Fiber Bragg Grating (FBG) Based Chemical Sensor

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FIBER BRAGG GRATING (FBG) BASED CHEMICAL SENSOR

A Thesis submitted in partial fulfillment of the requirements for the degree of
Master of Science at Virginia Commonwealth University.

by

GOPAKUMAR SETHURAMAN

Director: Dr. Afrodit V. Filippas
Department of Electrical & Computer Engineering

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, Virginia
August 2008
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Contents

Acknowledgements ii

List of Figures v

List of Tables vii

Physical Constants viii

Abstract ix

1 Introduction 1

2 Experimental Procedure 8
  2.1 Introduction .................................................. 8
  2.2 The Polymer .................................................... 9
  2.3 Procedure ..................................................... 11
  2.4 Results and Discussion ....................................... 14

3 Theoretical Analysis and Simulation 24
  3.1 Introduction .................................................... 24
  3.2 Formulation .................................................... 25
  3.3 Solution ......................................................... 40
  3.4 Transfer Matrix Model ......................................... 47
  3.5 Results and Discussion ....................................... 50

4 Conclusion and Future Work 55

A Code 58
Bibliography
List of Figures

1.1 A close up view of how the FBG reflects light at wavelengths that match the grating period and transmits other wavelengths. (Reproduced with permission from Understanding Fiber Optics by Jeff Hecht.) 2
1.2 A larger scale view of how the FBG reflects light at wavelengths that match the grating period and transmits other wavelengths. (Reproduced with permission from Understanding Fiber Optics by Jeff Hecht.) 2
1.3 Reflection and transmission in a fiber grating. (Reproduced with permission from Understanding Fiber Optics by Jeff Hecht.) 3

2.1 Cellulose acetate chemical structure. 10
2.2 Cellulose acetate synthesis reaction. 11
2.3 Striated CA coating. 13
2.4 Setup Schematic. 13
2.5 Baseline reflectance spectra for the 1550 nm nominal wavelength gratings in DI water. 15
2.6 Baseline reflectance spectra for the 1540 nm nominal wavelength gratings in DI water. 16
2.7 Figure showing the right edge transition shift and the change in response bandwidth from the DI water baseline. 17
2.8 Figure showing the right edge transition shift and the change in response bandwidth from the DI water baseline. 18
2.9 Chemical analyte signatures based on right-edge transition shifts and spectra bandwidth changes for the 1550 nm fiber. 21
2.10 Chemical analyte signatures based on right-edge transition shifts and spectra bandwidth changes for the 1540 nm fiber. 22

3.1 Planar Dielectric Waveguide. 28
3.2 Fiber Bragg Grating Profile. 34
3.3 Conceptual side view of polymer beads along the fiber with the gratings under stress. 48
3.4 Comparison of the experimental baseline to the theoretical baseline. 51
3.5 Comparison of the theoretical baseline to the perturbed response.
\[ \delta L = 0.0001/3 \text{ mm.} \]

3.6 Comparison of the theoretical baseline to the perturbed response.
\[ \delta L = 0.0002/3 \text{ mm.} \]

3.7 Comparison of the theoretical baseline to the perturbed response.
\[ \delta L > 0.0005/3 \text{ mm.} \]
List of Tables

2.1 List of chemical analytes tested. ........................................... 15
2.2 Right-edge transition shifts and bandwidth changes in 1550 nm FBG reflectance spectra .................................................. 19
2.3 Right-edge transition shifts and bandwidth changes in 1540 nm FBG reflectance spectra .................................................. 20
Physical Constants

Speed of Light \( c = 2.997 \, 924 \, 58 \times 10^8 \) ms\(^{-8}\) (exact)

Vacuum Permittivity \( \varepsilon = 8.854 \times 10^{-12} \) farads/meter

Vacuum Permeability \( \mu_0 = 4\pi \times 10^{-7} \) henrys/meter
Abstract

FIBER BRAGG GRATING (FBG) BASED CHEMICAL SENSOR

By Gopakumar Sethuraman

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Virginia Commonwealth University, 2008

Major Director: Dr. Afrodit V. Filippas

Department of Electrical & Computer Engineering

In this work, reagentless fiber optic-based chemical sensors for water quality testing were fabricated by coating fiber Bragg gratings with the glassy polymer cellulose acetate. With this polymeric matrix capable of localizing or concentrating chemical constituents within its structure, immersion of the coated grating in various chemical solutions causes the rigid polymer to expand and mechanically strain the glass fiber. The corresponding changes in the periodicity of the grating subsequently result in altered Bragg-reflected responses. A high-resolution tunable fiber ring laser interrogator is used to obtain room temperature reflectance spectrograms from two fiber gratings at 1550 nm and 1540 nm wavelengths. Rapidly swept measurements of the full spectral shapes yield real-time chemical detection and identification. With deionized water as a reference, wavelength shifts in the
reflectivity transition edge from -82 pm to +43 pm and changes in response band-
width from -27 pm to +42 pm are used to identify uniquely a diverse selection of
chemical analytes.
Chapter 1

Introduction

The global fiber optic sensors market is burgeoning and projected to exceed US$650 million by 2010. The need for technologically advanced sensors that are capable of providing rapid results is expected to lead to the increasing use of fiber optic sensors in various industries [1]. Though they started as merely a scientific curiosity, FBGs or fiber Bragg gratings has a broad and important role in optical communications and as sensors now attract attention from construction [2, 3], where it accounts for 70% to 80% of the optical sensors used in structural health monitoring [4], to aviation [5, 6]. They are also used as sensing devices for a wide range of physical and chemical phenomena [7, 8].

In a FBG, periodically spaced regions in the fiber core are altered to have refractive indexes slightly higher than the core. If the wavelength of the input matches the
spacing of these regions in the fiber, there is significant reflection. Fig. 1.1 shows a close up view and Fig. 1.2 shows a large scale view of this phenomenon. The non-resonant wavelengths are transmitted through the grating with low loss. Thus the FBG selectively reflects a very narrow range of wavelengths while transmitting others [9].

Figure 1.1: A close up view of how the FBG reflects light at wavelengths that match the grating period and transmits other wavelengths. (Reproduced with permission from Understanding Fiber Optics by Jeff Hecht.)

Figure 1.2: A larger scale view of how the FBG reflects light at wavelengths that match the grating period and transmits other wavelengths. (Reproduced with permission from Understanding Fiber Optics by Jeff Hecht.)

The output from a FBG is the reflection curve shown in Fig. 1.3. In this example, the peak reflection is in a band centered at 1538.19 nm. The transmission plot shows the transmission loss at that wavelength [9].
FBGs are fabricated by “writing” a fiber grating into the core of a germanium doped optical fiber. The most common method uses two short-wavelength laser beams that are angled to form an interference pattern through the side of the optical fiber. The interference pattern consists of bright and dark bands that represent local changes in the index of refraction in the core region of the fiber. Exposure time for making these gratings varies from minutes to hours, depending on the dopant concentration in the fiber, the wavelengths used, the optical power level, and the imaging optics. Other methods include the use of phase masks as well as the use of interference patterns induced by short, high energy laser pulses.
The short duration pulses have the potential to be used to write fiber gratings into the fiber as it is being drawn [10, 11].

A FBG based sensor system monitors the shift in the reflectance wavelength with the changes in the measurand (e.g. strain, temperature) on injecting a spectrally broadband source of light into the fiber. The response of the grating is due to the photoelastic effect arising from the physical elongation of the sensor, leading to a fractional change in the grating pitch or periodicity with a corresponding change in the fiber index. As the fiber grating is expanded or compressed, the grating period expands or contracts, changing the grating’s spectral response. For a grating operating at 1300 nm as a strain gauge, the change in wavelength is about $10^{-3}$ nm per microstrain. This type of resolution requires the use of spectral demodulation techniques that supersede conventional spectrometers. Several demodulation methods have been suggested using fiber gratings themselves, etalons and interferometers.

The variables measured by a FBG sensor can be expanded using an additional sensitive material, or a transducer, which strains the Bragg grating under an external influence. Several examples of chemical detection with FBGs include hydrogen gas sensing using a palladium-coated FBG, measuring salinity using hydrogels and detecting hydrocarbon leaks using polymers [12, 13, 14]. A fiber optic based
humidity sensor has been fabricated using a FBG coated with polymide, a moisture sensitive polymer, to assess moisture levels in 200 year old limestone walls around Worcester College, Oxford [15]. This humidity sensor was based on the strain effect induced in the Bragg grating through the swelling of the moisture sensitive polymer coating. A direct indication of the humidity level is given by the shift of the Bragg wavelength caused by the expansion of the sensing material. The polymer had an approximate coating thickness of 33 µm and was exposed to different humidity levels at room temperature. The sensitivity of the sensor was reported to be about 4.5 pm/‰ relative humidity at a wavelength of 1535 nm.

Because of the wavelength-encoded nature of the measurand, FBG based sensors offer several advantages over competing conventional assay methods. They can perform the functions of virtually any conventional sensor, often faster and with greater sensitivity, and they can perform measurement tasks that would be impractical with conventional sensors. They are real-time, reagentless, repeatable, reusable and have the ability to perform quasi-distributed (multipoint) sensing through the use of multiplexing. They also allow remote operation. In addition, the fiber is lightweight, small, cheap and immune to vibration, electromagnetic interference and explosive atmospheres. Compared to other variations of the fiber optic sensors, spectrally based sensors such as FBGs are inherently resistant to errors induced by intensity variations (potential error sources include variable losses
due to connectors and splices, microbending loss, macrobending loss, mechanical creep and misalignment of light sources and detectors).

