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Numerical simulation and characterization of photonic/plasmonic devices

by

FOO, Yishu

November 2011
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FOO, Yishu

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Abstract

Nano-scale optical materials are often difficult to fabricate for experimental characterization and too complex for analytical analysis. Numerical simulation is a more cost effective way to characterize nano-scale optical materials due to increasingly cost effective computers and the availability of commercial electromagnetic-simulation software. One of the electromagnetic simulation methods that become increasingly favorable due to the ability to simulate a wide variety of problems is the Finite-Difference Time-Domain (FDTD) method. However, FDTD is not an unconditionally stable numerical simulation method. To facilitate the use of FDTD to characterize nano-scale optical materials, knowing the conditions for a numerically stable simulation is necessary. The main focus of this project is to quantify the ability of FDTD to characterize thin films using simulations which mimics ellipsometry measurements using a chosen commercial FDTD software. Simulating polarization states of light reflected by thin films is chosen due to the availability of analytical solutions to the problem. In the second part, planar chiral metamaterials (PCM), a material with periodic structure and unit cell in the shape of (left-, or right- hand) gammadions which are shown to support surface plasmon resonance with the ability to excite circularly polarized light into super-chiral light is characterized. These structures are of interest as recently, PCM have been shown to enhance the detection of biomolecules using Circular Dichroism by up to six orders of magnitudes as compared to conventional chirality detection schemes.
1 Introduction

1.1 Finite Difference Time Domain (FDTD)

1.1.1 Overview

FDTD is a method of numerically simulating electromagnetic waves in the time domain using Maxwell’s Equations and is proposed by K.S.Yee [1]. FDTD was not widespread back in the days when computing power is expensive as time domain methods require a lot of computing power and computer memory. Today, FDTD can be performed on any personal computer with commercially available software and thus is a favorable choice. Some of the advantages of FDTD are that it can handle complex geometries, obtain broadband data in a single simulation and is capable of simulating real time EM pulse propagation.

However, FDTD is not an unconditionally stable numerical simulation method. To facilitate the use of FDTD to characterize nano-scale optical materials, knowing the conditions for a numerically stable simulation is necessary. There are a vast variety of FDTD algorithms and ways to implement the boundary conditions, and each of the algorithms has their own advantages and disadvantages [2]. It is thus important to know how which parameters contribute to the stability of a FDTD simulation of implementing a certain algorithm.

1.1.2 1D FDTD in Free Space

In Yee’s scheme [4], the E field and the H field are defined only at the points labeled in Figure 1.1. The E field and H field are not calculated simultaneously in the same time step; instead, a so-called leap-frog algorithm is used where the E field at time $t=1/2$ is calculated from H field at time $t=0$ and the H field at time $t=1$ is again calculated from the E field at time $t=1/2$.

![Figure 1.1: A single unit cell in FDTD (Yee Cell)](image)
For the sake of simplicity, we only formulate the FDTD method in 1D, which is sufficient for explaining the concepts of absorbing boundary conditions, periodic boundary conditions, propagation in dielectric medium and propagation in lossy medium. [5]

The time dependent Maxwell’s Curl Equations in free space are given by Eq. 1.1, 1.2,

\[
\frac{\partial E(x, y, z, t)}{\partial t} = \frac{1}{\varepsilon_0} \nabla \times H(x, y, z, t) \\
\frac{\partial H(x, y, z, t)}{\partial t} = -\frac{1}{\mu_0} \nabla \times E(x, y, z, t)
\]

And can be simplified to Eq. 1.3, 1.4 for 1D case,

\[
\frac{\partial E_x(z, t)}{\partial t} = -\frac{1}{\varepsilon_0} \frac{\partial H_y(z, t)}{\partial z} \\
\frac{\partial H_y(z, t)}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x(z, t)}{\partial z}
\]

The most important step in formulating a simulation scheme is to choose a way to discretize continuous functions. Both temporal and spatial derivatives are discretized using the central difference approximations.

\[
\frac{E_x(k, n + \frac{1}{2}) - E_x(k, n - \frac{1}{2})}{\Delta t} = -\frac{1}{\varepsilon_0} \frac{H_y(k + \frac{1}{2}, n) - H_y(k - \frac{1}{2}, n)}{\Delta z}
\]

\[
\frac{H_y(k + \frac{1}{2}, n + 1) - H_y(k + \frac{1}{2}, n)}{\Delta t} = -\frac{1}{\mu_0} \frac{E_x(k + 1, n + \frac{1}{2}) - E_x(k, n + \frac{1}{2})}{\Delta z}
\]

Note that \(k\) and \(n\) are integers for space and time step. Rearranging, Eq. 1.5, 1.6 then we have an algorithm to simulate \(E\) and \(H\) by iterating in discrete time steps.

\[
E_x(k, n + \frac{1}{2}) = E_x(k, n - \frac{1}{2}) - \frac{\Delta t}{\varepsilon_0 \Delta z} \left[ H_y(k + \frac{1}{2}, n) - H_y(k - \frac{1}{2}, n) \right]
\]

\[
H_y(k + \frac{1}{2}, n + 1) = H_y(k + \frac{1}{2}, n) - \frac{\Delta t}{\mu_0 \Delta z} \left[ E_x(k + 1, n + \frac{1}{2}) - E_x(k, n + \frac{1}{2}) \right]
\]
1.1.3 Stability (Time Step and Mesh Size)

Since, space and time is discretize there will be numerical errors associated with it and it is important to know the limit of $\Delta x$, $\Delta t$ to maximize accuracy and speed. For FDTD simulations to be stable, the Courant Condition [6] [7] must be met,

$$\Delta t \leq \frac{1}{c \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$ \hspace{1cm} (1.9)

Eq. 1.9 implies that the time step is limited by $c$ and the mesh size $\Delta x$, $\Delta y$ and $\Delta z$, as for one dimensional simulation, the above condition can be simplified to,

$$c \leq \frac{\Delta x}{\Delta t}$$ \hspace{1cm} (1.10)

Figure 1.2, Figure 1.3 is used to gain some physical insight of this stability condition, in Figure 1.2 a 1D sine wave is at $t=0$, Figure 1.3 shows the sine wave at time $\Delta t$ for $\Delta t > \frac{\Delta x}{c}$, assuming that it is free space, the sine wave will move with speed $c$ with node 1 moving slightly pass the $k = 1$ mesh point at time $\Delta t$, this causes node 2, 3 to be indistinguishable and node 4, 5 to be indistinguishable with each other and thus results in an unstable solution.
1.1.4 Boundary Conditions (Absorbing & Periodic)

Absorbing Boundary Conditions

There will be undefined E, H values at the edges of the simulation mesh, if a propagating wave is to propagate outward without reflection, these values at the boundary needs to be adjusted to artificially create this kind of effect, if the values at the boundary are left to be 0, reflection will occur and ruin the simulation. The absorbing boundary condition used by FDTD solutions is the Perfectly Matched Layer (PML) [8]. The PML is quite accurate when used in simulations with normal incidence light but not so accurate when used for simulations with oblique incidence light.

Periodic Boundary Conditions

When simulating periodic structures, we want to set periodic boundary conditions so that by only simulating one cell we can imitate results from a whole set of arrays. However, the simplest periodic boundary conditions does not account for the phase change of oblique incidence plane wave. For this, we need a type of periodic boundary condition that accounts for this phase change [9]. The boundary condition will be referred to as the Bloch boundary condition. The Bloch boundary condition can be implemented in many ways, a simple illustration of the phase shift needed for a plane wave that is incident on a periodic structure is shown.

