is representative of the total thickness of GaN nucleation layer, n-GaN template, MQWs and the planarized top p-layer. The material is assumed to be non-dispersive because it can be observed from Fig. 4.3 that the variation of refractive index of GaN grown on sapphire by MOCVD technique is negligible around the emission wavelength of 460nm.

4. In practical samples, the thickness of sapphire substrate ranges from 330\(\mu m\) - 430\(\mu m\) for a 2” wafer diameter indicating its large thickness compared to the epitaxial layers and less reflections within it for a Gaussian input pulse [35-37]. In case of substrate thickness ranging from 25\(\mu m\) – 100\(\mu m\), there are no accountable reflections at the air-sapphire interface. Hence to be within the computational memory limit, we define it with a thickness of 25\(\mu m\) at the bottom of GaN layer. The substrate’s refractive index is set to 1.7 and is also assumed to be non-dispersive in nature because of its transparency to the emission wavelength. The rest of the computational cell is filled with air to model the sapphire-air interface of the sample.

5. A resolution of 53 is set for the computational cell such that each base unit of 1\(\mu m\) is
divided into 53 Yee-cells and the electric and magnetic fields are distributed on their boundaries as per the Yee’s algorithm. Each Yee cell is therefore 1/53 meep units long implying $\Delta x = 1/53$, which in turn determines the upper limit for the time stepping in algorithm. Hence a given spatial resolution affects the time-stepping of the algorithm and the simulation time. One of the important factors that dictate the behavior of fields during the simulation is the Courant number which is set to 0.5 by default in MEEP. This value is within the Courant factor of $1/\sqrt{2} = 0.707$ for a 2D computational cell. With $\Delta x = 1/53$, the upper limit for our time-stepping defined by the stability criterion would
be:

\[
\Delta t \leq \frac{(1/53)}{\sqrt{2}} \leq 0.013341 \tag{4.1}
\]

Since we are working with GaN which has a refractive index of 2.4, the emission wavelength in the material would be:

\[
\lambda_{\text{emission}}(\text{meep units}) = \frac{460 \times 10^{-9}}{1 \times 10^{-6} (\text{base unit})} = 0.46 \text{ meep units} \tag{4.2}
\]

\[
\lambda_{\text{emission}} \frac{n_{\text{GaN}}}{2.4} = 0.19167 \text{ meep units} \tag{4.3}
\]

It is required to have a minimum of 8-10 pixels per wavelength in the high dielectric material to get results with a relative error of the order of $10^{-2}$. So a minimum resolution of $8/0.19167 = 41.738$ is needed and it is taken care of with the chosen spatial resolution.

### 4.2 Modeling of Voids

The striking feature of the In$_{0.2}$Ga$_{0.8}$N/GaN LED structure is the presence of embedded voids after the overgrowth on GaN NWs. The embedded voids network is arranged with random spacing and sizes as a consequence of the random nature of etching process at etching sites (dislocations) and difference in the growth rates on semi-polar and non-polar planes. The range of dimensions of embedded voids is shown in table 4.1. In our 2D computational cell, ten periodic voids are modeled as cylinders with height $h$, cross sectional radius $r$ and a spacing of $d$ between them as illustrated in Figs. 4.4 and 4.5. The refractive index of the medium in embedded voids
Table 4.1 Dimensions of embedded voids.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Dimension range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>0.5 – 2.0µm</td>
</tr>
<tr>
<td>Cross-sectional radius</td>
<td>0.1 – 0.25µm</td>
</tr>
<tr>
<td>Spacing between adjacent voids</td>
<td>0.5 – 2.0µm</td>
</tr>
</tbody>
</table>

in the sample was close to that of air and hence the cylinders in our model has a refractive index of 1. It can be observed in Fig. 4.5 that the PML is not as conspicuous as in the schematic but

Figure 4.4 Cross-section schematic used in the simulation of InGaN/GaN multiple quantum well light emitting diode with 10 embedded voids.

its presence can be observed during the simulation when the fields incident on it are absorbed.
Figure 4.5 Cross-sectional dielectric profile output from the simulation with 10 voids ($d = 1.5\mu m, h = 1.2\mu m$ and $r = 0.175\mu m$).