Even with these advantages, fiber sensing technology has to compete against more mature, proven and entrenched technologies. Fiber optics has to identify the niche that only fiber sensing can address and solve specific problems within that niche [16, 17]. One such specialization is environmental sensing. Currently, more than 80,000 chemicals are being produced in the United States. It has become a monumental task to monitor and regulate chemicals, such as those found on the OSHA Toxic Industrial Chemicals (TIC) list [18], that are hazardous to humans and the environment. Since the 1970’s, the U.S. Environmental Protection Agency (EPA) has maintained a Priority Pollutants List (PPL) that identifies those agents based on toxicity, commonality, concentration characteristics, and methods of circulation in the environment [19, 20]. As improvements are made in analytical instrumentation, more compounds are being analyzed and added to the EPA’s Candidate Contaminant List (CCL). Further complicating matters is the need to detect what have previously been considered rather benign chemicals. Common household agents, such as pharmaceuticals, antiseptics, and personal hygiene products, are increasingly becoming environmental hazards [21]. Municipal public works authorities monitor levels of chloramines, a disinfectant commonly used in water across the nation. Ironically, the constituents of this compound, chlorine and ammonia, are known to dissociate in water, and are both TICs with a high
hazard rating. As potential pollutants continue to emerge, low-cost, sensitive, and versatile detection and identification methods will be needed. FBG sensors can be adapted to meet the required characteristics for detecting hazardous chemicals in water.

In this work, fiber optic based chemical sensors are created by coating FBGs with the glassy polymer cellulose acetate (CA), examines the sensor response to many aqueous chemical analytes which are chemicals commonly found in industrial settings and declared Toxic Industrial Chemicals (TICs)—all in the liquid phase and reports on characteristic spectral behavior of these chemicals [22].
Chapter 2

Experimental Procedure

2.1 Introduction

In this section, we describe the polymer used, cellulose actuate and the experimental procedure. The principle of the chemical sensor in this study uses applying a polymer to the cladding of an optical fibers containing an FBG section to form a transducer that, upon exposure to various chemicals, expands in size and exerts strain on the underlying fiber. Because polymers demonstrate selectivity to various analytes based on physicochemical properties, we feel that this device can be used as a chemical sensor. For organic analytes, absorption and swelling are influenced by the interaction of the analyte with the polymer based on dispersion forces, polarity and hydrogen bonding. For inorganic analytes such as acids and
bases, pH factor is important. Given a desired selection of multiple chemical analytes, a polymer having appropriate functional groups in the side chains is needed to obtain the appropriate cross-selectivity. The polymer should also be rigid i.e. have a high Young’s modulus, in order to produce enough stress on the glass fiber so that a sufficient level of strain is imparted to the FBG. In addition, a polymer with controlled cross-linking is a good choice so that it can be used in harsh conditions with a long lifetime [23]. These are important considerations in selecting a polymer to develop the chemical sensor.

2.2 The Polymer

Cellulose acetate, a glassy polymer having a relatively high Young’s modulus, strongly adheres to the cladding of the fiber, ensuring that any physical deformation of the polymer is transferred to the fiber. The transferred axial elongation modulates the Bragg period, resulting in an increase or decrease in the Bragg (reflectance) wavelength and a shift to longer or shorter wavelengths on a spectral display. A benefit of this type of sensor is that no alteration of the optical architecture is required, such as stripping the cladding, which is done when evanescent field sampling or change in effective refractive index is used for sensing [24, 25]. This ensures that the mechanical strength of the fiber is not degraded and structural integrity is maintained. This is important considering the harsh environments,
for example high vibration and high temperature, in which the sensors might be employed.

The chemical structure of cellulose acetate is shown in Fig. 2.1. Cellulose acetate is produced by treating cellulose with acetic anhydride and pyridine [26]. The chemical reaction is shown in Fig. 2.2.

![Cellulose acetate chemical structure](image)

**Figure 2.1:** Cellulose acetate chemical structure.

By composition, CA can have different numbers of acetyl groups per monomer unit, which is referred to as degree of substitution (DS). The maximum DS value is 3 in triacetate, which does not have available hydroxyl groups. We use CA with a DS of 2.45, which provides higher affinity analytes with hydrogen bonding abilities and good adhesion to glass cladding. Average molecular weight ($M_n$) of CA is approximately 30000. Hydrogen bonding takes place at the side-chains on the hydroxyl groups (–OH). Pyridine and acetic anhydride cause a reaction whereby the hydroxyl groups are blocked from any further hydrogen bonding. The resulting polymer, cellulose acetate, has chains that are able to fold in upon
themselves and tangle with other chains to create a matrix. It is this matrix that absorbs and concentrates the various chemical analytes of interest.

### 2.3 Procedure

Two optical fibers, one with an acrylate buffer (1540 nm grating) and the other with a polyimide buffer (1550 nm grating) (Model no.’s: OEFBG-100, SN’s: 881-1-1, 881-2-1, O/E Land Inc., Quebec, Canada) were used in this experiment. The
polyimide and acrylate buffers were stripped in the region of the gratings and cleaned with tetrahydrofuran (THF). This enables to coat the cladding directly with cellulose acetate and the fiber is strained. A 10% cellulose acetate (Aldrich part #180955, CAS Number:9004-35-7, average Mn~30,000 by GPC, 39.3-40.3 wt.% acetyl by titration) in dioxane solution was applied to the fiber cladding at room temperature using an applicator and then allowed to air dry for 20 minutes. After drying, the polymer/FBG section was immersed in deionized water to remove any impurities from the coating process. The dried CA does not adhere to the fiber in a uniform fashion, but rather presents a striated and non-uniform appearance as is visible in Fig. 2.3.

The fibers were fixed in position between two optical base mounts with the polymer/FBG regions suspended above a petri dish as shown in Fig. 2.4. The optical mounts ensure that the fiber is loose and no additional strain is created. The petri dish is used to contain the liquid analytes under test. One end of the fiber was connected using an optical coupler to the optical interrogator, a Micron si720 model containing a swept fiber laser source and large dynamic range photo detectors. The optical interrogator is used to interrogate and demodulate reflected optical signals from the FBG. It allows real-time, full-spectrum data acquisition and data transfer to a PC via an Ethernet remote utility. With the sweep rate set to 5Hz, a 50nm-wide spectrum displays the entire reflectance profile in real time. Spectral resolution of the system is approximately 1 pm. The opposite end of the
Figure 2.3: Striated CA coating.

Figure 2.4: Setup Schematic.
fiber was terminated by bending the fiber and capping it with index matching fluid. After initial instrument calibration, base line measurements for both fibers were measured in deionized water as the reference and the reflectance spectrogram was recorded. When the fibers were immersed in petri dishes of analytes, a shift in wavelength was observed. The two polymer/FBG sensors are tested on a wide variety of chemical analytes, listed in Table 2.1. The selection was partly based on a TIC list and partly on the polar nature of the chemicals. The polymer coated FBG sensor was immersed in each of the different analytes for 10 minutes and the results recorded. Each analyte was tested only once. Between the tests of each analyte, the grating reflectance is allowed to return to its initial recorded baseline response by immersion in clean deionized water for 10 minutes. This ensures that the sensor is clean of any residual analyte before proceeding to the next analyte. The return to baseline after each test also establishes the re-usability of the polymer coated FBG sensor.

2.4 Results and Discussion

The baseline spectrograms for the CA coated fiber gratings in deionized water with nominal measured center wavelengths of 1550.321 nm and 1540.4 nm, are shown in Fig. 2.5 and Fig. 2.6, respectively.
Table 2.1: List of chemical analytes tested.

<table>
<thead>
<tr>
<th>1540nm FBG</th>
<th>1550nm FBG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (deionized)</td>
<td>Water (deionized)</td>
</tr>
<tr>
<td>Hydrogen Peroxide (3%)</td>
<td>Hydrogen Peroxide (3%)</td>
</tr>
<tr>
<td>Sodium Chloride solution (0.9%)</td>
<td>Sodium Chloride solution (0.9%)</td>
</tr>
<tr>
<td>Ammonium Hydroxide (21%)</td>
<td>Ammonium Hydroxide (21%)</td>
</tr>
<tr>
<td>Isopropanol (70%)</td>
<td>Isopropanol (70%)</td>
</tr>
<tr>
<td>Isopropanol w/Methyl Salicylate (70%)</td>
<td>Isopropanol w/Methyl Salicylate (70%)</td>
</tr>
<tr>
<td>Ethanol (100%)</td>
<td>Ethanol (100%)</td>
</tr>
<tr>
<td>Potassium Hydroxide (20 %)</td>
<td>Potassium Hydroxide (20 %)</td>
</tr>
<tr>
<td>Oxalic Acid (10%)</td>
<td>Oxalic Acid (10%)</td>
</tr>
<tr>
<td>Hydrochloric Acid (HCl) (1M)</td>
<td>Sodium Hypochlorite (5.25%)</td>
</tr>
<tr>
<td></td>
<td>Ethanol (50%)</td>
</tr>
<tr>
<td></td>
<td>Dimethylformamide</td>
</tr>
<tr>
<td></td>
<td>Gasoline (87 Octane)</td>
</tr>
<tr>
<td></td>
<td>Acetonitrile</td>
</tr>
<tr>
<td></td>
<td>Ethylene Glycol</td>
</tr>
<tr>
<td></td>
<td>Dimethyl Sulfoxide (DMSO)</td>
</tr>
<tr>
<td></td>
<td>Methylene Chloride</td>
</tr>
</tbody>
</table>

Figure 2.5: Baseline reflectance spectra for the 1550 nm nominal wavelength gratings in DI water.
In Fig.s 2.7 and 2.8, the right edge transitions and response bandwidths at the reference –10 dBm reflectance are shown for the 1550 nm grating sensor for two chemical analytes from the table of analytes tested. For the purpose of analyzing the experimental spectral results, the “absolute” 10 dBm power value as opposed to the “relative” 10 dBm power value is chosen as a reference reflectance for the sake of simplicity. This is acceptable because the peak of the response does not change significantly from response to response. We identify the different responses in the experiment by the shift in the right edge wavelength and a change in the bandwidth because given the broad profile of the peak, no unique, easily identifiable center wavelength is available to quantify the shift in center wavelength. The absolute –10 dBm power value provides an easy visual marker with which to note the shift in right edge wavelength and change in the bandwidth. The right edge transition
and changes in response bandwidth are used in order to provide two parameters with which to distinguish the response of the fiber upon immersion in the analyte.