If the red, green, blue and black lines represents different phase of a wave, and on any point on the same line the phase is the same, it can be seen that at level P, phase at point P2 is black, and phase at point P1 is green, so there is a phase difference, if the simulation region is periodic in the x direction, the phase change of the oblique incident light must be accounted.
1.1.5 1D FDTD in Constant Dielectric Materials

One of the advantages of FDTD is to be able to simulate arbitrary structures and a wide variety of materials, to simulate a dielectric material instead of free space [10], Eq. 1.1 can simply be changed to,

\[
\frac{\partial E}{\partial t} = \frac{1}{\varepsilon_r \varepsilon_0} \nabla \times H
\]

While Eq. 1.2 remains as is assuming a non-magnetic material; in this conditions the discretization process would be the same as demonstrated earlier.

1.1.6 Resolving a Curved Surface Containing Two or more Materials in a Single Cell

Since FDTD needs a finite mesh size, the dielectric function used in a cell that contains 2 or more materials has to be decided. The simplest method used is the staircase approximation that approximates a curved surface shown in Figure 1.5.

The staircase approximation although decent for dielectric materials, is very unstable when applied to Metal-Dielectric Interfaces; in these cases, a Conformal Meshing Technique (CMT) [11] is preferred. Several CMT have been developed, here only the Yu-Mittra [12] method is discussed to exemplify the approaches used in CMTs. The Yu-Mittra CMT is a good method for interfaces between dielectrics and Perfect Electric Conductors (PEC).
The Yu-Mittra method uses Faraday’s Induction Law to update the magnetic field in time, instead of integrating all the electric field along the cell wall, the Yu-Mittra method discards the electric field within the PEC.

1.1.7 1D FDTD in Frequency Dependent Materials using Debye Formulation

To simulate a frequency dependent material, there are lots of formulations to choose from, some methods gives better approximation of the dielectric function, some methods are easier to implement and requires less computation. Here, we will try to analyze the general steps to formulate the algorithm without actually deriving it. [13]

A more general form of Maxwell’s Equations are given by,

\[ \frac{\partial D}{\partial t} = \nabla \times H \]  \hfill (1.12)
\[ D(\omega) = \varepsilon_0 \varepsilon_r(\omega) E(\omega) \]  \hfill (1.13)
\[ \frac{\partial H}{\partial t} = -\frac{1}{\mu_0} \nabla \times E \]  \hfill (1.14)

Where \( D \) is the electric flux density,

Since Eq. 1.14 is same as Eq. 1.2 it does not need to be changed, and Eq. 1.12 looks similar to Eq. 1.1. The only thing left is to discretize Eq. 1.13, which is not an easy step as \( \varepsilon_r(\omega) \) is different for different optical models. For frequency dependent materials, \( \varepsilon_r(\omega) \) can be represented by the Debye formulation, or Lorentz Model. Eq. 1.15 shows the Debye Formulation which is simpler of the two,

\[ \varepsilon_r(\omega) = \varepsilon_r + \frac{\sigma}{i\omega \varepsilon_0} + \frac{\chi_1}{1 + i\omega t_0} \]  \hfill (1.15)
\[ D(\omega) = \varepsilon_0 \varepsilon_r E(\omega) + \frac{\sigma}{i\omega} E(\omega) + \frac{\varepsilon_0 \chi_1}{1 + i\omega t_0} E(\omega) \]  \hfill (1.16)

Eq. 1.16 is obtained by substituting Eq. 1.15 into Eq. 1.13, further transforming Eq. 1.16 to the time domain gives Eq. 1.17

\[ D(t) = \varepsilon_0 \varepsilon_r \cdot E(t) + \sigma \int_0^t E(t') \cdot dt' + \frac{\varepsilon_0 \chi_1}{t_0} \int_0^t e^{-\frac{t'-t}{t_0}} E(t') \cdot dt' \]  \hfill (1.17)
\( \mathbf{D}(t) \) in Eq. 1.17 can be discretized into \( \mathbf{D}(n\Delta t) \) by approximating the integrals by summations. (See reference [13] for details)

<table>
<thead>
<tr>
<th>N(time step no.)</th>
<th>N=0</th>
<th>N=1/2</th>
<th>N=1</th>
<th>N=3/2</th>
<th>N=2</th>
<th>N=......</th>
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<tbody>
<tr>
<td>( \sum_{0}^{N} \mathbf{E}(n) )</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<tr>
<td>( \mathbf{E}(n) )</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>( \mathbf{D}(n) )</td>
<td>Initial Condition</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \mathbf{H}(n) )</td>
<td>Initial Condition</td>
<td></td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>

Table 1.1: Relationship between \( \mathbf{E}, \mathbf{D} \) and \( \mathbf{H} \) values

Before rearranging Eq. 1.17 that is discretized, the relationship of \( \mathbf{E}, \mathbf{D} \) and \( \mathbf{H} \) values are examined in Table 1.1: Relationship between \( \mathbf{E}, \mathbf{D} \) and \( \mathbf{H} \) values. It is seen that to obtain \( \mathbf{E}(N) \), the values \( \sum_{0}^{N} \mathbf{E}(n) \) and \( \mathbf{D}(N) \) are required. Thus, the discretized Eq. 1.17 is arranged with \( \mathbf{E}(N) \) at the left side and everything else at the right side and the formulation is complete.

1.1.8 Time Domain Results to Frequency Domain Results

For most applications, it is often more useful to obtain the results of the simulation in the frequency domain; this could be obtained, albeit in an unpractical way, by iterating the simulation at every frequency until a stable condition is reached. It is much more convenient to follow system theory, in which case it is possible to input an impulse and get output data from all frequencies. Due to the discretized nature of FDTD, it is impossible to create a perfect impulse function. However, a Gaussian pulse, if narrow enough, can be approximated as an impulse. Thus, a Gaussian pulse can be propagated throughout the system until it dies out from the simulation region at which point the frequency domain data can be obtained by applying a Fast
Fourier Transform on time domain data at any point in space. This method, however, requires large amount of memory as all the time domain data has to be recorded. [14]

A more practical approach to obtain the frequency domain response follows. The Fourier Transform is written as Eq. 1.18,

$$E(\omega) = \int_0^t E(t').e^{-i\omega t'}dt'$$  \hspace{1cm} 1.18

Discretizing and then separating into real and imaginary parts to get Eq. 1.19,

$$E(\omega) = \sum_{n=0}^{t/\Delta t} E(n \cdot \Delta t) \cdot \cos(\omega_1 \cdot n \cdot \Delta t) - \sum_{n=0}^{t/\Delta t} E(n \cdot \Delta t) \sin (\omega_1 n \cdot \Delta t)$$  \hspace{1cm} 1.19

Eq. 1.19 if implemented in computer code, frees up the memory required to record all the data in the time domain, as the Fourier Transform can be performed in real time.

1.1.9 Far Field Analysis

Many applications require results in the far field, although FDTD is a general electromagnetic simulation technique, extension of the simulation area incurs heavy computational time (as constraints, Eq 1.9, 1.10, need to be satisfied) and is not practical. However, there are methods to calculate the far field from near field. [15] Normally, $E_x, E_y, E_z, H_x, H_y, H_z, P_x, P_y$ and $P_z$ at the desired points in space are recorded. Where $E$ is the electric field, $H$ is the magnetic field and $P$ is the Poynting Vector. Since the Poynting vector is recorded, the far field can then be calculated using the near field data. [16] The direction, amplitude and phase of the electric field is also recorded, that makes finding the polarization state of light possible too [17].

For 2D monitor in FDTD Solutions, the far field data is obtained by projecting the field as a function of angle into the half space above the 2D monitor. This is possible because at the far
field (~1m), the source (E field on 2D monitor) can be seen as a point source. Due to this reason this method of far field projection is not accurate at intermediate distance of a few wavelengths.

