Doctoral Thesis

Analysis and design of metamaterials

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Analysis and Design of Metamaterials

A dissertation submitted to the
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Doctor of Sciences

presented by
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2010
Abstract

Metamaterials can be engineered to provide new and useful electromagnetic devices. These range from extremely practical antireflective coatings to state of the art superlenses and cloaks. Their special properties often arise from resonances or crystal effects like electromagnetic bandgaps. It is exactly because of these behaviors that metamaterials are not simple to analyze or design. The utility of metamaterials for scientific and industrial applications warrants a description of the tools and numerical techniques available to deconstruct their functionality and synthesize or optimize new designs.

Two powerful tools are suitable for these purposes. Band diagrams can be used for infinitely periodic structures, and scattering spectra for semiperiodic ones. We demonstrate the generation of reliable finite-difference time-domain generated (FDTD) band diagrams using a systematic brute-force algorithm that generates node maps and performance statistics for photonic crystals and their band diagram simulations, respectively. From these we are able to draw conclusions about the placement of sensors and detectors for the optimal detection of harmonic modes.

We also need scattering spectra to study the reflection and transmission of metamaterial scatterers. FDTD is useful for generating these spectra for one, two, and three dimensional scatterers. As we demonstrate, this also works well for obliquely incident polarized fields, resulting in broadband, broad angle scattering surface plots.

Even with these tools, it is still necessary to reduce very large problems using effective media approximations. We provide a numerical procedure for evaluating and visualizing the accuracy of mixing formulas for these computations. For photonic crystal systems, we show how to increase the approximation accuracy for intermediate wavelengths on the order of a lattice constant.

We finally apply these tools to several practical design examples. We optimize a nanorod thin-film coating for low reflection optics, multiplying the previously published attainable bandwidth by a factor of three. The internal roughness morphology of a thin-film silicon solar cell is also investigated. Using simulations, we are able to draw conclusions about the fabrication process matching industrial expert-knowledge on the relationship between zinc oxide deposition and cell absorption. Another high-performance antireflective coating is analyzed for a three dimensional infrared application, where we compare the performance of FDTD to other methods. We also design an electromagnetic bandgap radiation seal for microwave ovens in a demonstration of all of the techniques necessary for the numerical analysis and design of metamaterials. This seal performs on-par with with conventional quarter-wave choke seals while providing several manufacturing advantages.
Zusammenfassung


Bei größeren Problemen reichen diese Werkzeuge manchmal nicht. In solche Fälle benutzen wir effektive Medien, um die Problemgröße zu verkleinern. Wir geben ein Prozedur an, um die Genauigkeit dieser Approximationen zu evaluieren und zu visualisieren. Für photonische Kristallsysteme zeigen wir wie die Genauigkeit mit Hilfe angepasster Grenzbedingungen gesteigert werden kann.

Many individuals helped me accomplish the work presented in this dissertation. I must first express my thanks to Rüdiger Vahldieck, who had the vision for a good initial project, and the encouragement for me to continue when it proved successful.

Christian Hafner, who supervised most of my work, provided me with invaluable advice. Not once was he too busy for an unscheduled question. I learned a lot from him, both on scientific level and a personal one. He was able to provide us with insight when we needed it, while at the same time allowing us the liberty to steer our own ships. I hope to be able to replicate that someday.

Daniel Erni helped me when I started at IFH and was learning about photonics, in the middle of my work when we published a paper with his valuable input, and at the end with valuable comments that greatly improved another paper and this dissertation. He is extremely knowledgeable and ready to help.

I am endlessly grateful to Steven Johnson’s group for generously providing the MEEP and MPB codes, and the members of their mailing lists for many hints and tips. It was truly a one-way benefit, in my favor. I hope to contribute back, now that I have more experience and time.

BSH funded our EBG radiation seal project, which provided me with a chance to work with Martin Thaler and his colleagues. My work on the project was supervised by Martin Gimersky, from whom I learned many things. He also helped make our patent application a successful one.