### 4.3 Modeling of the Active Layer

The electro-luminescence characteristics of embedded voids LED indicates that the semi-polar nature of five In$_{0.2}$Ga$_{0.8}$N/GaN MQWs contribute a broad emission spectra at high current injection level as shown in Fig. 4.6. Hence in our model, the active layer is modeled as broad Gaussian dipole point sources with its electric field component oscillating in X-direction (TE polarization). The parameters defining a Gaussian dipole point source such as center frequency and frequency width are calculated from the electro-luminescence spectra as follows:

1. **Center frequency**

   \[ \lambda_{\text{emission}} = 460nm \]

   Since our base unit is $1\mu m$ and the speed of light $c$ is 1 in MEEP,
Figure 4.6 Electro-luminescence spectra of embedded voids light emitting diode at different applied currents (Reprinted with the permission from [7]).

\[ f_{cen} (\text{meep units}) = \frac{c}{\lambda_{emission} (\text{meep units})} = \frac{1}{0.46} \quad (4.4) \]

2. Frequency width

From the Fig. 4.6 at a current injection level of 100mA,

\[ \lambda_{min} \approx 425nm = 0.425 \text{ meep units} \]

\[ \lambda_{max} \approx 535nm = 0.525 \text{ meep units} \]
Correspondingly,

\[
\begin{align*}
    f_{\text{max}} &= \frac{1}{0.425} \text{ meep units} \quad (4.5) \\
    f_{\text{min}} &= \frac{1}{0.535} \text{ meep units} \quad (4.6)
\end{align*}
\]

Frequency-width, \( df = f_{\text{max}} - f_{\text{min}} = 0.48 \text{ meep units} \quad (4.7) \)

In order to verify the behavior of a single TE polarized Gaussian dipole point source with above mentioned characteristics, it was placed near the top of GaN layer as shown in Fig. 4.7 and the flux was measured approximately 0.66\( \mu \)m away from it. After the measurement, the comma-delimited file was imported to MATLAB\textsuperscript{TM} to plot the flux values against frequencies as shown in Fig. 4.8. It can be observed that the Gaussian source behaves as intended and

![Figure 4.7](image)

**Figure 4.7** Simulation output of a single Gaussian point dipole source placed near the top of GaN layer.
the slight shift in the peak wavelength is due to the nature of this source in the software. The Gaussian sources in MEEP are not precisely Gaussian but the time derivative of it. This was done to ensure that the flux converges at the end of simulations for problems with periodic boundary conditions.

To average out the effect of emission from the MQWs, three Gaussian point dipole sources are placed between adjacent voids as shown in the Fig. 4.9. The triangular geometry is to replicate the cross-sectional view of semi-polar $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}/\text{GaN}$ MQWs. The placement of sources is calculated based on the angle between the dominant semi-polar planes and c-plane which is either $62^\circ$ or $58^\circ$ [1]. Choosing an angle of $58^\circ$ for a spacing between the voids of $0.5\mu m$ and radius of $0.1\mu m$, the height of top source is evaluated as follows:
Figure 4.9 Dielectric profile output showing the placement of three Gaussian point dipole sources $G_1$, $G_2$ and $G_3$ above voids in GaN on sapphire substrate.

Let the sources be named as $G_1$, $G_2$ and $G_3$, voids be $V_1$ and $V_2$. If $\theta$ is the angle between semi-polar plane and the c-plane and $x$ is the distance between $G_1$ and top of $V_1$ as shown in Fig. 4.9 then the height, $H$, of $G_1$ is,

\[
x \cos \theta = 0.5 \times (r + d + r) = 0.5 \times (0.1 + 0.5 + 0.1) = 0.35 \mu m = 0.35 \text{ meep units}
\]

\[
x \cos 58^\circ = 0.66 \mu m = 0.66 \text{ meep units}
\]
Hence,

\[ H = x \sin \theta \]
\[ = 0.66 \sin 58^\circ \]
\[ H = 0.56 \mu m = 0.56 \text{ meep units} \] (4.9)

The sources \( G_1, G_2 \) and \( G_3 \) are placed roughly at the same geometric locations for different spacing between and radii of the voids since we are considering the average emission from the quantum wells. Fig. 4.10 displays the epsilon profile output of the simulation model for ten periodic voids when all the sources are switched on simultaneously at the start of simulation.