The far field projection also assumes that

\[ \omega = ck \]  

So no numerical dispersion is involved, however, if the far field is calculated directly using FDTD instead of far field projection, there is numerical dispersion, and the results obtained will be slightly different. Figure 1.7 to Figure 1.10 shows how the how the far field projection is done.

---

**Figure 1.7**: Simple far field projection setup [18]

**Figure 1.8**: Near field data obtain at 2D monitor [18]

**Figure 1.9**: Far field projection as a function of angle [18]

**Figure 1.10**: Far field data obtained at ~1m away in spherical coordinates, it can be seen that the power is $10^{-13}$ smaller than the near field [18]
1.2 Ellipsometry

The main purpose of this project is to study the feasibility to use ellipsometry to provide a quantitative assessment of the accuracy of FDTD simulations. The principles of ellipsometry are discussed in this section. By relating the polarization state of light with the material properties, the fundamental equation of ellipsometry is shown and the two very important variables $\psi$ and $\Delta$ are defined. Finally, a simple explanation is given to show how the optical properties and thickness of thin films can be obtained by analyzing ellipsometry data. For the explanation of the polarization ellipse, and Circularly Polarized Light (CPL) please refer to Appendix 5.4.

1.2.1 Transverse Nature of Light

It is well known that an electromagnetic wave propagating in an isotropic media is a transverse wave; therefore the components of the electric field can be separated using vector calculations. This fundamental property of light makes ellipsometry possible.

1.2.2 Introduction to Ellipsometry

Ellipsometry is an indirect technique to find the thickness and optical properties of thin films by detecting the change in polarization state of light after reflection on a thin film [19]. It is also widely used for nano-scale topographic measurements. The advantage of ellipsometry is that it is inert to background disturbances, allows fast measurement of samples and has the ability to measure complex layers on thin films. However, the downside is that it does not directly measure the physical parameters and requires iterative analysis to get the desired results. Ellipsometry also allows measurement at multiple incident angles therefore the analysis can be more accurate.

1.2.3 The Fundamental Equation of Ellipsometry

An equation that is normally used in ellipsometry to relate the polarization state of light to the material properties is derived in this section [19].
Figure 1.11: Reflection on mono-layer thin film in ellipsometry

Eq. 1.21 to 1.24 represents the incident (E) and reflected (R) electric fields which are parallel (p) and perpendicular (s) to the incident plane.

\[
\begin{align*}
E_p &= E_{0p} e^{-i\alpha_p} \\
E_s &= E_{0s} e^{-i\alpha_s} \\
R_p &= R_{0p} e^{-i\beta_p} \\
R_s &= R_{0s} e^{-i\beta_s}
\end{align*}
\]

Traditionally, ψ, Δ and ρ is used while doing ellipsometry experiments, and they are defined as,

\[
\tan \psi = \frac{R_{0p}/E_{0p}}{R_{0s}/E_{0s}} \quad 1.25
\]

\[
\Delta = \beta - \alpha = (\beta_p - \beta_s) - (\alpha_p - \alpha_s) \quad 1.26
\]

\[
\rho = \tan \psi e^{-i\Delta} = f(n, k, d) \quad 1.27
\]

Eq. 1.27 is a general form that relates the change in polarization state of light to the material parameters. The goal of ellipsometry is to measure ψ, Δ and solve Eq. 1.27 to obtain n, k and d of the thin film. However, sample measured in ellipsometry consists of thin films that have several layers and also materials that are absorbing. Solving n, k and d analytically would be extremely difficult in this case. The approach normally taken is to first get a rough estimation of n, k and d of the measured thin film, and use them to numerically model the corresponding ψ
and Δ. Finally, perform a N dimensional optimization on the parameters \( n, k \) and \( d \) until the modeled \( \psi \) and \( \Delta \) matches the experimental \( \psi \) and \( \Delta \). In our FDTD measurements, we will follow this convention and express the change in polarization state of light in the form of \( \psi \) and \( \Delta \).

### 1.2.4 Modeling \( \psi, \Delta \) from theory

The process of modeling \( \psi, \Delta \) can be simplified into 4 components. First, treat parallel and perpendicular polarization independently. Second, find the amplitude and phase change induced by interfaces between different materials, which can be treated using Fresnel’s Coefficients. Third, find the amplitude and phase change induced by the absorbance of materials and the thickness of the thin film. Fourth, combine the above three steps and account for the interference between multiple reflections. [20] The modeling for multiple layers of thin film with complex refractive indexes will be long and exhausting and it is left out. For our calculations a commercial software WVASE from J. A. Wollam [21] is used to calculate the theoretical values of \( \psi, \Delta \) of selected film structures which are then used to compare against FDTD simulations.
2 Finding numerically stable conditions for Thin Film simulations

2.1 Objective

1) To increase the efficiency of Broadband Simulations (BB) and Single Wavelength Simulations (SW) by investigating the optimal mesh for the simulations.

2) To increase the accuracy of BB and SW by investigating the errors caused by incorrect indexes.

3) To optimize between performance and accuracy of BB by separating a BB of 200nm to 1400nm into few simulations that cover a smaller range of wavelengths.

4) To quantify FDTD performance using the Mean Square Error (MSE) (See Appendix 5.6) for $\psi, \Delta$ obtained for a wavelength of 200nm to 1400nm, angle of Incidence of 20 to 70 degree, Mesh Size in the Z direction of 5nm to 0.25nm and 8 different thin film structures.

2.2 Simulation Setup

The FDTD simulation software used throughout this project is a commercial FDTD simulation by Lumerical [22], thus most of the details of the implementation is not available. However, Lumerical does explain the limitations of their algorithms. Although low level optimization is not possible using Lumerical FDTD solutions, the high level parameters present in the software still allows a rage of optimization and must be dealt with carefully.

Both SW and BB will be conducted in this section, their setup differ only by the wavelength of the source used and the iterations required to cover all angle of incidence and wavelength required. Some additional post processing of the broadband data is also required.
**Materials and Structures:** A total of 8 samples are chosen, the structural order and the thickness of the thin films are tabulated in Table 5.2 in the Appendix. Samples are chosen to represent metal-dielectric interfaces and dielectric-dielectric interfaces with different thickness.

**Light Sources:** An oblique incidence plane wave is used in the simulation to mimic the incident light used in an ellipsometry measurement. Light sources can either be set to obtain data for a SW or BB. It is found that SW are simple and more accurate compared to BB as the index used does not have to be modeled over a large range of wavelengths. On the other hand, broadband data are also harder to analyze due to some restrictions on the Angle of Incidence ($\theta$) and Wavelength ($\lambda$), for details refer to Appendix 5.2.

**Mesh & Boundary:** Mesh Size in the z-direction is important as there are structural variations. Investigation is done on the mesh size near the interface to determine its effect on the accuracy of the data. There is only 1 cell in the x-y plane and thus the size can be set as small as possible without heavily compromising speed. FDTD Solutions has an automatic mesh generation system that will generate a non-uniform mesh according to the complexity of the structure involved. Accuracy problems related to the minimum mesh size and time step is taken care of automatically. However, due to the automatic mesh generation, the mesh does not always snap to the interfaces between layers and thus relies on averaging and conformal techniques to be
used at the interfaces. However, FDTD Solutions does provide a custom meshing scheme that allows users to override automatically generated mesh. This mesh overriding method is used to optimize the cells at the interfaces and also their size.

**Data Analysis**: Data recorded in the simulation are E and B field data at a certain plane in space. The data analysis process calculates the far field data from this near field data and averages the polarization state in space to get a single meaningful number that represents the polarization state of light which is then changed into $\psi$ and $\Delta$ to compare with theoretically modeled ellipsometry data.

### 2.3 Accuracy Optimization

Each material is represented by its corresponding set of index that is loaded into the simulation file from which FDTD Solutions models the index into a different parametric function depending on the details of the simulation. This modeling can affect the simulation results significantly which is especially critical in BB.