During the 2006 Christmas holidays, when everyone else was at home with their families, Glen Stark and I were in our offices hacking at bandgap diagram statistics code, running simulations, analyzing results, and trying to make a January paper deadline. It took a while, but all the hard work and stress eventually paid off.

Martin Lanz, Claudio Maccio, and Stephen Wheeler helped to fabricate EBG proof of concept prototype. That was no small job, and I believe it was only successful because of their meticulous precision. Hansruedi Benedickter helped us make measurements on that device, as well as for several projects for students I helped supervise. The workshop was my ‘office away from office,’ a place where I could enjoy a hot drink, post-lunch dessert, and the occasional calm and collected discussion about Swiss politics.

Many of my results, in particular those presented here on boundary conditions, came from working together with Leonid Braginsky, a physicist, and Valery Shklover, a materials scientist. I believe this was a really useful experience for me from an interdisciplinary collaboration standpoint. They were always encouraging, and always amiable.
I was lucky to benefit from Christian Engström’s experience with mixed media when he joined the IFH. His thoughts (and his dissertation) were a huge aid to me when I was investigating the topic. I also enjoyed chatting with him over lunch and coffee.

My awesome office mate, Arya Fallahi, helped me with many questions over the years. He has an impressive grasp of fundamentals and a patient and organized approach that I can only try to mimic. I will miss our regular “shay” breaks, as well the Persian sweets that he brought us.

For the infrared antireflective coatings, I compared my results with several colleagues, including Arya, Samuel Nosal, Patrick Leidenberger, and Sven Burger, all great collaborators. Patrick is also a great gourmand, and even knows a thing or two about carburetor repair.

Several others helped me remember that having a good time is an important part of grad school. I especially want to thank Claudio, Jean-George, Damir, the IFE crew (George, Lucio, David and Silvan), and Sib and Roger. I hope to keep in touch with all of you, even if I refuse to sign up for a Facebook account to prove it.

Finally I want to thank Martina and her family for being supportive and loving. I look forward to returning home to spend time with my own family before heading off for the next thing. That includes lots of cooking (and eating), catching up to Josh on the new piano, and prompting Mom and Dad to ask Mina about a baby girl.
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<th>Description</th>
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<tr>
<td>aSi</td>
<td>amorphous silicon</td>
</tr>
<tr>
<td>BCC</td>
<td>body-centered cubic</td>
</tr>
<tr>
<td>CAD</td>
<td>computer-aided design</td>
</tr>
<tr>
<td>DFT</td>
<td>discrete Fourier transform</td>
</tr>
<tr>
<td>EBG</td>
<td>electromagnetic bandgap</td>
</tr>
<tr>
<td>EFA</td>
<td>envelope function approximation</td>
</tr>
<tr>
<td>FCC</td>
<td>face-centered cubic</td>
</tr>
<tr>
<td>FDTD</td>
<td>finite-difference time-domain</td>
</tr>
<tr>
<td>FEM</td>
<td>finite element method</td>
</tr>
<tr>
<td>FE</td>
<td>finite element</td>
</tr>
<tr>
<td>FFT</td>
<td>fast Fourier transform</td>
</tr>
<tr>
<td>FSS</td>
<td>frequency selective surface</td>
</tr>
<tr>
<td>GMT</td>
<td>generalized multipole technique</td>
</tr>
<tr>
<td>HIS</td>
<td>high-impedance surface</td>
</tr>
<tr>
<td>hp-FEM</td>
<td>h- and p-refinement finite element method</td>
</tr>
<tr>
<td>IBZ</td>
<td>irreducible Brillouin zone</td>
</tr>
<tr>
<td>MBC</td>
<td>Maxwellian boundary condition</td>
</tr>
<tr>
<td>MBPE</td>
<td>model-based parameter estimation</td>
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<tr>
<td>mcSi</td>
<td>microcrystalline silicon</td>
</tr>
<tr>
<td>MEEP</td>
<td>MIT Electromagnetic Equation Propagation</td>
</tr>
<tr>
<td>MG</td>
<td>Maxwell-Garnett</td>
</tr>
<tr>
<td>MMP</td>
<td>multiple multipole program</td>
</tr>
<tr>
<td>MPB</td>
<td>MIT photonic bands</td>
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<table>
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<th>Acronym</th>
<th>Definition</th>
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<tr>
<td>MTL</td>
<td>multiconductor transmission line</td>
</tr>
<tr>
<td>NTFF</td>
<td>near-field to far-field</td>
</tr>
<tr>
<td>PCB</td>
<td>printed circuit board</td>
</tr>
<tr>
<td>PEC</td>
<td>perfect electric conductor</td>
</tr>
<tr>
<td>PMC</td>
<td>perfect magnetic conductor</td>
</tr>
<tr>
<td>PML</td>
<td>perfectly matched layer</td>
</tr>
<tr>
<td>PhC</td>
<td>photonic crystal</td>
</tr>
<tr>
<td>QE</td>
<td>quantum efficiency</td>
</tr>
<tr>
<td>QWC</td>
<td>quarter-wave choke</td>
</tr>
<tr>
<td>RCWA</td>
<td>rigorous coupled wave analysis</td>
</tr>
<tr>
<td>SEM</td>
<td>scanning electron microscope</td>
</tr>
<tr>
<td>SES</td>
<td>simple evolutionary strategy</td>
</tr>
<tr>
<td>SRR</td>
<td>split-ring resonator</td>
</tr>
<tr>
<td>SiO₂</td>
<td>silicon dioxide</td>
</tr>
<tr>
<td>TBC</td>
<td>thermal barrier coating</td>
</tr>
<tr>
<td>TEM</td>
<td>transverse electromagnetic</td>
</tr>
<tr>
<td>TE</td>
<td>transverse electric</td>
</tr>
<tr>
<td>TFSF</td>
<td>total-field scattered-field</td>
</tr>
<tr>
<td>TLM</td>
<td>transmission line matrix</td>
</tr>
<tr>
<td>TM</td>
<td>transverse magnetic</td>
</tr>
<tr>
<td>TiO₂</td>
<td>titanium dioxide</td>
</tr>
<tr>
<td>ZnO</td>
<td>zinc oxide</td>
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1.1 Metamaterials: usage and definition