In Fig 2.7, the response bandwidth of the deionized water is 220.3 pm and the right edge wavelength is 1550.454 nm, measured at the reference reflectance value. For hydrogen peroxide, the response bandwidth is 209.2 pm and the right edge wavelength is 1550.476 nm. This is a shift in bandwidth of 11.1 pm and right edge shift of 22 pm. Similarly in Fig 2.8, dimethylformamide (DMF) is added to the initial response of Fig. 2.7. DMF has a response bandwidth of 218 pm and right edge wavelength of 1550.496 nm. This is a bandwidth change of 7 pm and a right edge shift of 39 pm from the baseline of deionized water.

**Figure 2.7:** Figure showing the right edge transition shift and the change in response bandwidth from the DI water baseline.

Table 2.2 lists the measured values for shifts in right-edge transition and changes in bandwidth from the baseline deionized water values for the 1550 nm grating.
Table 2.3 lists the measured values for shifts in right edge transition and changes in bandwidth from the baseline deionized water values for the 1540 nm grating. As can be seen from the figures and tables, the right transition edge wavelength shifts range from \(-82\) pm to \(+43\) pm and bandwidth changes range from \(-27\) pm to \(+42\) pm.

The sensitivity is based on the minimum resolution obtainable with this particular experimental setup and is a function of the polymer swelling characteristic, the transfer of strain to the underlying grating, tunability of the laser, and averaging and interpolating algorithms of the signal processing. Shifts of 1 pm are easily resolvable and given the ranges observed in the experimental results, it is clear that reagentless multi-chemical detection and identification of different analytes is possible with an excellent degree of accuracy.
Table 2.2: Right-edge transition shifts and bandwidth changes in 1550 nm FBG reflectance spectra. Changes for the chemical analytes are measured with respect to the reference deionized water baseline spectrum.

<table>
<thead>
<tr>
<th>1550nm FBG</th>
<th>-10dBm right edge (nm)</th>
<th>right-edge shift (pm)</th>
<th>-10 dBm BW (pm)</th>
<th>Δ BW (pm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methylene Chloride</td>
<td>1550.372</td>
<td>-82</td>
<td>218.1</td>
<td>-2.2</td>
</tr>
<tr>
<td>87 Octane</td>
<td>1550.405</td>
<td>-49</td>
<td>260</td>
<td>39.7</td>
</tr>
<tr>
<td>Potassium Hydroxide (20%) (KOH)</td>
<td>1550.448</td>
<td>-5</td>
<td>245.5</td>
<td>25.2</td>
</tr>
<tr>
<td>Ethanol (100%)</td>
<td>1550.453</td>
<td>-1</td>
<td>197.5</td>
<td>-22.8</td>
</tr>
<tr>
<td>Acetonitrile</td>
<td>1550.453</td>
<td>-1</td>
<td>209.2</td>
<td>-11.1</td>
</tr>
<tr>
<td>Water (deionized)</td>
<td>1550.454</td>
<td>0</td>
<td>220.3</td>
<td>0</td>
</tr>
<tr>
<td>Ethylene Glycol</td>
<td>1550.455</td>
<td>+1</td>
<td>261.8</td>
<td>41.5</td>
</tr>
<tr>
<td>Ammonium Hydroxide</td>
<td>1550.458</td>
<td>+4</td>
<td>197.6</td>
<td>-22.7</td>
</tr>
<tr>
<td>Ethanol (50%)</td>
<td>1550.458</td>
<td>+4</td>
<td>209.3</td>
<td>-11</td>
</tr>
<tr>
<td>Isopropanol w/Methyl Salicylate (70%)</td>
<td>1550.463</td>
<td>+9</td>
<td>199.4</td>
<td>-20.9</td>
</tr>
<tr>
<td>Isopropanol (70%)</td>
<td>1550.471</td>
<td>+17</td>
<td>204.7</td>
<td>-15.6</td>
</tr>
<tr>
<td>Sodium Hypochlorite</td>
<td>1550.472</td>
<td>+18</td>
<td>201.3</td>
<td>-19</td>
</tr>
<tr>
<td>Sodium Chloride solution (0.9%)</td>
<td>1550.474</td>
<td>+20</td>
<td>208.7</td>
<td>-11.6</td>
</tr>
<tr>
<td>Oxalic Acid (10%)</td>
<td>1550.474</td>
<td>+20</td>
<td>193.4</td>
<td>-26.9</td>
</tr>
<tr>
<td>Hydrogen Peroxide (3%)</td>
<td>1550.476</td>
<td>+22</td>
<td>209.2</td>
<td>-11.1</td>
</tr>
<tr>
<td>Dimethyl Sulfoxide (DMSO)</td>
<td>1550.493</td>
<td>+39</td>
<td>213.3</td>
<td>-7</td>
</tr>
<tr>
<td>Dimethylformamide (DMF)</td>
<td>1550.496</td>
<td>+43</td>
<td>218</td>
<td>-2.3</td>
</tr>
</tbody>
</table>
Table 2.3: Right-edge transition shifts and bandwidth changes in 1540 nm FBG reflectance spectra. Changes for the chemical analytes are measured with respect to the reference deionized water baseline spectrum.

<table>
<thead>
<tr>
<th>ANALYTE</th>
<th>1540nm FBG</th>
<th>-10dBm right edge (nm)</th>
<th>right-edge shift (pm)</th>
<th>-10 dBm BW (pm)</th>
<th>Δ BW (pm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonium Hydroxide</td>
<td>1540.453</td>
<td>-18</td>
<td>113.65</td>
<td>-2.55</td>
<td></td>
</tr>
<tr>
<td>Isopropanol w/Methyl Salicylate (70%)</td>
<td>1540.457</td>
<td>-14</td>
<td>117.14</td>
<td>+0.94</td>
<td></td>
</tr>
<tr>
<td>Ethanol (100%)</td>
<td>1540.457</td>
<td>-14</td>
<td>119</td>
<td>-15.36</td>
<td></td>
</tr>
<tr>
<td>Isopropanol (70%)</td>
<td>1540.467</td>
<td>-4</td>
<td>117.1</td>
<td>+0.9</td>
<td></td>
</tr>
<tr>
<td>Water (deionized)</td>
<td>1540.471</td>
<td>0</td>
<td>116.2</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Hydrogen Peroxide (3%)</td>
<td>1540.479</td>
<td>+8</td>
<td>126.8</td>
<td>+10.6</td>
<td></td>
</tr>
<tr>
<td>Hydrochloric Acid (1M)</td>
<td>1540.487</td>
<td>+16</td>
<td>134.36</td>
<td>+18.16</td>
<td></td>
</tr>
<tr>
<td>Oxalic Acid (10%)</td>
<td>1540.490</td>
<td>+19</td>
<td>129.24</td>
<td>+13.04</td>
<td></td>
</tr>
<tr>
<td>Sodium Chloride solution (0.9%)</td>
<td>1540.491</td>
<td>+20</td>
<td>143.25</td>
<td>+27.05</td>
<td></td>
</tr>
<tr>
<td>Potassium Hydroxide (20%)</td>
<td>1540.494</td>
<td>+23</td>
<td>130.7</td>
<td>+14.5</td>
<td></td>
</tr>
</tbody>
</table>
Fig. 2.9 and Fig. 2.10 shows the significant spatial separation between chemical analytes in a two-dimensional parameter space of right-edge shifts and bandwidth changes. This two-dimensional representation reflects the fact that the altered spectral response from the non-uniformly modulated gratings can be characterized by these two independent parameters. Using these two degrees of freedom, the right edge transition shift along the $x$-axis and the change in response bandwidth ($\Delta BW$) along the $y$-axis, the various chemicals can be uniquely identified.
Using only one parameter would not have sufficed to uniquely distinguish the analytes. For example, in Fig. 2.9, had we used the right edge transition shift as the sole distinguishing parameter we would not have been able to differentiate between acetonitrile and 100% ethanol because they would have exhibited the same right edge transition shift. Correspondingly, had we used the change in response bandwidth as the sole distinguishing parameter, we would not have been able to distinguish between acetonitrile and 50% ethanol because they would have
exhibited an identical change in bandwidth.