Figure 2.2 shows the difference between the input material index (square symbols) and the FDTD software modeled index (solid line). As expected, fitting a function with a preset number of parameters is always more difficult when the fitting range is large and the function to be fitted has many local minima and maxima. In Figure 2.2 the fitting range is from 0.2$\mu$m to 0.8$\mu$m, which is quite large, and the fitted material index has an error of about $\pm0.1$. 

![Figure 2.2](image-url)
It is not sufficient to only decrease the fitting range to get a better fitting. It can be seen that in Figure 2.3 that the fitted material index is monotonous with a fitting range of 0.52μm to 0.58μm but in Figure 2.4 the fitted material index has a local minimum with a fitting range of 0.53μm to 0.58μm. Therefore, recording of the material index used in any simulation is necessary to identify the errors caused by inaccurate material index.

This type of parameter fitting is necessary in the FDTD implementation by Lumerical because the optical constants are not fitted using optical models like the Lorentz Oscillator Model. Although this method will compromise the accuracy of the modeled index, it has advantages for being able to speed up the simulations and is suitable for general use for a wide range of materials.
Single Wavelength Simulations

For SW, a simple interpolation is done between data points to obtain the index at the desired wavelength and thus it is relatively accurate compared to BB modeling.

The error of $\Delta$ is representative of the error of $\psi$ and thus only one set of data is shown. It is seen from Figure 2.6 that the accuracy of the simulation decreases as $\lambda$ decreases; this effect can be traced back to the inaccuracies of the index of the simulation shown in Figure 2.7. $n$ and $k$ generally have the same magnitude of error and thus only $n$ is showed.
**Broadband Simulations**

The fitting of $n$, $k$ is only done within a certain range of interest for BB. Thus, the smaller the range needed, the more accurate the index. Also, $\theta$ and $\lambda$ are not independent of each other in BB causing the need to split BB into several steps in $\lambda$ (See Appendix 5.2). The number of steps in $\lambda$ is set as $n_\lambda$. After testing with $n_\lambda$ of 5, 10 and 15, $n_\lambda$ of 10 gives optimal balance between accuracy and speed for a wavelength range from 200 nm to 1400 nm, and so the following BB are setup using $n_\lambda$ of 10.

![Image](image.png)

**Figure 2.8:** $\Delta$ of BB AuCr100 Aol-20 (see Appendix 5.1 Setup 2 for details of FDTD simulation setup)

**Figure 2.9:** Difference between $\Delta$ by FDTD and $\Delta$ by ellipsometry model (see Appendix 5.1 Setup 2 for details of FDTD simulation setup)

**Figure 2.10:** Difference between $n$ modeled by FDTD and $n$ by original optical models (see Appendix 5.1 Setup 2 for details of material index inputted and fitting range)

It is clearly seen in Figure 2.10 that due to the modeling of the indexes there is a large error in the index. The continuous profile of $\Delta n$ is due to the modeling and the discontinuity is because $\lambda$ of 200nm-1400nm is separated into 10 different simulations.
The error in index of BB is relatively large compared to SW by a factor of \( \sim 100 \). However, \( \Delta(\Delta) \) in Figure 2.6 and Figure 2.9 indicates that different structures are more or less sensitive to inaccuracies in index, with \( \Delta(\Delta)_{\text{max}} \approx 0.25^\circ \) for Au100Cr5 BB simulation and \( \Delta(\Delta)_{\text{max}} \approx 2^\circ \) for SiO\(_2\) 500 SW.

2.4 Efficiency Optimization

For FDTD method, finer mesh size and time step improves the accuracy of the results but only until a certain mesh size and time step after which the results converge and further reduction in mesh size and time step result only in minor improvements. Here we are trying to find an optimal mesh size that is accurate yet worth the simulation time.

The thin film is periodic in the x-y plane, so only one cell is required. The dimensions are only limited by wavelength of the source since there is no material variation in the x-y plane. Thus the mesh size does not need to be optimized in the x-y plane for this simulation.

In the z direction, there are changes in material and thus the mesh size is important especially at the interfaces between 2 materials. Local override of the mesh size of interfaces is applied instead of using a uniform mesh to prevent major increase in simulation time.

Increasing the mesh size to obtain accuracy is the last option of any FDTD simulations as the simulation time will be a function \( \frac{1}{dx^4} \). [23]
Figure 2.11: MSE obtained for simulations with different thin films and $\theta$ (see Appendix 5.1 Setup 1, 2 for details of FDTD simulation setup, Appendix 5.6 for definition of MSE)

Figure 2.12: MSE obtained for simulations with different thin films and $\theta$ (see Appendix 5.1 Setup 1, 2 for details of FDTD simulation setup)
From the second plot of Figure 2.12 it seems that there is a significant improvement for mesh size 1nm compared to mesh size 2.5nm, but further increasing the mesh size does not improve accuracy by much, although this is not true for all structures, mesh size of 1nm can be chosen as an optimal size when accuracy has high priority. The first plot of Figure 2.12 also shows that BB with $n_{\lambda}=10$ is far more accurate than with $n_{\lambda}=5$, whereas further increase to $n_{\lambda}=15$ does not give much improvement.

From Figure 2.11 and Figure 2.12, MSE increases as $\theta$ increases, this is a known problem for FDTD simulations using oblique incidence light with periodic materials. The problem could be due to the PML and the Bloch boundary conditions for the simulations.

2.5 Conclusion & Future Work

Indexes must be accurate for FDTD simulations to be accurate; it is important to note that there are no significant computation-time tradeoffs by using indexes with denser data points.

Decreasing the mesh size at interfaces between materials increases accuracy, with 1nm being the optimal mesh size for 200nm-1400nm frequencies, any mesh size smaller then 1nm does not increase accuracy by much. Decreasing the mesh size should be the last countermeasure as it increases simulation time significantly.

The error for simulations of oblique incidence plane wave on periodic structures increases with $\theta$, so with the MSE for $\theta=20,30,40,50,60,70$ and different thin films plotted, before doing any further simulations with complex geometries, the error tolerable can be first checked with Figure 2.11.

Future work includes understanding how PML and Bloch boundary conditions effect simulations for thin film with oblique incidence light and optimize the accuracy of the simulations so that other complex geometries could be explored with oblique incidence light with the FDTD method.
3 Simulations of PCM using FDTD

3.1 Objective
1) Introduce an example of future application of the results from Section 2 based on Planar Chiral Metamaterials (PCM)
2) Setup the FDTD to reproduce the normal-incidence calculations of near-field EM fields and circular dichroism transmission data in PCM

3.2 Introduction
The combined use of FDTD and ellipsometry can result in a powerful tool to study nanoscale materials by means of correlating optical numerical simulations (FDTD) with far-field optical measuring techniques (ellipsometry). On a first instance, this approach will enable quantitative confirmation of numerical model; however for simple cases it is possible to envision that it will be possible to extract near-field information based on far field-measurements (e.g. optical properties, morphology). Indeed a number of applications have been demonstrated in this regard including gratings [24] and photonic crystals [25], which, however use a different numerical algorithm (Rigorous Coupled-Wave Analysis, RCWA, which is ideally suitable for modeling periodic structures) [24]. In this part I wish to introduce an advanced application related to the detection of chirality in biomolecules that takes advantage of plasmonic resonances in specially designed chiral structures. While the full modeling of the ellipsometric data of such samples is out of the scope of this project, the initial steps in achieving a basic FDTD model (that is a model that reproduces published data and are thus deemed accurate) are demonstrated. The section will make a qualitative description of the next steps needed to achieve numerical simulations that can be compared to experimental data. We start with the definition of some basic concepts followed by a description of the modeling setup. The comparison between our simulations and those in the selected reference are presented in section 3.4.
**Optical Chirality:** An object is chiral if its mirror image cannot be superimposed on itself by way of 3-D rotations and translations. [26] For example, one could think of the alphabet S, with its front side coated with red and back side coated with blue. Electromagnetic fields can also be chiral, with circularly polarized light being the simplest example. Together with the concept that any electromagnetic wave can be separated into left circularly polarized light and right circularly polarized light, chirally sensitive spectroscopic techniques are invented. Biomolecules such as amino acids and sugars are chiral, so biomacromolecules formed from these units also exhibit chirality on molecular and supramolecular scales. Chirally sensitive (chiroptical) spectroscopic techniques such as circular dichroism (CD), optical rotatory dispersion (ORD) and Raman optical activity (ROA) are therefore good techniques to characterize the 3D structure of the biomolecules. [27, 28].