The term ‘metamaterial’ has become a buzzword in electromagnetics over the past decade. Partially due to its vague meaning, it has been used in a wide range of publications, with some applications less appropriate than others.

Sihvola discusses the word extensively and explains his reasoning for rejecting certain definitions [1, 2]. Specifically, he rejects the requirements that metamaterials exhibit properties not observed in the constituent materials, and that these properties are not observed in nature. These requirements are inherently subjective.

He goes on to discuss scale-based definitions. The mineral salt, when observed closely enough, is composed of sodium and chloride ions. Its electromagnetic properties are certainly different than those of its constituents. Their atomic scale is not a suitable criterion for labeling the compound as a normal material, because that choice is arbitrary. If we then try to exclude salt based on a ‘naturalness’ definition, do we then also exclude the widely cited examples of opal and the morpho butterfly wing?

We do not try to give a definition of metamaterials, but instead apply the term loosely to include materials that have been artificially engineered to provide some desirable electromagnetic properties. Their features can arise from their physical structure, as is the case for Yablonovite [3], a photonic crystal that exhibits a complete, three dimensional bandgap. Their properties may arise from circuit-like resonant behaviors (such as splitting resonators (SRRs) or Sievenpiper structures), or plasmonic resonances (including the well-known stained glass effect [4] created by nanospheres).

In conferences and journals on the topic, the term is used in more narrow contexts. Often times it is used synonymously with left-handed or negative-index materials (covered thoroughly in [5, 6]). These have generated much interest because of their potential for application such as superlensing.

In other instances the definition is stretched in a very general manner. Some microstrip publications [7, 8] refer to filters as ‘metamaterial-inspired’ because they incorporate SRRs like the ones used in Veselago-type materials [9, 10].

We apply the term metamaterial to electromagnetically engineered one, two and three dimensional structures. These are usually periodic structures because that simplifies the
1 Introduction

engineering process, but some irregular structures such as thermal barrier coatings (TBCs) may also be considered to be metamaterials. While some of these structures exhibit left-handedness for certain frequencies (e.g., the Sievenpiper structures of Chapter 5), we do not analyze these properties in any detail. The techniques shown here however can and have been used to focus on these aspects [5, 11].