Additionally, in Fig. 2.9, taking the $x = 17, 18$ and $y = -15.6, -19$ points of two close analytes, IPA and Sodium Hypochlorite and calculating the distance between two points gives us $d = 3.54$ pm which is well within the 1 pm resolution of the interrogator. Given the 1 pm resolution of this sensor system, the multiple chemical analytes can be uniquely identified by their ‘signature’ in this two dimensional space, using, for example, an artificial neural network.
Chapter 3

Theoretical Analysis and Simulation

3.1 Introduction

Coupled mode theory (CMT) provides an effective analytical method for understanding the influence of waveguide perturbations on light passing through an optical waveguide. The analysis of FBGs using CMT has been exhaustively covered by both [27] and [28]. The operating assumption behind coupled mode theory in FBGs is that the grating serves as a perturbation that couples power between the forward moving and backward moving modes [29, 30]. We proceed in this chapter by first formulating the equations characterizing the spatial spectrum of
the FBG, then describing a solution for them and deriving the crucial relationship between the reflectivity and wavelength. Finally we use the Transfer Matrix Method (TMM) to extend that solution to analyze and model the polymer coated grating used in this work. Using transfer matrix method, the grating may be broken up into smaller sections of uniform period and/or refractive index. Because of the beaded nature of the polymer, certain regions along the polymer are able to absorb more of the analyte under test and create concentration spots. This higher concentration causes greater swelling and as a consequence greater stretching of the fiber and a change in the periodicity of the grating. Overall, there is a nonlinear variation in the period along the length grating. The period varies as a function of location of the polymer on the grating, spectrally encoding displacement position and manifested in the spectrogram. A model coded with aforementioned criteria follows the output observed.

3.2 Formulation

We begin by analyzing wave propagation of uniform plane electromagnetic waves using Maxwell’s wave equations [31]. For a simple medium with constant, scalar permittivity and permeability, and one with no free charges and currents (charge density, \( \rho = 0 \) and current density, \( J = 0 \)), Maxwell’s equations are,
\( \nabla \cdot \mathbf{D} = 0 \) \hspace{1cm} (3.1)

\( \nabla \cdot \mathbf{B} = 0 \) \hspace{1cm} (3.2)

\( \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = -\mu \frac{\partial \mathbf{H}}{\partial t} \) \hspace{1cm} (3.3)

\( \nabla \times \mathbf{H} = -\frac{\partial \mathbf{D}}{\partial t} = -\varepsilon \frac{\partial \mathbf{E}}{\partial t} \) \hspace{1cm} (3.4)

In the above Eq.s 3.1–3.4, \( \mathbf{D} \) is the electric flux density and is related to the electric field intensity \( \mathbf{E} \) by the expression \( \varepsilon_r \varepsilon_0 \mathbf{E} \). \( \varepsilon_0 \) is the permittivity of space and is \( \approx 8.854 \times 10^{-12} \) F/m and \( \varepsilon_r \) characterizes the effect of the atomic and molecular dipoles in the material. \( \mathbf{H} \) is the magnetic intensity and is related to the magnetic flux density \( \mathbf{B} \) by the relation \( \mu_r \mu_0 \mathbf{H} \) where \( \mu_0 \) is the permeability of space and is \( = 4\pi \times 10^{-7} \) H/m and \( \mu_r \) measures the effect of the magnetic dipole moments of the atoms compromising the medium.
For wave behavior in three dimensions, taking the curl of Eq. 3.3 and interchanging the time and space partial derivatives, we get,

$$\nabla \times \nabla \times \textbf{E} = -\mu \frac{\partial}{\partial t} (\nabla \times \textbf{H})$$  \hfill (3.5)

Using the Laplacian vector identity and Eq. 3.4 on the left hand side and the right hand side of Eq. 3.5 respectively, Eq. 3.5 can be written as,

$$\nabla^2 \textbf{E} = \mu \frac{\partial^2 \textbf{D}}{\partial t^2}$$  \hfill (3.6)

Eq. 3.6 is the three dimensional wave equation. For planar dielectric waveguides, shown in Fig. 3.1, the TE or transverse electric wave (waves that contain magnetic field but no electric field) mode \((E_y, H_x, H_z)\) is dominant and is most similar to the \(LP_{01}\) mode of weakly guiding optical fiber [32]. Therefore Eq. 3.6 can be rewritten as,

$$\nabla^2 \hat{\textbf{E}}_T = \mu \frac{\partial^2 \hat{\textbf{D}}_t}{\partial t^2}$$  \hfill (3.7)

In Eq. 3.7 \(\hat{\textbf{E}}_T(x, y, z)\) is the transverse electric field component where \(\hat{\textbf{D}}_t\), the electric flux density is equal to \(\varepsilon_0 \hat{\textbf{E}}_t + \hat{\textbf{P}}_t\), \(\hat{\textbf{P}}\) is polarization and is equal to \(\varepsilon_0 \chi_e \hat{\textbf{E}}\) or \(\varepsilon [\chi_0 + \delta \chi_e(x, y, z)] \hat{\textbf{E}}\) and \(\chi_e\) is electric susceptibility, a constant. Coupling between the forward moving and backward moving modes occurs through the
**Figure 3.1**: Planar Dielectric Waveguide.

**perturbation** term \(\delta \chi_e(x, y, z)\) via polarization. Substituting these terms into Eq. 3.7 we get,

\[
\nabla^2 E = \mu \frac{\partial^2}{\partial t^2} \left[ \varepsilon_0 E (1 + \chi_0 + \varepsilon_0 \delta \chi_e) + \varepsilon_0 \delta \chi_e E \right] \tag{3.8}
\]

In Eq. 3.8, \(1 + \chi_e = \varepsilon_r\), where \(\varepsilon_r\) is the dielectric constant. Also, \(\varepsilon_r = n^2\) where \(n\) is the refractive index. Now, \(\delta \varepsilon_r = \delta \chi_e = \delta(n^2)\) and \(\varepsilon_0 \delta \varepsilon_r = \delta(\varepsilon_0 \varepsilon_r) = \delta \varepsilon\) where \(\delta \varepsilon\) is the perturbed permittivity. Therefore, \(\delta \varepsilon(x, y, z) = \varepsilon_0 \delta \chi_e(x, y, z)\). Making the substitutions, Eq. 3.8 simplifies to the form seen in Eq. 3.9,

\[
\left( \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2} \right) E = \mu_0 [\varepsilon + \delta \varepsilon] \frac{\partial^2}{\partial t^2} E \tag{3.9}
\]
The electric field, $E$, can now be written in the form shown in Eq. 3.10,

$$E = \sum_j [A_j e^{i\beta_j z} + B_j e^{-i\beta_j z}] e_j(x, y)e^{-i\omega t} \quad (3.10)$$

where the summation is over the unperturbed mode solutions and the constants $A_j$ and $B_j$ are the amplitudes of the waves traveling in the positive (+) and the negative (−) directions respectively.

In order to model the perturbed case, the amplitudes $A_j$ and $B_j$ in Eq. 3.4 are now chosen to be slowly varying functions in $z$, as shown in Eq. 3.11

$$E = \sum_j [A_j(z) e^{i\beta_j z} + B_j(z) e^{-i\beta_j z}] e_j(x, y)e^{-i\omega t} \quad (3.11)$$

This variation in $z$ allows the exchange of energy between the modes and accounts for mode coupling.

In order to substitute Eq. 3.11 into Eq. 3.9, we need to evaluate the second order $x$, $y$ and $z$ derivatives. These evaluations are shown in Eq.s 3.12– 3.15.

$$\frac{\partial^2}{\partial x^2} E = (A_j(z) e^{i\beta_j z} + B_j(z) e^{-i\beta_j z}) e^{-i\omega t} \frac{\partial^2}{\partial x^2} e_j \quad (3.12)$$

$$\frac{\partial^2}{\partial y^2} E = (A_j(z) e^{i\beta_j z} + B_j(z) e^{-i\beta_j z}) e^{-i\omega t} \frac{\partial^2}{\partial y^2} e_j \quad (3.13)$$
Evaluating $z$-derivatives, we obtain the first derivative,

$$\frac{\partial}{\partial z} E = e_j e^{-i\omega t} \left[ \frac{\partial A_j}{\partial z} e^{i\beta_j z} + A_j i\beta_j e^{i\beta_j z} + \frac{\partial B_j}{\partial z} e^{-i\beta_j z} + B_j i\beta_j e^{-i\beta_j z} \right]$$  \hspace{1cm} (3.14)

and the second derivative,

$$\frac{\partial^2}{\partial z^2} E = e_j e^{-i\omega t} \left[ \frac{\partial^2 A_j}{\partial z^2} e^{i\beta_j z} + \frac{\partial A_j}{\partial z} 2i\beta_j e^{i\beta_j z} - A_j \beta_j^2 e^{i\beta_j z} 
+ \frac{\partial^2 B_j}{\partial z^2} e^{-i\beta_j z} - \frac{\partial B_j}{\partial z} 2i\beta_j e^{-i\beta_j z} - B_j \beta_j^2 e^{-i\beta_j z} \right]$$  \hspace{1cm} (3.15)

Additionally one must evaluate the $t$ derivative, shown in Eq. 3.16,

$$\mu_0 (\varepsilon + \delta \varepsilon) \frac{\partial^2 E}{\partial t^2} = -\omega^2 \mu_0 (\varepsilon + \delta \varepsilon) \left[ A_j e^{i\beta_j z} + B_j e^{-i\beta_j z} \right] e_j e^{-i\omega t}$$  \hspace{1cm} (3.16)