**Figure 4.10** Epsilon profile output of the simulation model containing 10 periodic voids \((d = 1.5 \mu m, h = 1.2 \mu m \text{ and } r = 0.175 \mu m)\) when the sources are just switched on.
4.4 Assumptions of the Model

With the constraints of computational resources, memory and the need for only a basic investigation on the light output efficiency of voids LED structure, some assumptions and considerations were employed in the simulation model. Following are the assumptions of our model:

1. A two dimensional model is designed for all simulation runs with a computational cell dimension of $25\mu m \times 33\mu m$ which provides enough room for ten voids with a maximum spacing of $1.5\mu m$ between them.

2. All the epilayers (GaN and sapphire) and voids of the LED structure are non-dispersive and linear materials characterized only by their refractive index or dielectric constant. The thickness of these layers are imported from the reported experimental data.

3. The embedded voids are modeled as cross-sectional cylinders filled with air having a finite height $h$ and radius $r$ due to limited availability of geometric shapes supported by the software.

4. The emission profile of semi-polar In$_{0.2}$Ga$_{0.8}$N/GaN MQWs is modeled as an ideal point dipole Gaussian source centered at a wavelength of 460nm. As a result, the variations in the internal quantum efficiency is not considered in our model and is assumed to be unity.

5. The dielectric interfaces in this model are smooth and there are no defects in the GaN NW template layers.
Chapter 5

Simulation Results and Discussion

After designing a model for the InGaN/GaN LED system with embedded voids as described in chapter 4, iterative simulations were performed to study the interaction of incident light source on some of the void parameters. This chapter explains different configurations of the simulation model and their respective results to analyze its suitability for light output enhancement.

5.1 Light Output

The outgoing flux calculation is performed by defining flux regions at specific locations in the computational cell. Flux line $S_1^B$ is placed at the end of the sapphire substrate, $S_1^R$ is placed vertically on the right edge of substrate and $S_1^L$ is placed vertically on the left edge of substrate. The flux values measured at these three lines are added such that $S_1^B + S_1^L + S_1^R = S_1$ denotes the total outgoing flux through the substrate. To measure the source flux, $T_2$ flux line is placed approximately 0.5$\mu$m below the bottom two sources for voids structure and approximately 0.66$\mu$m below the single source in case of c-plane structure as shown in Figs. 5.1a and 5.1b.

In MEEP, when a flux region is defined the integral of the Poynting vector of the Fourier-
(a) c-plane structure with a single Gaussian point dipole source.

(b) Embedded voids structure with 10 voids ($d = 1\mu m$, $h = 1.2\mu m$ and $r = 0.175\mu m$) and three Gaussian point dipole sources.

Figure 5.1 Epsilon profile output showing the flux regions $S_1^B$, $S_1^L$, $S_1^R$ and $T_2$. 

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transformed fields is computed at each point of the flux region as:

\[ P(\omega) = \text{Re} \; \hat{n} \cdot \int E_{\omega}^x(x) \times H_{\omega}(x) dx \] (5.1)

Thus the flux output can be calculated in a single computation by Fourier-transforming the response to a Gaussian pulse provided the simulation is run for a time till the fields at the measuring point decay away by a given tolerance. In all our simulations, the program was made to run for an extra time of 20 meep units after the sources had turned-off until the \( |E_x|^2 \) at the end of sapphire substrate had decayed by at least 1/1000th of its maximum previous value. MEEP always computes the flux values in the positive normal direction of the flux region and hence the flux values are multiplied with a weight of -1 to get the outward flux in opposite direction (i.e. coming out of sapphire substrate).