1.2 FDTD: A general-purpose electromagnetic field solver

The finite-difference time-domain (FDTD) algorithm is a well-studied general-purpose electromagnetic field solver. Several books are available on the method, including the most famous one by Taflove and Hagness [12], but also many others [13–16]. Each year there is a large number of new publications on the method itself, with thousands more on results that come from FDTD codes.

Because it is a simple discretization in time and space of Maxwell’s equations, it can be used as a brute-force field solver. Like most numerical methods however, FDTD is not optimal for solving all problems. Other methods, such as the semi-analytic generalized multipole technique (GMT) are able to generate results with much higher accuracy in a fraction of the time for certain problems [17].

Most methods slow for large problem sizes. For these problems it is beneficial to use parallelization. FDTD allows for easy parallelization by means of domain decomposition. Sections of a problem are divvied up among several processors to handily divide and conquer the computation domain.

FDTD does present some disadvantages. Because it usually operates on a rectilinear grid, curved boundaries become ‘staircased’ when discretized. This leads to inaccuracies, especially in some plasmonic problems where sharp corners engender large field singularities. For dielectric problems, this can be mitigated by using pixel smoothing techniques [18, 19]. Some work has been done to show that smoothing is also possible for plasmonic problems, but so far only for flat interfaces [20].

Additionally, the entire domain must be discretized. This is not the case for boundary methods [21, 22]. If the FDTD code does not have a subgridding or irregular gridding feature, this means that areas of the computation domain will be over-discretized. This is especially the case with certain metamaterials, such as resonant electromagnetic bandgap (EBG) structures, where critical geometric features are finer than the normal wavelength discretizations.

The standard FDTD algorithm uses second order differences to compute field updates. This limits the error convergence in a way that disadvantages FDTD with respect to other methods, such as the finite element method (FEM) which can allow for mesh (h) and order (p) refinement (hp-FEM). This is not to say that higher order finite differences cannot be used. There are implementations of higher-order difference algorithms such as in [23], but this is
far from standard. This is because higher-order differences are more difficult to implement, and require much more memory since field values must be kept track of over multiple time steps. These time steps are for stability reasons necessarily shorter (by a factor of $6/7$ for fourth-order FDTD), but the accuracy benefits allow for the solving of electrically larger problems [12].

As a time-domain method, FDTD is useful for studying the time evolution of fields. With the fast Fourier transform (FFT), we can aggregate high frequency-resolution spectra with a single simulation. It can also be used for narrowband simulations, but using FDTD as a frequency domain sampler is unideal; in this case it would be better to simply use a true frequency domain method. Other solver concepts are also more naturally represented in the frequency domain, such as the representation of dispersive media, and periodic boundary conditions. That does not mean that time domain codes cannot handle these features, but it does mean their implementation is more complex.

Despite these significant drawbacks, FDTD presents a useful approach for studying a wide range of metamaterial problems because of its parallelizability, its ability to handle difficult and non-linear materials, and support for features like Bloch periodicity (vital for metamaterials), and two-, and three-dimensional simulation domains.

For our work we use an open-source FDTD code named MIT Electromagnetic Equation Propagation (MEEP) that allows us to take advantage of parallelization and subpixel averaging, as well as the harminv program for harmonic mode detection [24, 25]. This code is available as C++ libraries, but also comes with a handy Scheme-like programming interface that allows simple scripts to control the simulation and the output of results.

1.3 Goal, scope, and overview of the dissertation

Numerical approaches are vital for the design and analysis of metamaterials. This dissertation aims to demonstrate that thesis.

Despite several books available on FDTD, and several on the topic of metamaterials, and even a recent book titled ‘FDTD modeling of metamaterials: theory and applications’ [5], a large number of details remain undiscussed. We address a few of the important ones in the following chapters.