Since $A(z)$ and $B(z)$ are slowly varying due to mode coupling, the second order terms in Eq. 3.16 are small and can be neglected. Therefore Eq. 3.16 reduces to the form $\nabla_e^2 e_j - \beta_j^2 e_j = -\mu_0 \varepsilon \omega^2 e_j$ and since $e_j$ are the solutions to the unperturbed Helmholtz wave equation, given by $k^2 = \omega^2 \mu \varepsilon$, we are left with the following perturbed wave equation,

$$\sum_j e_j(x, y) \left( 2i\beta_j \frac{\partial A_j}{\partial z} e^{i\beta_j z} - 2i\beta_j \frac{\partial B_j}{\partial z} e^{-i\beta_j z} \right) =$$

$$\sum_m -\omega^2 \mu_0 \delta \varepsilon (A_m e^{i\beta_m z} + B_m e^{-i\beta_m z}) e_m(x, y)$$  \hspace{1cm} (3.17)
Multiplying Eq. 3.17 by the complex conjugate $e^*_k$ and integrating with respect to $x$ and $y$ yields Eq. 3.18,

$$
\sum_j \int e_j e^*_k \, dx \, dy \left( 2i\beta_j \frac{\partial A_j}{\partial z} e^{i\beta_j z} - 2i\beta_j \frac{\partial B_j}{\partial z} e^{-i\beta_j z} \right) = -\omega^2 \mu_0 \sum_m \left( A_m e^{i\beta_m z} + B_m e^{-i\beta_m z} \right) \int \delta\varepsilon(x, y, z) e_m e^*_k \, dx \, dy
$$

(3.18)

Using the orthogonality of the transverse field modes, defined in Eq. 3.19,

$$
\int e_j e^*_k \, dx \, dy = \begin{cases} 0, & j \neq k \\ \text{constant,} & j = k \end{cases}
$$

(3.19)

In order to identify the constant, in Eq. 3.19, we use the fact that for TE waves, the wave impedance $Z_{TE}$ is given by Eq. 3.20,

$$
\frac{E_x}{H_y} = Z_{TE} = \frac{\omega \mu_0}{\beta}
$$

(3.20)

where $\beta$ is the mode propagation constant [33].

Additionally, from the Poynting vector equation, which governs the flow of electromagnetic power, we get Eq. 3.21,

$$
\frac{1}{2} \int E_x H^*_y \, dx \, dy = P
$$

(3.21)
By convention, the fields are “normalized” for unit power flow. Thus, combining Eq. 3.20 and Eq. 3.21 yields Eq. 3.22

\[ \int E_x E_x^* dxdy = \frac{2\omega \mu_0}{\beta} \] (3.22)

Therefore, the constant in Eq. 3.19 is,

\[ \int e_j e_k^* dxdy = \begin{cases} 0, & j \neq k \text{ orthogonal functions} \\ \frac{2\omega \mu_0}{\beta_k}, & j = k \end{cases} \] (3.23)

By combining the results in Eq. 3.23 with Eq. 3.18, we obtain Eq. 3.24,

\[ \frac{2\omega \mu_0}{\beta_k} 2i\beta_k \left( \frac{\partial A_k}{\partial z} e^{i\beta_k z} - \frac{\partial B_k}{\partial z} e^{-i\beta_k z} \right) = -\omega^2 \mu_0 \sum_m \left( A_m e^{i\beta_m z} + B_m e^{-i\beta_m z} \right) K_{m,k} \] (3.24)

where \( K_{m,k} \) in Eq. 3.24 is defined as shown in Eq. 3.25,

\[ K_{m,k} \equiv \int \int_{-\infty}^{\infty} \delta(x, y, z) e_m(x, y) e_k^*(x, y) dxdy \] (3.25)

Further simplifying Eq. 3.24 and multiplying by \( e^{-i\beta_k z} \), we may derive Eq. 3.26,

\[ \frac{\partial A_k}{\partial z} - \frac{\partial B_k}{\partial z} e^{-2i\beta_k z} = \frac{i\omega}{4} \sum_m \left( A_m e^{i(\beta_m - \beta_k)z} + B_m e^{-i(\beta_m + \beta_k)z} \right) K_{m,k} \] (3.26)
The term involving $e^{-2i\beta_k z}$ is neglected through “synchronous approximation” which neglects rapid variation in a complex exponential term that does not contribute to the gradual growth or decay in $A(z)$ or $B(z)$. Thus, Eq. 3.26 further simplifies to Eq. 3.27,

$$\frac{\partial A_k}{\partial z} = \frac{i\omega}{4} \sum_m (A_m e^{i(\beta_m - \beta_k)z} + B_m e^{-i(\beta_m + \beta_k)z}) K_{m,k}$$ (3.27)

Similarly, multiplying Eq. 3.25 by $e^{i\beta_k z}$ and neglecting the $e^{2i\beta_k z}$ term through “synchronous approximation” yields Eq. 3.28,

$$\frac{\partial B_k}{\partial z} = -\frac{i\omega}{4} \sum_m (A_m e^{i(\beta_m + \beta_k)z} + B_m e^{-i(\beta_m - \beta_k)z}) K_{m,k}$$ (3.28)

For a short period fiber Bragg grating (FBG), we look at two dominant modes $A_1$ and $B_1$, where $A_1$ is the positive-traveling wave amplitude of the fundamental mode and $B_1$ is the negative-traveling wave amplitude of the fundamental mode.

From 3.27 and 3.28, for $k = m = 1$, we derive Eq. 3.29 and Eq. 3.30,

$$\frac{\partial A_1}{\partial z} = \frac{i\omega}{4} [A_1 K_{1,1} + B_1 e^{-2i\beta_1 z} K_{1,1}]$$ (3.29)

$$\frac{\partial B_1}{\partial z} = -\frac{i\omega}{4} [A_1 K_{1,1} e^{2i\beta_1 z} + B_1 K_{1,1}]$$ (3.30)
Specifically for a FBG, the grating is written into the fiber core with the general profile defined in Eq. 3.31, and shown in Fig. 3.2,

\[
\delta n_{\text{eff}}(z) = \overline{\delta n_{\text{eff}}(z)} \left[ 1 + v \cos \left( \frac{2\pi}{\Lambda} z + \phi(z) \right) \right]
\]  

(3.31)

where \( \overline{\delta n_{\text{eff}}(z)} \) is the “dc” index change spatially averaged over many grating periods, \( v \) is the fringe visibility of the index change and is \(< 1\), \( \Lambda \) is the nominal period of the grating and \( \phi(z) \) is a continuously varying function known as “chirp”. Chirp is a non-uniform periodicity in the fiber Bragg grating. It is a function of wavelength and it’s effect is to disperse light by introducing a delay into the wavelength.

Figure 3.2: Fiber Bragg Grating Profile.
From Eq. 3.25 and assuming variation in $\delta \varepsilon$ that only depends on $z$ (as shown in Fig. 3.2) we derive Eq. 3.32,

$$K_{1,1} = \int \int_{-\infty}^{\infty} \delta \varepsilon e_1 e_1^* dxdy = \delta \varepsilon(z) \int \int e_1 e_1^* dxdy = \delta \varepsilon(z) \frac{2 \omega \mu_0}{\beta_1}$$ (3.32)

The perturbation in the fiber core can be written as shown in Eq. 3.33,

$$\delta \varepsilon = \varepsilon_0 \delta \varepsilon_r = \varepsilon_0 \delta (n_{eff}^2) = \varepsilon_0 2 n_{eff} \delta n_{eff}$$ (3.33)

Given Eq. 3.32 and Eq. 3.33, we can now simplify the double integral $K_{1,1}$ to the form shown in Eq. 3.34,

$$K_{1,1} = 2 \varepsilon_0 n_{eff} \delta n_{eff}(z) \frac{2 \omega \mu_0}{\beta_1}$$ (3.34)

By replacing $\beta_1 = \frac{\omega}{c} n_{eff}$ in Eq. 3.34, we can further simplify Eq. 3.34 as shown in Eq. 3.35,

$$K_{1,1} = \frac{4}{c} \delta n_{eff}$$ (3.35)
Eq. 3.35 is now expressed in terms of $\delta n_{\text{eff}}$, which has previously been defined
Eq. 3.31. Thus Eq. 3.35 evolves into Eq. 3.36,

$$K_{1,1} = \frac{4}{c} \delta n_{\text{eff}}(z) \left[ 1 + v \cos \left( \frac{2\pi}{\Lambda} z + \phi(z) \right) \right]$$

(3.36)

Multiplying by $\frac{\omega}{4}$ on both sides and letting $\theta = \frac{2\pi}{\Lambda} z + \phi(z)$, yields Eq. 3.37,

$$\frac{\omega}{4} K_{1,1} = \frac{\omega}{c} \delta n_{\text{eff}}(z) + \frac{\omega}{c} \delta n_{\text{eff}}(z) v \cos(\theta)$$

(3.37)

Defining, $\sigma(z) \equiv \frac{\omega}{c} \delta n_{\text{eff}}(z)$ and $k(z) \equiv \frac{v}{2} \sigma(z)$, Eq. 3.37 further develops into Eq. 3.38,

$$\frac{\omega}{4} K_{1,1} = \sigma(z) + 2k(z) \cos(\theta)$$

(3.38)

For uniform gratings, $\delta n_{\text{eff}}(z)$ is constant, making $\sigma$ and $k$ constants as well.