Initial simulations with a thicker sapphire substrate of approximately 330\(\mu m\), 200\(\mu m\), 100\(\mu m\) and 50\(\mu m\) were performed and was found out that the flux output measured at the end of sapphire substrate was negligible even with higher intensities of the sources. This is because our Gaussian point dipole source has broad frequency width which makes it a very short pulse in time-domain and the time-averaged Poynting vector is a function of the input frequency and dipole moment. Moreover, it was evident from their field patterns that the pulse decayed away after propagating for 20 – 30\(\mu m\) through the sapphire substrate. Hence a substrate thickness of 25\(\mu m\) was used for measuring the outgoing flux.

The color scale of field patterns used for all simulation outputs in this chapter go from dark blue (negative) to white (zero) to dark red (positive). From Fig. 5.1 (b) diffraction effects can be observed near the voids as the incident field is traveling through a medium with varying refractive index (from \(n_{\text{GaN}}\) to \(n_{\text{air}}\) in voids). Dense interference fringes can also be seen along the length of the voids which are mainly because of simultaneous switching on of all Gaussian point dipole sources and these fringes are guided along GaN-void interface towards sapphire
substrate. In an actual LED sample, this interface can be pretty rough due to termination of threading dislocations and act as scattering points for the incident photons. Scattered reflections at these points will ultimately direct the photons into the narrow light escape cone. There is also a significant trapping of field inside the voids which are guided almost normally towards the substrate. In case of c-plane structure, the source field propagates towards the sapphire substrate undisturbed except for minute reflections from the interfaces. Hence the peak of output flux is higher for voids structure compared to that of c-plane one.

5.1.1 Study of Effect of Number of Voids

The effect of number of voids on the outgoing flux is illustrated in the Fig. 5.2. It can be observed that the peak value of the flux increases initially with increase in number of voids and saturates after 4 voids. The simulation was performed for a constant voids height of $1.2\, \mu m$ and radius of $0.175\, \mu m$. As the individual graphs in this figure are very close to each other, the number of identification marks used for each graph are much less than the number of data points obtained from simulation.

5.1.2 Study of Effect of Spacing between the Voids

The simulation of variation of flux output with changing spacing between the voids is shown in Fig. 5.3. The number of voids was fixed to ten with their height $h = 1.2\, \mu m$ and radii $r = 0.175\, \mu m$. From the plot the flux enhancement improves initially with increase in the spacing between the voids ($0.5 - 0.75\, \mu m$), reaches a high value for $d = 1\, \mu m$ and then decreases with further increase in the spacing. This nature depends on the position of standing wave pattern of electromagnetic field in the structure where strong constructive interference is created.
5.1.3 Study of Effect of Height of voids

Similar to the spacing between the voids, the variation of flux output with changing height of the voids is shown in Fig. 5.4. The number of voids was fixed to ten with their adjacent spacing $d = 1\mu m$ and radii $r = 0.175\mu m$. It can be observed from the Fig. 5.4 that there is not much flux enhancement with increase in height of the voids. However, a high flux output is observed for a height of $1.25\mu m$.

5.1.4 Study of Effect of Source Amplitude

Since LED is an optoelectronic device, the dependence of light flux output on the source current is to be studied. The source amplitude is varied by changing the amplitude of the current source modeled with Gaussian profile. From Fig. 5.5 it can be observed that, with variation of the source
amplitude while keeping the center frequency fixed, the peak of the output light flux enhances more for the voids LED structure than the conventional c-plane one. For voids structure, 10 voids with height $1.2\mu m$, adjacent spacing of $1\mu m$ and cross-sectional radii of $0.175\mu m$ are used during output flux measurement.

5.2 Transmission Spectrum

As discussed in the previous section, the field profiles showed that there are reflections, scattering and guiding phenomena happening in the voids structure compared to the c-plane one. Hence, all the flux regions defined in the voids structure will measure the input power and the reflected/scattered power from the voids. Since we are interested in transmission relative to the power the source couples into voids network, a “control” simulation without the voids (i.e.
scatterers) is required for normalization of each structure (with voids) run. Hence a normalization run without the voids as illustrated in the Fig. 5.6(b) is performed where all the other parameters in the cell remains same as that of the structure run with voids. For both structure and normalization runs, the Fourier-transformed fields at $S_1^B$, $S_1^L$ and $S_1^R$ are accumulated at every point as the simulation progresses to get the total flux $S_1$ coming out of the substrate.