**Circular Dichroism:** Circular dichroism [29] describes the differential absorption of left and right-circularly polarized light by chiral molecules. CD is therefore a tool to identify such structural information of molecules. One might think that CD might not be significant as there could be little molecules that could be described as chiral. However, the fact is most biomolecules including DNA and most proteins are chiral and can be identified using CD spectroscopy. The downside is that CD output signals are often very weak, due to the small size of most molecules relative to the wavelength of light. One could think that the twisting of light is barely noticeable to the molecule due to the small size of the molecule compare to circularly polarized light.

**Surface plasmon resonances:** By solving Maxwell’s Equations at the interfaces between 2 materials, the results show that the incident wave is separated into transmitted and reflected components. For a special case when the real part of the dielectric constant ($\varepsilon_1$) of a metal is negative with a magnitude larger than the $\varepsilon_1$ of another dielectric, a third kind of resulting wave can be possible: one that propagates along the surface of the metal. This wave is normally referred as the surface plasmon or evanescent waves as its amplitude decreases exponentially with distance from the metal surface thus making it relatively hard to detect compared to the
reflected or transmitted waves. Localized surface plasmon resonance (LSPR) refers to the enhancement in amplitude of surface plasmon resonance at some resonance frequencies in a physically bounded (with dimensions of few 10s to few 100s nm) metallic structure. Effects that depend on the E field amplitude can therefore be enhanced by LSPR. Normally, LSPR is achieved by exciting metallic nanoparticles by light. [30]

**Superchiral Electromagnetic Field Excitation by Planar Chiral Metamaterial (PCM):** Efforts have been made to excite some kind of EM field that satisfies Maxwell’s Equations and significantly twists more within a smaller space compared to CPL light, quantification of such twist cannot be done without first defining optical chirality [27]. Periodic gold gammadions (a type of PCM) with CPL light of same handedness is shown to give rise to local EM fields that have a high degree of chirality [31]. This EM field is then used for CD spectroscopy on biomolecules and shows a significant increase in the sensitivity of CD spectroscopy [28].

**Measuring scheme:** as previously described, PCM generate high chirality EM fields that can be detected in the far field as resonances in CD. When chiral molecules are located on the surface of PCM, the interaction between them produces a shift in such resonances. The cited work, Ref [28], uses a sensing scheme based on the differential shift of such resonance position (L-PCM vs R-PCM). While great improvement (6 orders of magnitude) in sensitivity was demonstrated, it is noted that such sensing scheme is very simple and enhanced sensing capabilities could be made available by using a full simulation of the CD signal. In the proposed scheme, simulation of the ellipsometric data of PCM is expected to provide such information.
3.3 Simulation Setup

Figure 3.1: Overview of Simulation Setup in the x-z plane

Figure 3.2: Overview of Simulation Setup in the x-y plane

Figure 3.3: 3D Overview, water immersion removed for a clear view
3.4 Comparing CD Data

Normalized CD Data from Different Sources

Figure 3.4: Comparison of Normalized CD data from various sources, the FEM model and Experiment data is obtained from Figure 3a of Nature Nanotechnology [28], the y-axis is not shown as the scale of the result from our FDTD model is off by a factor of 2 to 3, the CD data are normalized for comparison. (see Appendix 5.1 Setup 3 for details of FDTD simulation setup, Appendix 5.5 for how CD(deg) is measured)

It is seen from Figure 3.4 that data from FDTD model fits better to the experiment data compared to the FEM model, as the local minima and maxima at 560nm, 600nm and 800nm matches better.

Figure 3.5: Enhancement of E field intensity at the substrate interface of left-handed PCM excited using left-circularly polarized light for a wavelength of 760nm, left side shows FEM model from reference [28] and right side reproduced using FDTD. (see Appendix 5.1 Setup 3 for details of FDTD simulation setup)
It is seen from Figure 3.5 that the $E$ field intensity that is reproduced using FDTD model has many features that resemble the data from the FEM model.

### 3.5 Conclusion & Future Work

A FDTD model was setup to reproduce the expected EM fields and CD transmission data as recently published [28] for the case of normal incidence. The $E$ field is qualitatively reproduced for 760nm wavelength. However there are differences in the calculated CD and local chirality, more work needs to be done to understand these observations. Incidentally, it is observed that our CD calculation provides a better fit to the experimental data reported in reference [28] in particular in determining the resonance position below 650 nm. Future work includes optimizing simulation setup for complex geometries like PCM, especially through obtaining reliable optical functions and optimizing mesh size in 3D instead of 1D as in the thin film case. Also, ellipsometric data $\psi$ and $\Delta$ with expected accuracy could be obtained from simulations with PCM geometry. A question arises on whether oblique incidence light incident on PCM can excite a similar superchiral light, changing the symmetry of the PCM could be a possible way to achieve this.
4 Conclusion

In the first part, different setup conditions that affect accuracy of thin film simulations are investigated. The errors from different setup conditions are quantified. These results are specific for certain implementation of FDTD algorithm as the software used is Lumerical FDTD Solutions 7.5. Firstly, more accurate modeling of indexes gives more accurate results with no significant computation-time tradeoffs by using indexes with denser data points. Secondly, shrinking the mesh size at interfaces between materials increases accuracy, with 1nm being the optimal mesh size for 200nm-1400nm wavelengths, any mesh size smaller then 1nm does not increase the accuracy by much but significantly increases simulation time. At last, the error for simulations of oblique incidence plane wave on periodic structures increases with $\theta$. Future work includes understanding how PML and Bloch boundary conditions effect simulations for thin films with oblique incidence light and optimizing the accuracy of the simulations so that other complex geometries could be explored with oblique incidence light using the FDTD method.

In the second part, a FDTD model was setup to reproduce the expected EM fields and CD transmission data as recently published [28] for the case of normal incidence. The E field is qualitatively reproduced for 760nm wavelength. However there are differences in the calculated CD and local chirality, more work needs to be done to understand these observations. Incidentally, it is observed that our CD calculation provides a better fit to the experimental data reported in reference [28] in particular in determining the resonance position below 650 nm. Future work includes optimizing simulation setup for complex geometries like PCM, especially through obtaining reliable optical functions and optimizing mesh size in 3D instead of 1D as in the thin film case. Also, ellipsometric data $\psi$ and $\Delta$ with expected accuracy could be obtained from simulations with PCM geometry. A question arises on whether oblique incidence light incident on PCM can excite a similar superchiral light, changing the symmetry of the PCM could be a possible way to achieve this.