Thus, we can finally define the integral $K_{1,1}$ through Eq. 3.39,

$$\frac{\omega}{4} K_{1,1} = \sigma + 2k \left( \frac{e^{i\theta} + e^{-i\theta}}{2} \right)$$

(3.39)
The expression for $K_{1,1}$ given in Eq. 3.39 can now be substituted into Eq. 3.29 to get Eq. 3.40,

$$\frac{\partial A_1}{\partial z} = i \left[ \sigma + 2k \left( \frac{e^{i\theta} + e^{-i\theta}}{2} \right) \right] A_1 + i \left[ \sigma + 2k \left( \frac{e^{i\theta} + e^{-i\theta}}{2} \right) \right] B_1 e^{-2i\beta_1 z} \quad (3.40)$$

Eq. 3.40 further simplifies to Eq. 3.41,

$$\frac{\partial A_1}{\partial z} = i \left[ \sigma + 2k \left( \frac{e^{i\theta} + e^{-i\theta}}{2} \right) \right] A_1 + i \left[ \sigma e^{-2i\beta_1 z} + k (e^{i\theta} + e^{-i\theta}) e^{-2i\beta_1 z} \right] B_1 \quad (3.41)$$

Letting $\theta = \frac{2\pi}{\lambda} z + \phi(z)$ and removing the term $\sigma e^{-2i\beta_1 z}$ using “synchronous approximation”, Eq. 3.41 is simplified to Eq. 3.42,

$$\frac{\partial A_1}{\partial z} = i \left[ \sigma + k \left( e^{i\theta} + e^{-i\theta} \right) \right] A_1 + i \left[ k \left( e^{-i(2\beta_1 z - \theta)} \left[ 1 + e^{-i(\frac{4\pi}{\lambda} z + 2z)} \right] \right) \right] B_1 \quad (3.42)$$

The term involving $e^{-i(\frac{4\pi}{\lambda} z + \phi)}$ can be removed using “synchronous approximation”.

However, the other complex exponential term in Eq. 3.42, $e^{-i(2\beta_1 z - \theta)}$, must be retained because $\beta_1 = \frac{2\pi}{\lambda} n$ and following the Bragg equation, $\lambda_B = 2n\Lambda$, at near Bragg resonance condition ($\lambda \approx \lambda_B$), $\beta_1 = \frac{\pi}{\Lambda}$, and these terms are not rapidly varying.
Therefore Eq. 3.42 simplifies to Eq. 3.43,

\[
\frac{\partial A_1}{\partial z} = i \left[ \sigma + k \left( e^{i\theta} + e^{-i\theta} \right) \right] A_1 + i \left[ k \left( e^{-i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \cdot e^{-i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \right) \right] B_1 \tag{3.43}
\]

Multiplying both sides of Eq. 3.43 by \( e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \),

\[
e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \frac{\partial A_1}{\partial z} = i \left[ \sigma e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} + k(e^{i\theta} + e^{-i\theta})e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \right] A_1 + \ i k B_1 e^{-i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \tag{3.44}
\]

Eq. 3.44 is simplified to,

\[
e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \frac{\partial A_1}{\partial z} =
\]

\[
i \left[ \sigma e^{i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} + k(e^{i(\beta_1 z + \frac{\pi}{2} z + \phi)} + e^{i(\beta_1 z - \frac{3\pi}{2} z - \frac{3\phi}{4})}) \right] A_1 + \ i k B_1 e^{-i(\beta_1 z - \frac{\pi}{2} z - \frac{\phi}{4})} \tag{3.45}
\]

Again, near the Bragg resonance condition \( \beta_1 \approx \frac{\pi}{\Lambda} \) and the two terms involving \( e^{i(\beta_1 z + \frac{\pi}{2} z + \phi)} \approx e^{i(\frac{2\pi}{\Lambda} z + \frac{\phi}{2})} \) and \( e^{i(\beta_1 z - \frac{3\pi}{2} z - \frac{3\phi}{4})} \approx e^{i(\frac{-2\pi}{\Lambda} z - \frac{3\phi}{4})} \) can be removed by “synchronous approximation”.

Adding $iA_1 \left( \beta_1 - \frac{\pi}{\Lambda} - \frac{1}{2} \frac{d\phi}{dz} \right) e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$ on both sides of Eq 3.45,

$$e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})} \frac{\partial A_1}{\partial z} + iA_1 \left( \beta_1 - \frac{\pi}{\Lambda} - \frac{1}{2} \frac{d\phi}{dz} \right) e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})} =$$

$$i\sigma e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})} A_1 + ikB_1 e^{-i(\beta_1 - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

$$+ iA_1 \left( \beta_1 - \frac{\pi}{\Lambda} - \frac{1}{2} \frac{d\phi}{dz} \right) e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

(3.46)

The left hand side of Eq. 3.46 is the total derivative. Thus, Eq. 3.46 simplifies to Eq. 3.47,

$$\frac{d}{dz} \left( A_1(z)e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})} \right) = i \left( \sigma + \beta_1 - \frac{\pi}{\Lambda} - \frac{1}{2} \frac{d\phi}{dz} \right) A_1 e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

$$+ ikB_1 e^{-i(\beta_1 - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

(3.47)

We can simplify Eq. 3.47 in terms of the amplitude of the forward going ("+") wave, $R(z)$ and the amplitude of the backward going wave ("") $S(z)$ shown in Eq. 3.48 and Eq. 3.49 respectively,

$$R(z) \equiv A_1(z)e^{i(\beta_1 z - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

(3.48)

and

$$S(z) \equiv B_1(z)e^{-i(\beta_1 - \frac{\pi}{\Lambda} z - \frac{\phi}{2})}$$

(3.49)
The equations Eq. 3.48 and Eq. 3.49 can be substituted into Eq. 3.47 to yield the much simpler Eq. 3.50,

$$\frac{d}{dz} R(z) = i \hat{\sigma} R(z) + ik S(z)$$

(3.50)

where $\hat{\sigma} = \sigma + \delta - \frac{1}{2} \frac{d \phi}{dz}$ and $\delta = \beta_1 - \frac{\pi}{\Lambda}$ is a “detuning” factor.

Starting from Eq. 3.39, it can be shown in similar fashion to Eq.s 3.41–3.50 that,

$$\frac{d}{dz} S(z) = -i \hat{\sigma} S(z) - i k R(z)$$

(3.51)

These two equations, Eq. 3.50 and Eq. 3.51 represent the Coupled Mode Equations for a FBG.

### 3.3 Solution

To solve the coupled equations for a FBG, we will take a column vector, $\bar{V}$ and relate that to $R$ and $S$, the amplitudes of the forward going wave and the backward going waves respectively.

$$\bar{V} = \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} R \\ S \end{bmatrix}$$

(3.52)
Eq. 3.52 can be expanded to the matrix Eq. 3.53,

\[
\begin{bmatrix}
\frac{dV_1}{dz} \\
\frac{dV_2}{dz}
\end{bmatrix} = \begin{bmatrix}
 i\hat{\sigma} & ik \\
-ik & -i\hat{\sigma}
\end{bmatrix} \begin{bmatrix}
 V_1 \\
 V_2
\end{bmatrix}
\] (3.53)

\[
\frac{d\bar{V}}{dz} = [M] \bar{V}
\] (3.54)

From [34], the solution to the system defined in Eq. 3.54 is Eq. 3.55,

\[
\bar{V}(z) = \bar{V}(0)e^{[M]z}
\] (3.55)

where the matrix exponential is defined by the series Eq. 3.56 and converges to a 2 \times 2 matrix,

\[
e^{[M]z} = I + [M] z + \frac{1}{2} [M]^2 z^2 + \cdots
\] (3.56)

A method for efficiently evaluating the matrix exponential is described in [34] and is presented here. Let \( p(\lambda) \) be given by, Eq. 3.57,

\[
p(\lambda) = \det \{M - \lambda I\}
\] (3.57)
Then, from Eq. 3.57,

\[
p(\lambda) = \det \begin{bmatrix} i\hat{\sigma} - \lambda & ik \\ -ik & -i\hat{\sigma} - \lambda \end{bmatrix}
\]

(3.58)

By evaluating the determinant defined in Eq. 3.58, the eigen values are \( \lambda \) and \( \hat{\sigma}^2 - k^2 \), as shown in Eq. 3.59,

\[
p(\lambda) = \lambda^2 + (\hat{\sigma}^2 - k^2) = c_2\lambda^2 + c_1\lambda + c_0
\]

(3.59)

Therefore, the polynomial coefficients are \( c_2 = 1 \), \( c_1 = 0 \) and \( c_0 = \hat{\sigma}^2 - k^2 \)

Now, Eq. 3.56 can be written as,

\[
e^{[M]z} = f_1(z) [I] + f_2(z) [M]
\]

(3.60)

where,

\[
c_2 \frac{d^2 f}{dz^2} + c_1 \frac{df}{dz} + c_0 z = 0
\]

(3.61)

Eq. 3.60 has two solutions \( f_1 \) and \( f_2 \) with two boundary conditions, as shown below,

\[
f_1(0) = 1
\]

\[
f_1'(0) = 0
\]

(3.62)
\[ f_2(0) = 0 \]  
\[ f_2'(0) = 1 \]  