Thus for a given number of voids the simulation is ran twice, once with and once without voids. The output files containing the flux values are then imported to MATLAB\textsuperscript{TM} where a code is written to calculate the ratio of flux values of structure run and normalization run as a function of frequency.

Figure 5.4 Light output as a function of frequency for different heights of ten voids ($d = 1 \mu m$ and $r = 0.175 \mu m$) and the c-plane structure.
5.2.1 Study of Effect of Spacing between the Voids

After understanding the procedure to get a quantitative transmission spectrum, the effect spacing between embedded voids on it was analyzed. The number of voids was fixed to ten and the spacing varied from 0.5\( \mu m \) to 1.5\( \mu m \) for a height of 1.2\( \mu m \) and radius of 0.175\( \mu m \). At first, a structure run with ten voids having an adjacent spacing of 0.5\( \mu m \) was performed followed by its normalization run by removing the voids. Flux values measured at the sapphire substrate from the structure run were normalized by the corresponding measured flux values from its normalization run to get the transmission flux value corresponding to 652.1 THz.

The spacing between the voids was increased gradually and the same procedure was repeated to get the transmitted flux value corresponding to 652.1 THz for each increment as a function of spacing between the voids as shown in Fig. 5.7. It can be observed from the graph that,
(a) Structure run with voids and flux regions.

(b) Normalization run with the same flux regions but without voids.

**Figure 5.6** Transmission field profile of embedded voids LED structure containing 10 voids ($d = 1\mu m$, $h = 1.2\mu m$, $r = 0.175\mu m$).
there is an optimum spacing between the voids (1µm) for which the normalized transmission of emission wavelength is enhanced. Since the spacing between voids was varied for a given number of voids the same results are applicable for the variation in cross-sectional radius of the voids because effectively for a given spacing between voids changing their cross-sectional radius will only change the amount of material present between the voids.

5.2.2 Study of Effect of Height of Voids

The range of void height variation inside the LED sample is same as the spacing between them i.e. from \( h = 0.5\mu m \) to \( h = 2.0\mu m \). The effect of this height variation in ten periodic voids on the transmission spectra for \( d = 1\mu m \) and \( r = 0.175\mu m \) is studied for a resolution of 53 using the same methodology discussed in the previous section. The field pattern for two extreme
cases are discussed here i.e. for shorter voids and longer voids. With a height of $h = 0.5\mu m$, the length of field trap is reduced and less diffraction is observed due to increased distance between top source and voids as shown in Fig. 5.8 (a). For $h = 1.2\mu m$, comparatively more field is trapped owing to its increased height and strong diffraction effects at the top edge of the voids as illustrated in Fig. 5.8 (b). The transmission of wavelength of 460nm in the ten voids structure does not improve much with their height as shown in Fig. 5.9 which was also observed in case of flux output in the previous section.

5.3 Light Output Efficiency

As per the definition mentioned in chapter 2, the calculation of light output efficiency for embedded voids can be challenging. The additional flux line $T_2$ placed right after the triangular Gaussian sources helps in measuring the input flux. It is defined at a distance of $\approx 3$ times the wavelength of light in the material to avoid irrelevant near-field measurements. The output flux is measured as a summation of flux lines $S_{B1}^1$, $S_{L1}^1$ and $S_{R1}^1$ in the substrate and the percentage of light output for each voids structure is then calculated by taking the ratio of flux values $T_2/(S_{B1}^1 + S_{L1}^1 + S_{R1}^1)$.

5.3.1 Study of Effect of Spacing between the Voids

In this part of the work, the effect of spacing between the voids ($d$) on the light output efficiency of $E_x$ component of the sources is studied. Fig. 5.10 (a) plots the light output efficiency of 10 voids as a function of spacing between them for an emission wavelength of $\lambda = 460\text{nm}$. It can be observed from Fig. 5.10 (a) that the change in light output efficiency is not significant with smaller spacing between the voids ($0.5\mu m - 1.0\mu m$) and saturates for larger spacing of $d > 1\mu m$. 