## 5.1 Details of Simulation Setup

<table>
<thead>
<tr>
<th>Structure</th>
<th>Simulation A</th>
<th>Simulation B</th>
<th>Simulation C</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Structure</td>
<td>See Thin Film 1-8 of Table 5.2</td>
<td>See Thin Film 1 of Table 5.2</td>
<td>See Figure 3.1, Figure 3.2</td>
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<table>
<thead>
<tr>
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<th>Simulation B</th>
<th>Simulation C</th>
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<table>
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<th>Simulation A</th>
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<th>Simulation C</th>
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<tr>
<td>3. X: Bloch</td>
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<td>X: Bloch</td>
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<tr>
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<td>Y: Bloch</td>
<td>Y: Bloch</td>
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<tr>
<td>Z: PML</td>
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<table>
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<th>1</th>
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</table>

<table>
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<tr>
<th>Criteria to terminate simulation</th>
<th>Simulation A</th>
<th>Simulation B</th>
<th>Simulation C</th>
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<tr>
<td>4. SIMT (fs):100</td>
<td>SIMT:100</td>
<td>SIMT:100</td>
<td></td>
</tr>
<tr>
<td>ASL: 1x10^-5</td>
<td>ASL: 1x10^-5</td>
<td>ASL: 1x10^-5</td>
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<table>
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<th>Light Source</th>
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<th>Simulation B</th>
<th>Simulation C</th>
</tr>
</thead>
<tbody>
<tr>
<td>5. POLA(°): 45</td>
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<td>POLA: 45</td>
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</tr>
<tr>
<td>AMP#4:1</td>
<td>AMP:1</td>
<td>AMP:1</td>
<td></td>
</tr>
<tr>
<td>θ(°) : 20-70-10</td>
<td>θ: 20-50</td>
<td>θ: 0</td>
<td></td>
</tr>
<tr>
<td>λ(nm) : 200-1400-10</td>
<td>λ: 200-1400</td>
<td>λ: 400-900-10</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Analysis &amp; Script (see Appendix 5.3)</th>
<th>Simulation A</th>
<th>Simulation B</th>
<th>Simulation C</th>
</tr>
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<tr>
<td>6. 1) SW ψ, Δ Extraction</td>
<td>1) BB Source Optimization</td>
<td>Same method as SW ψ, Δ Extraction</td>
<td></td>
</tr>
<tr>
<td>2) BB ψ, Δ Extraction</td>
<td>2) BB ψ, Δ Extraction</td>
<td>further processing using Eq. 5.16 for CD data</td>
<td></td>
</tr>
<tr>
<td>3) BB ψ, Δ Interpolation</td>
<td>3) BB ψ, Δ Interpolation</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 5.1: Parameters for all Simulations

1. **Structure**: 8 Thin Film samples are shown in Table 5.2, each labeled with a number for identification
2. **Boundary**: Refer to Section 1.1.4
3. **Mesh Size**: Mesh size in the z-direction at the interface between 2 materials, spanning a range of 5nm from the interface.
4. **Simulation Time (SIMT)**: Time to terminate the simulation. Section 1.1.8 shows that Fourier Transform is required to obtain the frequency domain data. The accuracy of this frequency domain data is thus related to the completeness of the time domain data. If the simulation terminates too early, there will be errors and if the simulation terminates too late, it will be a waste of resources.
5. **Auto shutoff level (ASL)**: FDTD Solutions terminates the simulation when total power within the simulation region reaches that fraction of power to save simulation time.
6. **Light Source**: Figure 2.1 shows plane wave source incident on the thin film is normal in the y direction, and oblique in the x-direction, with θ representing the angle of incidence. Pulse length, pulse delay and other parameters related to the light source is automatically decided by FDTD solutions.
7. **Polarization Angle (POLA)**: The polarization angle is set to 45° to give an equal E field in the S-plane and P-plane.
8. **E Field Amplitude (AMP)**: The amplitude of the plane wave source can be set to any value as the results will be normalized, in this project it is set to be 1.
9. **Angle of Incidence (θ) & Wavelength (λ)**: For SW, θ and λ are independent of each other. θ is illustrated clearly in Figure 2.1: Overview of Simulation Setup. λ of SW can be set to any value. However, for BB simulations using Bloch Boundary Conditions, θ is a function of frequency instead of independent variables because the in-plane k-vector must be a constant, details refer to Appendix 5.2.
10. Iterations with a change of variable will be written as ‘Start Number-End Number-Intervals’ or ‘Num1, Num2,...’
Table 5.2: Thin Film samples for FDTD simulation used throughout this project

<table>
<thead>
<tr>
<th>5) SiO2_0</th>
<th>6) SiO2_5</th>
<th>7) SiO2_50</th>
<th>8) SiO2_500</th>
</tr>
</thead>
<tbody>
<tr>
<td>Free Space</td>
<td>Free Space</td>
<td>Free Space</td>
<td>Free Space</td>
</tr>
<tr>
<td>Si Substrate</td>
<td>SiO2 5nm</td>
<td>SiO2 50nm</td>
<td>SiO2 500nm</td>
</tr>
</tbody>
</table>

5.2 Broadband Oblique Incidence Setup

\[ k_{in} = k_c \sin \theta_c \]  
\[ k_{in} = k \sin \theta \]  
\[ k_c \sin \theta_c = k \sin \theta \]  
\[ \lambda = \frac{\lambda_c}{\sin \theta_c} \sin \theta \]  

In order to obtain a set of data with constant \( \theta \) and variable \( \lambda \) two procedures were followed. The first calculates a single wavelength (SW) at each AoI and iterated the calculation over \( \lambda \) and
θ sequentially; the second uses a broad band (BB) approximation where a nominal AoI ($\theta_N$) is used but the actual AoI is a function of $\lambda$ and $\theta_N$, then data at the desired $\lambda$ and $\theta$ obtained through interpolation. If the wavelength region of interest is too large, it must also be separated into smaller intervals because $\theta$ will reach 90° at a certain wavelength according to Eq. 5.4. As the simulation in this project spans a wavelength range from 200nm to 1400nm, more than 5 steps are required to cover this range. The density of data points affects the accuracy of interpolation but a set of overly dense data points is not favorable as it will take more time than running SW which has better accuracy. [33]

From Figure 5.4: Data Points Obtained for a Series of Broadband Simulations with Wavelength Steps, in the first wavelength step from 200nm to 400nm, the angle varies significantly compared to other wavelength steps, causing uneven data point distribution, this will reduce the accuracy of interpolation. Since Eq. 5.4 shows the relation of $\theta$ and $\lambda$, optimization can be done to solve this problem.

Firstly, a factor that makes errors in angles constant is defined.

$$\alpha = \left(\frac{f_{\text{max}}}{f_{\text{min}}}\right)^\frac{1}{\lambda}$$  \hspace{1cm} (5.5)
Where \( f_{\text{max}}, f_{\text{min}} \) is the max and min frequency of interest (note that \( \lambda_{\text{min}} = c \times f_{\text{max}} \) and vice versa) and \( n_\lambda \) is the number of wavelength steps. \( \alpha \) allows the separation of the broadband into few uneven spaced wavelength steps which makes errors in angles constant. (See BB Source Optimization Script of Appendix 5.3)

Next, the min and max angle of interest \( \theta_{\text{min}}, \theta_{\text{max}} \) needs to be chosen. From Figure 5.3, \( \theta_{\text{min}}, \theta_{\text{max}} \) is defined as 30 and 40. It can be seen that there are data points that have not been calculated yet (e.g., \( \theta_{\text{max}} \) at \( \lambda_{\text{min}} \)). To have data points equal or larger than \( \theta_{\text{max}} \) near \( \lambda_{\text{min}} \), so that the interpolation can be done, \( \theta_{\text{cmax}} \) has to be calculated using Eq. 5.4 since only the angles at the center wavelength can be controlled.