By substituting the solutions for \( c_0, c_1 \) and \( c_2 \) into Eq. 3.61 we derive,

\[ \frac{d^2 f}{dz^2} + (\hat{\sigma}^2 - k^2) = 0 \]  

(3.64)

The solution to Eq. 3.64 is,

\[ f(z) = a_1 e^{\sqrt{k^2 - \hat{\sigma}^2}z} + a_2 e^{-\sqrt{k^2 - \hat{\sigma}^2}z} \]  

(3.65)

Using the first set of boundary conditions shown in Eq. 3.62 we obtain,

\[ f_1(0) = a_1 + a_2 = 1 \]  

(3.66)

and

\[ f_1'(0) = a_1(k^2 - \hat{\sigma}^2) - a_2(k^2 - \hat{\sigma}^2) = 0 \]  

(3.67)

for which,

\[ a_1 = a_2 = \frac{1}{2} \]
Therefore, the solution for the first set of boundary conditions is,

\[ f_1(z) = \frac{1}{2} e^{\sqrt{k^2 - \hat{\sigma}^2} z} + \frac{1}{2} e^{-\sqrt{k^2 - \hat{\sigma}^2} z} \]  
(3.68)

or

\[ f_1(z) = \cosh \sqrt{k^2 - \hat{\sigma}^2} z \]  
(3.69)

Similarly, for the second set of boundary conditions from Eq. 3.63,

\[ f_2(0) = a_1 + a_2 = 0 \]  
(3.70)

and

\[ f'_2(0) = a_1(\sqrt{k^2 - \hat{\sigma}^2}) - a_2(\sqrt{k^2 - \hat{\sigma}^2}) = 1 \]
\[ f'_2(0) = a_2(-\sqrt{k^2 - \hat{\sigma}^2} - (\sqrt{k^2 - \hat{\sigma}^2})) = 1 \]  
(3.71)

for which,

\[ a_2 = \frac{-1}{2(\sqrt{k^2 - \hat{\sigma}^2})} \]
\[ a_1 = \frac{1}{2(\sqrt{k^2 - \hat{\sigma}^2})} \]

Therefore,

\[ f_2(z) = \frac{1}{2(\sqrt{k^2 - \hat{\sigma}^2})} e^{(\sqrt{k^2 - \hat{\sigma}^2})z} - \frac{1}{2(\sqrt{k^2 - \hat{\sigma}^2})} e^{-\sqrt{k^2 - \hat{\sigma}^2}z} \]
\[ f_2(z) = \frac{1}{(\sqrt{k^2 - \hat{\sigma}^2})} \sinh((\sqrt{k^2 - \hat{\sigma}^2})z) \]  
(3.72)
From 3.56, the matrix exponential now becomes,

\[
e^{[M]z} = \cosh((\sqrt{k^2 - \sigma^2})z) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{1}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z) \begin{bmatrix} i\sigma & ik \\ -ik & -i\sigma \end{bmatrix}
\]

(3.73)

\[
e^{[M]z} = \begin{bmatrix} \cosh((\sqrt{k^2 - \sigma^2})z) & 0 \\ 0 & \cosh((\sqrt{k^2 - \sigma^2})z) \end{bmatrix}
\]

\[\quad + \begin{bmatrix} \frac{1}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z) \cdot i\sigma & \frac{1}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z) \cdot ik \\ \frac{1}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z) \cdot -ik & \frac{1}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z) \cdot -i\sigma \end{bmatrix}
\]

(3.74)

\[
e^{[M]z} \equiv \begin{bmatrix} A & B \\ C & D \end{bmatrix}
\]

(3.75)

where

\[
A = \cosh((\sqrt{k^2 - \sigma^2})z) + \frac{i\sigma}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z)
\]

\[
B = \frac{ik}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z)
\]

\[
C = \frac{-ik}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z)
\]

\[
D = \cosh((\sqrt{k^2 - \sigma^2})z) + \frac{-i\sigma}{(\sqrt{k^2 - \sigma^2})} \sinh((\sqrt{k^2 - \sigma^2})z)
\]
Therefore,

\[
\begin{bmatrix}
V_1(z) \\
V_2(z)
\end{bmatrix} = e^{[M]z} \begin{bmatrix}
V_1(0) \\
V_2(0)
\end{bmatrix}
\]  

(3.76)

The two boundary conditions are \(V_1(0)\) which is the incident “positive (+)” wave at the input and \(V_2(L)\) which is the “negative (−)” wave at the output. Both \(V_1(0)\) and \(V_2(L)\) are known. The unknown of interest is \(V_2(0)\) which is the reflected wave at the input. The boundary condition are thus provided in Eq. 3.77,

\[
V_2(L) = 0 = C|_{z=L} V_1(0) + D|_{z=L} V_2(0)
\]  

(3.77)

By applying this boundary condition, we derive the result in Eq. 3.78,

\[
V_2(0) = \frac{-CV_1(0)}{D}
\]  

(3.78)

By definition of Field Reflectivity,

\[
\frac{S(0)}{R(0)} = \frac{V_2(0)}{V_1(0)} = \rho = \left. \frac{-C}{D} \right|_{z=L} = \left. \frac{ik}{\sqrt{k^2 - \sigma^2}} \sinh(\sqrt{k^2 - \sigma^2}L) \right|_{z=L} = \left. \frac{i\sigma}{\sqrt{k^2 - \sigma^2}} \sinh(\sqrt{k^2 - \sigma^2}L) \right|_{z=L}
\]  

(3.79)
In terms of the original wave amplitudes, $A$ and $B$ this reflectivity is from Eq. 3.51 and Eq. 3.52,

$$\rho = \frac{S(0)}{R(0)} = \frac{B_1(0)e^{i\phi(0)}}{A_1(0)e^{-i\phi(0)}} = \frac{B_1(0)}{A_1(0)}e^{i\phi(0)} \quad (3.80)$$

If the reference phase for any chirp is taken as $\phi(0) = 0$, then we see that the field reflection coefficient is just the ratio of (–) wave amplitude to the (+) wave amplitude at the input to the grating.

For Intensity Reflectance,

$$|\rho|^2 = \left| \frac{B_1(0)}{A_1(0)} \right|^2 = \frac{k^2}{k^2 - \hat{\sigma}^2} \sinh^2(\sqrt{k^2 - \hat{\sigma}^2}L) \left( \cosh^2(\sqrt{k^2 - \hat{\sigma}^2}L) + \frac{\hat{\sigma}^2}{k^2} \sinh^2(\sqrt{k^2 - \hat{\sigma}^2}L) \right)$$

$$= \frac{k^2 - \hat{\sigma}^2}{k^2} \cosh^2(\sqrt{k^2 - \hat{\sigma}^2}L) + \frac{\hat{\sigma}^2}{k^2} \sinh^2(\sqrt{k^2 - \hat{\sigma}^2}L) \quad (3.81)$$

By definition $\cosh^2(x) - \sinh^2(x) = 1$, and therefore we derive the reflectance for a uniform FBG as,

$$|\rho|^2 = \frac{\sinh^2(\sqrt{k^2 - \hat{\sigma}^2}L)}{\cosh^2(\sqrt{k^2 - \hat{\sigma}^2}L) - \frac{\hat{\sigma}^2}{k^2}} \quad (3.82)$$

### 3.4 Transfer Matrix Model

The polymer coating on our FBG tends to be beaded in nature. Therefore, what the light wave encounters along the FBG would be a periodic, non-uniform grating. Hence, the resultant non-uniform strain that would be produced along the FBG
would also be affected by this beading property. For the sake of simplicity, in our analysis we assume the beads alternate along the length of the FBG in a periodic fashion as shown in Fig. 3.3. The beaded section (Sections 1 and 3) corresponds to the perturbed FBG and the non-beaded section corresponds to the unperturbed FBG.

The numerical method used to simulate the FBG model is the Transfer Matrix model (TMM). In the TMM method, we assume the entire grating is made up
of sections of ABCD matrices. The coupled mode equations are modified for the sensor as in Eq. 3.4 for one section, with \( V_1 \) representing the incident wave and \( V_2 \) representing the reflected wave.

\[
\begin{bmatrix}
V_1(z_1) \\
V_2(z_1)
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_1
\begin{bmatrix}
V_1(0) \\
V_2(0)
\end{bmatrix}
\]

In a similar fashion to Eq. 3.4, the other sections can be written out as follows,

\[
\begin{bmatrix}
V_1(z_2) \\
V_2(z_2)
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_2
\begin{bmatrix}
V_1(z_1) \\
V_2(z_1)
\end{bmatrix}
\]

\[\vdots\]

\[
\begin{bmatrix}
V_1(z_{n+1}) \\
V_2(z_{n+1})
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_{(n+1)}
\begin{bmatrix}
V_1(z_n) \\
V_2(z_n)
\end{bmatrix}
\]

By cascading these matrices, the entire grating response can be modeled. Hence, noting \( L = z_{n+1} \) we get,

\[
\begin{bmatrix}
V_1(L) \\
V_2(L)
\end{bmatrix} =
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_{(n+1)}
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_n
\ldots
\begin{bmatrix}
A & B \\
C & D
\end{bmatrix}_1
\begin{bmatrix}
V_1(0) \\
V_2(0)
\end{bmatrix}
\]
The entire grating can be represented by one sum ABCD matrix.

\[
\begin{bmatrix}
V_1(L) \\
V_2(L)
\end{bmatrix} =
\begin{bmatrix}
A' & B' \\
C' & D'
\end{bmatrix}
\begin{bmatrix}
V_1(0) \\
V_2(0)
\end{bmatrix}
\]

The new expression for the intensity reflectance is

\[
|\rho|^2 = \left| -\frac{C'}{D'} \right|^2
\]

(3.83)

3.5 Results and Discussion

A non-uniformly strained model consisting of three equal sections shown in Fig. 3.3 was created in MATLAB. The manufacturer’s data sheet provided only the center wavelengths. To generate the parameters in this model the 1550 nm center wavelength was picked. The grating length was assumed to be in the range of millimeters and a total grating length of 1 mm divided into three sections was used. The total number of gratings was taken to be 10000. The effective refractive index, \( n_{eff} \) was calculated using the Bragg equation, \( \lambda_B = 2n_{eff}\Lambda \). The change in refractive index, \( \delta n_{eff} \) was set to be an arbitrarily small value of 0.0006 and adjusted to closely match as possible the unperturbed condition. As shown in
Fig. 3.4, the center wavelength and the envelope of the numerical model approach the experimental baseline.