(a) Less light trapping and guiding in shorter voids ($h = 0.5 \mu m$) just after the sources are turned off.

(b) More light trapping and guiding in longer voids ($h = 1.2 \mu m$) just after the sources are turned off.

**Figure 5.8** Transmission field pattern of embedded voids structure with 10 voids for two different heights.
5.3.2 Study of Effect of Height of Voids

The effect of height of voids \((h)\) on the light output efficiency of \(E_x\) component of the sources is illustrated in the figure Fig. 5.10 (b). It was plotted for 10 voids as a function of height of the voids for an emission wavelength of \(\lambda = 460\,\text{nm}\). From the figure Fig. 5.10 (b), it can be observed that light output efficiency almost remains constant with the height variation. This was the same behavior observed in case of output flux variation with voids height. The simulated enhancement in measured light output flux of up to 2.88 times was achieved when the spacing between the voids was \(1\,\mu\text{m}\) for 10 voids and this can be attributed to increased reflections/scattering and guiding between the voids.
(a) Variation with spacing between the voids ($h = 1.2\mu m$ and $r = 0.175\mu m$).

(b) Variation with height of voids ($d = 1\mu m$ and $r = 0.175\mu m$).

Figure 5.10 Light output efficiency for 10 voids corresponding to $\lambda = 460 nm$. 
Chapter 6

Conclusion

Simulations based on FDTD method were conducted to compare the light output of embedded voids InGaN/GaN MQW light emitting diode with that of the conventional c-plane one. A free software package called MEEP was used to design different simulation models through Scheme coding interface.

The electric field profiles of the embedded voids structure suggested the enhancement in guiding and trapping of light with increase in number of voids whereas no such exclusive trait was observed in the c-plane structure. The light transmission at $\lambda = 460\text{nm}$ was found to be higher for ten periodic voids at a spacing of $1\mu\text{m}$ whereas there was a 5% increase in the light transmission with increase in height of voids.

The important observation was the light output enhancement of up to 2.88 times in the periodic voids structure compared to the c-plane one at a spacing of $1\mu\text{m}$. An increase in the light transmission was also obtained due to variations in the embedded voids size. All these simulation results indicate that there is an improvement in the light output measured in the sapphire substrate for $\lambda = 460\text{nm}$ in the embedded voids LED structure due to reflections, scattering and guiding events of light in it.

Since this was an initial step towards modeling such a complex structure using MEEP
software, there is room for some future work which are suggested as follows:

1. The material parameters such as $\epsilon(x)$ and $\mu(x)$ were assumed to be linear and non-dispersive in nature. Frequency dependent and incident electric field dependent $\epsilon(x)$ and $\mu(x)$ can be incorporated in the simulation model using Drude susceptibility model along with other anisotropic material characteristics.

2. Similar computations can be performed using other field components of the Gaussian source such as $E_y$ and $E_z$. On the other hand, a custom source function can be specified corresponding to the nature of emission of In$_{0.2}$Ga$_{0.8}$N/GaN MQWs which will take care of variations in the internal quantum efficiency of the model.

3. Modeling of embedded voids as geometric objects with random geometry and increasing the spatial resolution may cooperate in visualizing the field interaction with them more clearly.

4. In case of periodic voids, the model has periodic modulation of dielectric constant which may give excite some resonant modes inside the cell. Detailed study of the supported modes and their quality factor will help in understanding modal extraction due to voids.
REFERENCES


APPENDICES
Appendix A

Comments on the software

A.1 Hardware information

MEEP software was installed on a linux-based university computer at NCSU and the machine information is as follows:

Operating System: RedHat Enterprise Server 6.6
Architecture: x86_64
Kernelrelease: 2.6.32-504.8.1.el6.x86_64
Memorysize: 15.56 GB
CPU: Intel(R) Xeon(R) CPU X5550 @ 2.67GHz 16 cores
HDD: 160GB (this is split among several volumes)

A.2 Units in MEEP

In MEEP, all the constants involved in Maxwell’s equations are treated as dimensionless units with $\epsilon_0 = \mu_0 = c = 1$. This choice emphasizes the scale invariance of Maxwell’s equations i.e., multiplying the sizes of everything by 10 just divides the corresponding solution frequencies
by 10. Also in most of the electromagnetic problems, meaningful quantities are always dimensionless ratios such as transmitted power over incident power or scattered power over incident power.