### 5.3 Data Recording and Analysis

#### 5.3.1 SW \( \psi, \Delta \) Extraction

```plaintext
#folder containing simulation files with wavelength as variable
strfilehead = "E:\Users\yishu\G_Au100Cr5 LNP0_AoI5 SW400-900 M5 ovz1nm_Wavelength"+"\Wavelength_";
#name of the monitor
mn = "fieldMonR";

#total wavelengths
totalsim = 120;
#frequency of choice, ignore this for SW simulations
f=300e+15;
#CREATE ARRAY TO STORE RESULTS FOR ALL WAVELENGTHS
wavelen = linspace(0,0, totalsim);
theta = linspace(0,0, totalsim);
psi = linspace(0,0, totalsim);
delta = linspace(0,0, totalsim);

#LOOP FOR ALL WAVELENGTHS
for(x=1:totalsim){

#LOAD SIMULATION FILE
strfile = strfilehead+num2str(x)+".fsp";
load(strfile);
#SEARCH FOR FREQUENCY SPECIFIED
f_vec=getdata(mn,"f");
fi=find(f_vec,f);
#PROJECT FAR FIELD DATA, FIND POLARIZATION STATE OF 0th ORDER
G_vec = gratingpolar(mn,fi,1,1);  #gratingpolar - Returns E field(with phase) with polarization expressed in spherical coordinates(Radial,Theta,Phi) of far field for all directions(orders), 0th order being the direction which most of the light is scattered towards
```
Gtheta = pinch(G_vec,3,2); #select E field(with phase) of Theta polarization of all orders
Gphi = pinch(G_vec,3,3); #select E field(with phase) of Phi polarization of all orders
Gs=Gphi(0,0); #select E field of 0th order
Gp=Gtheta(0,0); #select E field of 0th order
ux = gratingu1(mn,fi); #get the direction(in unit vectors) of all orders
uy = gratingu2(mn,fi); #get the direction(in unit vectors) of all orders

#CALCULATE PSI & DELTA

#calculate Wavelength from frequency selected
wavelen(x) = 299792458/f_vec(fi) * 1e+9;
#calculate Reflection Angle of 0th order scattered light
theta(x) = acos(sqrt(1-ux(ni)^2-uy(mi)^2))*180/pi;
#calculate Psi from E field(with phase)
psi(x) = atan(abs(Gp)/abs(Gs)) * 180 / pi;
#calculate Delta from E field(with phase)
delta(x) = ((angle(Gs) - angle(Gp)) * 180 / pi)+180;
    #shift all delta to the range of 0 < delta < 360
    if(delta(x) > 360){
        delta(x) = delta(x) - (360 * floor(delta(x)/360));
    }elseif(delta(x) < 0){
        delta(x) = delta(x) - (360 * (floor(delta(x)/360) - 1));
    }
}

#END OF LOOP FOR ALL WAVELENGTHS

#OUTPUT TO MATLAB FILE
matlabsave(“F_Data”,wavelen,theta,psi,delta);

5.3.2 BB Source Optimization

#DEFINED PARAMETERS
start_wavelength = 200e-9;
stop_wavelength = 1400e-9;
N_wavelength = 10;
theta_max = 50;
theta_min = 20;
N_angle = 10;

#AUTOMATICALLY ITERATED PARAMETERS
#i_wavelength
#i_angle

    # ensure that the angle error is the same for each section of the frequency
    fmax = c/start_wavelength;
    fmin = c/stop_wavelength;
    alpha = (fmax/fmin)^((1/N_wavelength);

    #separate the whole wavelength band into N_wavelength steps, saving values into f
    f = matrix(N_wavelength+1);
    f(1) = fmin;
    for(i=2:(N_wavelength+1)) {
f(i) = f(i-1)*alpha;

# find the min and max angle needed at the center frequency to cover the min
# and max angle of interest
# only the 1st wavelength step is used to estimate the max and min angle
# needed at the center freq because the variation in max and min angle is
# larger at smaller wavelengths as the wavelength changes
fc = 0.5*(f(1)+f(2));          # center freq of 1st wavelength step
df = f(2)-f(1);               # range of 1st wavelength step
min_factor = fc/(fc+df/2);     # factor to calc the max angle at the center
max_factor = fc/(fc-df/2);     # factor to calc the min angle at the center

true_theta_min = asin(sin(theta_min*pi/180) / max_factor) * 180/pi; # calc
the max angle at center freq
true_theta_max = asin(sin(theta_max*pi/180) / min_factor) * 180/pi; # calc
the min angle at center freq
theta = linspace(true_theta_min, true_theta_max, N_angle);

# set the wavelengths based on the target interval
selectall;
set("frequency start", f(i_wavelength));
set("frequency stop", f(i_wavelength+1));
set("angle theta", theta(i_angle));

# report for the user
?"Summary of settings"
?" The wavelength range is " + num2str(c/fmax*1e9) + "nm to " +
+ num2str(c/fmin*1e9) + "nm";
?" This range will be covered in " + num2str(N_wavelength) + " steps of
+ unequal spacing";
?" The angles will vary from " + num2str(min(theta)) + " to " +
+ num2str(max(theta)) + " degrees in " + num2str(N_angle) + " steps";
?" in order to cover the desired wavelength range at all frequencies";

5.3.3 BB ψ, Δ Extraction

f_vector = getdata(mn,"f");
delta = matrix(length(f_vector));
psi = matrix(length(f_vector));
theta_vector = matrix(length(f_vector));
for(fi=1:length(f_vector)){
    # test if light can propagate at this wavelength, will be a future script
    command
    Ux = meshgridx(gratingul(mn,fi,10,1)*10,gratingul(mn,fi,10,1)*10);
    Uy = meshgridy(gratingu2(mn,fi,10,1)*10,gratingu2(mn,fi,10,1)*10);
    if(min(Ux^2 + Uy^2) < 1) {
        G_vec = gratingpolar(mn,fi,1,1);
        n = gratingn(mn,fi);
        m = gratingm(mn,fi);
ux= gratingu1(mn,fi);
uy= gratingu2(mn,fi);
Gtheta = pinch(G_vec,3,2);
Gphi = pinch(G_vec,3,3);
G=abs(Gtheta)^2+abs(Gphi)^2;  # grating order strength

# find index of selected grating order
ni = find(n,0);
mi = find(m,0);

# convert spherical coordinates polarization into S,P polarization and select grating order
Gs=Gphi(ni,mi);
Gp=Gtheta(ni,mi);

delta(fi) = (angle(Gs) - angle(Gp)) * 180 / pi;
psi(fi) = atan(abs(Gp)/abs(Gs)) * 180 / pi;
theta_vector(fi) = acos(sqrt(1-ux(ni)^2-uy(mi)^2))*180/pi;
else {
    theta_vector(fi) = 90;
}

5.3.4 BB ψ, Δ Interpolation

##COLLECT DATA FROM the 3D SWEEP (ANGLE x FREQUENCY x WAVELENGTH STEPS) FOR INTERPOLATION
sweepname = sweepname;
?"Data in sweep object is: ";
?getsweepdata(sweepname) + endl;
# get data and remove extra singleton dimension that was inserted during the sweep data collection
f_matrix = pinch( getsweepdata(sweepname,"f_matrix") ,2);
theta_matrix = pinch( getsweepdata(sweepname,"theta_matrix"),2);
psi_matrix = pinch( getsweepdata(sweepname,"psi_matrix") ,2);
delta_matrix = pinch( getsweepdata(sweepname,"delta_matrix"),2);
# save original data
savedata("broadband_results.ldf",f_matrix,theta_matrix,psi_matrix,delta_matrix);
matlabsave("broadband_results",
    f_matrix,theta_matrix,psi_matrix,delta_matrix);