![Graph showing comparison of experimental and theoretical baselines.]

**Figure 3.4:** Comparison of the experimental baseline to the theoretical baseline.

A minute perturbation is introduced into the theoretical model by varying by a small amount the length of the section corresponding to the beaded section, thus simulating the effect of the polymer bead swelling and straining the fiber upon absorbing the analyte. Fig. 3.5 shows the comparison between the theoretical baseline and the perturbed response upon increasing the length of section 1 as well as section 3 by $3.33 \times 10^{-5}$ mm. As with the experimental data, there is a shift in the right edge transition wavelength and a change in the bandwidth with respect to the theoretical baseline. Using the –10 dBm reference value, there’s a shift of approximately 70 pm in the right edge wavelength and change in the bandwidth of approximately 100 pm.
Figure 3.5: Comparison of the theoretical baseline to the perturbed response. 
$\delta L = 0.0001/3$ mm.

On increasing the perturbation, i.e., on increasing the length of the beaded section in the model to 0.3334 mm from 0.3333, we see a further shift in the right edge transition wavelength as seen in Fig 3.6. We also see a change in the shape of the envelope which is a change in the bandwidth. For large increases in the length of a beaded section, there is no discernible peak in the range of interest. This can be seen in Fig. 3.7, where the analysis was performed for a length increase of the beaded section to 0.3335 mm.

We can conclude that the transfer matrix model adequately models the response of the perturbed waveguide in the qualitative sense. Further analysis is necessary in order to verify whether this model could be used to accurately model the response of the polymer coated FBG to specific analytes and specific concentrations of
Figure 3.6: Comparison of the theoretical baseline to the perturbed response. 
\[ \delta L = 0.0002/3 \text{ mm}. \]

Figure 3.7: Comparison of the theoretical baseline to the perturbed response. 
\[ \delta L > 0.0005/3 \text{ mm}. \]
analytes.
This work demonstrates the proof of concept of a polymer coated fiber Bragg grating (FBG) based chemical sensor, its desirable characteristics and its operation in the detection and identification of multiple chemical analytes. FBGs are used as sensors to measure many types of physical phenomena including strain, temperature, vibration, and pressure in a variety of diverse applications but use of FBGs as chemical sensors is less prevalent and this work is unique in attempting to devise a sensor to detect chemical analytes in the liquid state. There’s significant potential for this type of sensor to be used as an “optical tongue” for chemical sensing in water quality assurance systems.

The chemical sensor was devised by coating the FBG section of a commercial optical fiber with cellulose acetate (CA) and it was tested with variety of analytes.
Experimental data showed significant shifts in FBG transition edge wavelength and changes in response bandwidth. The right transition edge wavelength shifts range from –82 pm to +43 pm and bandwidth changes range from –27 pm to +42 pm with reference to the baseline deionized water at an “absolute” –10 dBm power value. This dual approach was used because it provided a way to uniquely distinguish between the different analytes in a two parameter space.

To describe the experimental results, a theoretical and numerical framework was set up. Starting from first principles, an alternate elegant solution was derived for the Coupled Mode Theory (CMT). Modifying the coupled mode equations, the numerical model of the Transfer Matrix Method (TMM) was developed. In the TMM model, the fiber Bragg grating is assumed to be made up of equal sections, each of which is modeled as an ABCD matrix. Furthermore, when there is a change in the length of these sections and therefore a change in the periodicity due to the FBG being strained there is a shift in the center wavelength as well as a change in bandwidth. To verify this, the numerical model was implemented in MATLAB. The numerical model was perturbed by changing the length of the two beaded sections, according to Fig. 3.3. We observed that the output from the numerical model approximates the experimental results qualitatively in that there’s a shift in the right edge transition wavelength and change in the response bandwidth upon perturbation.
What is presented here is an exploratory study of devising and testing a polymer coated fiber Bragg grating as a chemical sensor. Following this work, there are several recommendations for further investigation. Crucially, the reproducibility and the maximum absorbency of the sensor need to be quantitatively determined. This will improve the sensitivity and selectivity of the sensor. Any external parameters such as temperature that might affect the sensor would need to be deconvolved. The theoretical/numerical model presented here is a good approximation of the FBG response but future work can possibly increase its sophistication to predict the behavior of different analytes and on that basis sort them into distinct groups for easy tagging.
Appendix A

Code

MATLAB code for the numerical model.

```matlab
%clear all;
%close all;
clc

%L = input ('Enter length of FBG in m ');
%N = input ('Enter number of gratings ');

L1=1.e-3/3; %Length of Section 1 in m
N1=10000/3; %Number of gratings in Section 1

L2=1.e-3/3; %Length of Section 2
N2=10000/3; %Number of gratings in Section 2

%Constants:
n_eff = 7.7510; %core index of fiber
deltan_eff = .0006;
v = 1; %Fringe visibility

%Periodicity of FBG:
Lambda0 = L1/N1; %Periodicity of Section 1
Lambda1 = L2/N2; %Periodicity of Section 2
```
%Design periodicity:
 lambda_d = 2*n_eff*Lambda_0;
 lambda_e = 2*n_eff*Lambda_1;

% Set wavelength lambda up as an array:
 lambdam = 1548:0.01:1552;
 lambda = lambdam*1e-9;
 delta_0 = 2*pi*n_eff/lambda - pi/Lambda_0;
 delta_1 = 2*pi*n_eff/lambda - pi/Lambda_1;

sigma = 2*pi*deltan_eff/lambda;
 sigmahat_0 = sigma + delta_0; %DC/self-coupling co-efficient
 sigmahat_1 = sigma + delta_1; %DC/self-coupling co-efficient

k = (v*pi*deltan_eff/lambda); %AC/cross-coupling co-efficient
ksqsigsq_0 = sqrt((k.*k)-(sigmahat_0.*sigmahat_0));
ksqsigsq_1 = sqrt((k.*k)-(sigmahat_1.*sigmahat_1));

A_1 = cosh(ksqsigsq_0*L_1) + j*((sigmahat_0./ksqsigsq_0).*sinh(ksqsigsq_0*L_1));
B_1 = -j*(k./ksqsigsq_0).*sinh(ksqsigsq_0*L_1);
C_1 = -B_1;
D_1 = conj(A_1);

M_1 = [A_1, B_1; C_1, D_1];

A_2 = cosh(ksqsigsq_1*L_2) + j*((sigmahat_1./ksqsigsq_1).*sinh(ksqsigsq_1*L_2));
B_2 = -j*(k./ksqsigsq_1).*sinh(ksqsigsq_1*L_2);
C_2 = -B_2;
D_2 = conj(A_2);

M_2 = [A_2, B_2; C_2, D_2];

%Multiplying the two segments together
A_3 = (A_1.*A_2) + (B_1.*C_2);
B_3 = (A_1.*B_2) + (B_1.*D_2);
C_3 = (C_1.*A_2) + (D_1.*C_2);
D_3 = (C_1.*B_2) + (D_1.*D_2);

M_3 = [A_3, B_3; C_3, D_3];

%The third segment
\[ A_4 = (A_3 \cdot A_1) + (B_3 \cdot C_1); \]
\[ B_4 = (A_3 \cdot B_1) + (B_3 \cdot D_1); \]
\[ C_4 = (C_3 \cdot A_1) + (D_3 \cdot C_1); \]
\[ D_4 = (C_3 \cdot B_1) + (D_3 \cdot D_1); \]
\[ M_4 = [A_4, B_4; C_4, D_4]; \]
\[ \rho = \frac{|C_4|}{|D_4|}; \quad \text{\%Intensity Reflectance} \]
\[ \rho_1 = \frac{|C_1|}{|D_1|}; \]
\[ \rho_2 = \frac{|C_2|}{|D_2|}; \]
\[ R = \rho \cdot \rho_c; \]
\[ R_{\text{base}} = 10 \cdot \log_{10}(R); \]
\[ \text{figure();} \]
\[ \text{plot(lambdanm, R_{base});} \]
\[ \text{axis([1548 1552 -inf 0]);} \]
\[ \text{hold on;} \]
\[ \text{plot(exp\_wavelength, exp\_power, '}r'\text{);} \quad \text{\%Experimental baseline} \]
\[ \text{xlabel('Wavelength (nm)');} \]
\[ \text{ylabel('Reflectance all');} \]
Bibliography