As users, we have the flexibility of choosing any desired unit of distance $a$ (may be $1\mu m$, 10nm or 1mm) for the given problem and express all distances in units of $a$. Hence we can express our characteristic wavelength in units of $a$. Since $c = 1$ in meep units, all times are expressed in units of $a/c$ and frequencies in the units of $c/a$ which is equivalent to specifying $f$ as $1/T$.

For example, let the base unit for our system be $a = 1\mu m$. If the wavelength ($\lambda$) of our source is 400nm then,

$$\lambda(\text{meep units}) = \frac{\lambda(\text{SI units})}{a} = \frac{400 \times 10^{-9}}{1 \times 10^{-6}} = 0.4 \quad (A.1)$$

As $c = 1$, frequency will be specified in meep units as $1/0.4 = 2.5$ and if we want to run the simulation for 100 periods, then time is specified as 40 meep units ($=100/f$).
A.3 Acronyms

The list of acronyms used in this dissertation are as follows:

- **LED**: Light Emitting Diode
- **SSL**: Solid-State Lighting
- **EQE**: External Quantum Efficiency
- **FDTD**: Finite-Difference Time-Domain
- **MQW**: Multiple Quantum Well
- **EVA**: Embedded Voids Approach
- **IQE**: Internal Quantum Efficiency
- **QCSE**: Quantum Confined Stark Effect
- **NW**: Nano-Wire
- **MOCVD**: Metal Organic Chemical Vapor Deposition
- **ICP-RIE**: Inductively Coupled Plasma Reactive Ion Etching
- **TE**: Transverse Electric
- **TM**: Transverse Magnetic
- **PEG**: Polyethylene Glycol
- **PC**: Photonic Crystal
- **GPL**: General Public License
- **PML**: Perfectly Matched Layer
- **MEEP**: MIT Electromagnetic Equation Propagation
- **HDF**: Hierarchical Data Format
Appendix B

Scheme and MATLAB™ Codes

This appendix consists of fully commented Scheme and MATLAB™ codes used for our simulation. Codes are tweaked accordingly as per the changes in the simulation.

B.1 Scheme Code

; Modeling of light output in GaN LEDs with embedded voids by FDTD simulations
; 2-D simulation
; Choosing the base unit as a=1um

; Parameters to describe the geometry
(reset-meep)
(define-param n-saph 1.7) ; Refractive index of Sapphire
(define-param n-gan 2.4) ; Refractive index of GaN
(define-param r 0.175); Radius of the voids
(define-param d 1.0); Spacing between the voids
(define-param h 1.2); Height of each void
(define-param x1 (+(/ d 2) r))
(define-param x2 (+(+ r d) r))
(define-param res 53) ;Resolution

; The cell dimensions
(define-param sx 25) ; X- dimension
(define-param sy 33) ;Y- dimension
(define-param t-gan 4.7)
(define-param t-saph 25)
(define-param pmlt 1) ; PML thickness

; Defining the size of the computational cell
(set! geometry-lattice (make lattice (size sx sy no-size)))

; Geometric objects to create structures in the computational cell
; cylinder axis parallel to y-axis
(print "Setting the geometries\n")
(set! geometry
(append
(list(make block (center 0 -14.15) (size sx t-gan infinity)
(material (make dielectric (index n-gan)))))
(make block (center 0 0.3) (size sx t-saph infinity)
(material (make dielectric (index n-saph)))))
(make cylinder (center x1 -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (+ x1 x2) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (+ x1 (* 2 x2)) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (+ x1 (* 3 x2)) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (+ x1 (* 4 x2)) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (* -1 x1) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (* -1 (+ x1 x2)) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (* -1 (+ x1 (* 2 x2))) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (* -1 (+ x1 (* 3 x2))) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))
(make cylinder (center (* -1 (+ x1 (* 4 x2))) -13.03) (radius r) (height h)
(material air) (axis 0 1 0))))