##INTERPOLATE PSI AND DELTA VALUES FOR DESIRED AoI
n = size(theta_matrix);
?" Size of results corresponds to frequency X angle X wavelength steps and is ";
?n;
#choose the desired AoI to interpolate onto
theta = 20:10:50;
#declare 2D arrays to hold the interpolated data
f = matrix(n(1)*n(3));
psi = matrix(length(f),length(theta));
delta = matrix(length(f),length(theta));
# LOOP THROUGH (FREQUENCY x WAVELENGTH STEPS)
for (i=1:n(1)) {
    for (j=1:n(3)) {
        # select psi and delta at all AoI available
        theta_orig = pinch(theta_matrix(i,1:n(2),j));
        psi_orig = pinch(psi_matrix(i,1:n(2),j));
        delta_orig = pinch(delta_matrix(i,1:n(2),j));
        # exclude any angles above 80 degrees as they are likely to be inaccurate
        psi_orig = psi_orig(find(theta_orig <= 80));
        delta_orig = delta_orig(find(theta_orig <= 80));
        theta_orig = theta_orig(find(theta_orig <= 80));
        # shift discontinuied data back to 0 < x < 360 range
        psi_orig = 180/pi * unwrap(psi_orig * pi/180);
        delta_orig = 180/pi * unwrap(delta_orig * pi/180);
        fp = I + n(i)*(j-1);  # the index to store interpolated results at
        f(fp) = f_matrix(i,1,j);  # copy the frequency
        # Interpolate psi and delta to the desired AoI
        psi(fp,1:length(theta)) = interp(psi_orig,theta_orig,theta);
        delta(fp,1:length(theta)) = interp(delta_orig,theta_orig,theta);
    }
}  # END OF LOOP

### FINAL ADJUSTMENTS
# shift discontinuied data back to 0 < x < 360 range
psi = 180/pi * unwrap(psi * pi/180);
delta = 180/pi * unwrap(delta * pi/180) + 180;  # shift 180 deg to match ellipsometry model
# change frequency to lambda
lambda = c//f;

### SAVE AND PLOT
matlabsave("F_Data", lambda, psi, delta);
plot(lambda*1e9,psi,"lambda","psi");
legend("20","30","40","50");
plot(lambda*1e9,delta,"lambda","delta");
legend("20","30","40","50");

5.4 The Polarization Ellipse

A beam of light in free space or dielectric consists of a large number of pulses, if all the pulses have the same frequency (coherent), is propagating in the same direction, and has its E field orientated only in one direction then it can be represented by a sine wave. To simplify things, assume that the direction of propagation is the positive z-direction and the E field is orientated in the x or y direction, we can then have the following equations [34],

\[
E_x(z,t) = E_x \cos(\omega t - k_z z + \delta_x) \quad 5.6
\]

\[
E_y(z,t) = E_y \cos(\omega t - k_z z + \delta_y) \quad 5.7
\]
If we stack these 2 beams \( E_x(z, t) \) and \( E_y(z, t) \) using the superposition principle we could see that at any point in space, there is an E field that changes in time, by plotting this E field at a single point in space in Ex and Ey coordinates, after \( \omega t = 2\pi \) amount of time there is a definite trajectory that describes this E field. Now we try and derive the curve generated by the E field. The objective is to relate Ex and Ey in an equation and observe how the amplitude changes in a certain point in space. First, to simplify things a little, we let,

\[
\tau = \omega t - k_z z \tag{5.8}
\]

Substituting Eq. 5.8 into Eq. 5.6 and 5.7, then move the amplitude term to the left,

\[
\frac{E_x}{E_{0x}} = \cos \tau \cos \delta_x - \sin \tau \sin \delta_x \tag{5.9}
\]

\[
\frac{E_y}{E_{0y}} = \cos \tau \cos \delta_y - \sin \tau \sin \delta_y \tag{5.10}
\]

By multiplying Eq. 5.10 by \( \sin \delta_x \) and Eq. 5.9 by \( \sin \delta_y \), and then squaring both equations and add them together gives,

\[
\frac{E_x^2}{E_{0x}^2} + \frac{E_y^2}{E_{0y}^2} - 2\frac{E_x}{E_{0x}} \frac{E_y}{E_{0y}} \cos \delta = \sin \delta \tag{5.11}
\]

Where,

\[
\delta = \delta_y - \delta_x \tag{5.12}
\]

Eq. 5.11 shows how the relationship between \( E_x \) and \( E_y \) changes at a particular point in space as light propagates through space, with \( E_{0x}, E_{0y} \) and \( \delta \) as input parameters. If we try and draw Eq. 5.11, it will look like an ellipse (see Figure 5.9). It can be shown that the polarization ellipse is unique for different polarization states of light. Examining the ellipse in Figure 5.9, there are 2
important parameters that define this ellipse, the major axis angle $V_{xy}$, and the ratio between the major and minor axis $\gamma$.

**Specialized Forms of the Polarization Ellipse** [35]

<table>
<thead>
<tr>
<th>Amplitude</th>
<th>Phase Difference $\delta$</th>
<th>Plot</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Linearly Polarized Light</strong></td>
<td>$E_{0x} = 0$ OR $E_{0y} = 0$</td>
<td>$0, \pi$</td>
</tr>
<tr>
<td>$E_{0x} = E_{0y}$</td>
<td>$0, \pi$</td>
<td>Same as for the case of $E_{0x} = 0$ OR $E_{0y} = 0$, the only difference is the E field is orientated $45^\circ$ with respect to both x and y axis.</td>
</tr>
<tr>
<td><strong>Left Circularly Polarized Light</strong></td>
<td>$E_{0x} = E_{0y}$</td>
<td>$\frac{\pi}{2}, \frac{3\pi}{2}$</td>
</tr>
<tr>
<td><strong>Right Circularly Polarized Light</strong></td>
<td>$E_{0x} = E_{0y}$</td>
<td>$\frac{\pi}{2}, \frac{3\pi}{2}$</td>
</tr>
</tbody>
</table>

*Table 5.3: Specialized Forms of the Polarization Ellipse*
5.5 Molar Ellipticity

Circular Dichroism is mostly reported in molar ellipticity ($\theta$). Molar ellipticity is given by,

\[
\theta \text{ (degrees)} = \Delta A \left( \frac{\ln 10}{4} \right) \left( \frac{180}{\pi} \right)
\]

Eq. 5.13 is an approximation of $\theta$ which can be derived by first defining ellipticity of polarization [29], $\theta$ of Eq. 5.13 is illustrated in Figure 5.8: Combining left-CPL light and right-CPL light to form a polarization ellipse

\[
\tan \theta = \frac{E_R - E_L}{E_R + E_L}
\]

It seems like $\theta$ from Eq. 5.15 as a function of E field amplitude is not directly measurable, but by using $\psi$ and $\Delta$ from ellipsometry measurements, $\theta$ can be calculated using Eq. 5.16 [38]

\[
\theta = \frac{1}{2} \tan^{-1} \left( \frac{\sin 2\psi_{xy} \sin \Delta_{xy}}{\sqrt{1 - \sin^2 2\psi_{xy} \sin^2 \Delta_{xy}}} \right), \quad \theta \in \left[ -\frac{\pi}{4}, \frac{\pi}{4} \right]
\]

In this project, $\theta$ is calculated using Eq. 5.16.
5.6 Mean Square Error

The MSE used throughout this project is defined as the following,

\[
MSE = \sqrt{\frac{\sum_{n=1}^{N} (|\psi_{Tn} - \psi_{Sn}|^2 + |\Delta_{Tn} - \Delta_{Sn}|^2)}{4N}}
\]

5.17

Where \(\psi_{Tn}, \Delta_{Tn}\) is psi calculated from theory, \(\psi_{Sn}, \Delta_{Sn}\) is the FDTD simulated data and \(N\) being the number of wavelength data points. The usual definition of MSE used in the field of ellipsometry is

\[
MSE = \sqrt{\frac{\sum_{n=1}^{N} (|\psi_{Tn} - \psi_{Sn}|^2 + |\Delta_{Tn} - \Delta_{Sn}|^2)}{2N}}
\]

5.18
6 References