(set! pml-layers (list (make pml (thickness pmlt))))

(set-param! resolution res)

; Modelling emission from semi-polar quantum wells as Gaussian sources
(define-param fcen (/ 1 0.46)); center frequency in meep units
(define-param df 0.48); frequency width in meep units
APPENDIX B. SCHEME AND MATLAB\textsuperscript{TM} CODES

(define-param nfreq 400) ; number of frequencies at which flux is calculated
(print "Setting up sources\n")
(set! sources (list
(make source
(src (make gaussian-src (frequency fcen) (fwidth df)))
(component Ex) (center 0 -15.13) (size 0 0) (amplitude 10.0))
(make source
(src (make gaussian-src (frequency fcen) (fwidth df)))
(component Ex) (center x1 -14.63) (size 0 0) (amplitude 10.0))
(make source
(src (make gaussian-src (frequency fcen) (fwidth df)))
(component Ex) (center (* -1 x1) -14.63) (size 0 0) (amplitude 10.0))))

; Defining the flux regions
(define T1 (add-flux fcen df nfreq
(make flux-region (center 0 -15.3)
(size (* (- (- (/ sx 2) pmlt) 2) 2) 2) 0) (weight -1))))
(define T2 (add-flux fcen df nfreq
(make flux-region (center 0 -14.13)
(size (* (- (- (/ sx 2) pmlt) 2) 2) 2) 0))))
(define T3 (add-flux fcen df nfreq
(make flux-region (center 0 -10.2)
(size (* (- (- (/ sx 2) pmlt) 2) 2) 2) 0))))
(define S1 (add-flux fcen df nfreq
(make flux-region (center 0 12.8)
(size (* (- (- (/ sx 2) pmlt) 2) 2) 2) 0))
(make flux-region (center -9.5 0.3)
(size 0 t-saph) (weight -1))

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APPENDIX B. SCHEME AND MATLAB™ CODES

(make flux-region (center 9.5 0.3)
  (size 0 t-saph)))

(define B1 (add-flux fcen df nfreq(make flux-region (center 0 15.3)
  (size (* (- (- (/ sx 2) pmlt) 2) 2) 2) 0))))

; Output the fields
(use-output-directory "Withex_10voidssameD")
(run-sources+
  (stop-when-fields-decayed 20 Ex
   (vector3 0 12.8) 1e-3)
  (at-beginning output-epsilon)
  (during-sources
   (to-appended "ex" (at-every 2 output-efield-x)))
  (display-fluxes T1 T2 T3 S1 B1)
  (print "Simulation done!\n")
  (print "dt= " (meep-fields-dt-get fields) "\n")

B.2 MATLAB™ Code

% Author: Narendra Honnalli
clc;

x = dlmread('with10voids_cplane.dat',',',[0 1 399 5]);
y = dlmread('with10voids_diffD_norm.dat',',',[0 1 399 5]);
freq = x(:,1);
T2 = x(:,3);
T2_0 = y(:,3);
S1 = x(:,4);
S1_0 = y(:,4);

freq_mks = (freq.*(3e8))./(1e-6); \% frequency in mks units

norm_T2 = (T2./T2_0));

norm_S1 = (S1./(S1_0));

dlmwrite ('output.txt', [freq_mks norm_S1], 'delimiter', ',');

type('output.txt')

figure(1);clf;

plot(freq_mks,norm_S1,'b','linewidth',1.2);

legend({{'Normalized $S_1$'}},'interpreter','latex','fontsize',12);

grid on

axis square

xlabel('Frequency in Hz','interpreter','latex','fontsize',12);

ylabel('Transmitted spectrum (a.u)','interpreter','latex','fontsize',12);

title({{'Normalized $S_1$ with 10 voids($d = 1.0\mu m,r = 0.175\mu m,$
h = 1.25\mu m$) for $E_x$ component'}},'interpreter','latex','fontsize',12);