While FDTD is a key element to this work, we also discuss a few other methods. Specifically, because FDTD is too cumbersome for some optimizations where thousands of simulations must be run, we address the topic of model reduction by use of effective media for metamaterial design. We also look at analytic alternatives or other models where suitable. Finally results from other codes such as the MIT photonic bands (MPB) program allow us to check the performance of FDTD against a high-accuracy reference.

We present these results by using numerous examples with practical applications. These
1 Introduction

include optical and infrared antireflective coatings, thin-film solar cell design, and EBG microwave shielding.

The basic FDTD approach used in several sections is developed in Chapter 2. Here we look at the use of FDTD to generate reliable band diagrams. Specifically we develop a system that rigorously analyzes how and why modes are sometimes missed when generating band diagrams. Next we outline the generation of broadband, broad-angle scattering spectra plots for two- and three-dimensional grating structures using FDTD.

Chapter 3 focuses on the validity of mixed media approximations that are often useful when designing metamaterials. We present a method for checking the validity of mixed media formulas against results that come from numerical simulations. We go on to show how boundary conditions can be adjusted in photonic crystal models to provide more accurate results at shorter wavelengths, where mixing formulas otherwise lose validity.

Multiple examples of optical and infrared thin-films in Chapter 4 take advantage of the FDTD approach of Chapter 2. The first example is of a nanorod thin-film coating optimization using an evolutionary strategy. The second example is an iterative design of a solar energy cell with real, lossy materials. We finally show a three-dimensional coating for infrared applications.

On the lower end of the frequency spectrum, Chapter 5 presents the design, fabrication and measurement of microwave EBG radiation seals. This important example helps emphasize the utility of numerical approaches. It also highlights the importance of metamaterials for industrial applications, but also the difficulties in understanding and analyzing their behavior.

We finally summarize our findings and give directions for future work in Chapter 6.
Chapter 2

Band diagram and scattering spectra computation using FDTD

The most powerful metamaterial design tools available to us are 1) band diagrams (or dispersion diagrams), for infinite photonic crystal structures, and 2) power reflection, transmission, and absorption spectra, for finite ones.

Band diagrams are useful for determining the position and size of photonic bandgaps. Gap maps which aggregate gap information from several band diagrams also help in the design process. Band diagrams also allow us to characterize so called ‘slow wave’ regions close to band edges. They provide particular ways to manipulate and slow down light, and their application is discussed in [26] and [27].

For finite metamaterials, we can no longer refer to a bandgap, but instead identify a stop band. In the limit, as the number of periods increases towards infinity, the stop band will approach the bandgap in position and attenuation.

There are several computational methods that are able to compute band diagrams or scattering spectra. In this chapter we present how to compute them using the FDTD method. In particular, we highlight the reliable detection of photonic crystal modes, and the computation of broadband, broad-angle power spectra for gratings.

2.1 Reliable band diagram computation using FDTD

Photonic crystals (PhCs) can be used to control the flow of light. Devices such as photonic crystal (PhC) waveguides can be created by introducing defects into photonic crystals. These devices can be used in a wide range of applications, such as integrated optics [27, 28], lasing [29], and all-optical switching [30].

When designing a PhC device such as a PhC waveguide bend, we may want to minimize return loss or maximize the bandgap. In these situations, an optimization algorithm such as downhill-simplex or evolutionary strategy can be taken advantage of. The robustness, computational cost, and accuracy of simulation techniques become critical when applying these types of optimizers. A false mode (the erroneous detection of a non-existent mode), or missed mode (an existing mode that fails to be detected) will cause optimization algorithms to fail.
The FDTD algorithm is one simulation tool that is useful for PhC design. It supports broad-band simulations, metallic and absorbing boundary conditions, dispersive, non-linear, and inhomogeneous materials with complicated geometries. Traditional approaches for computing band spectra such as the planewave expansion method solve an eigenvalue problem requiring the diagonalization of a Hermitian matrix and therefore $O(N^3)$ operations. FDTD however scales linearly with the number of grid points in the Yee lattice, making it a computationally more efficient method for larger problems like crystals with defects or unideal nonperiodic disorder (see the discussion in [31]). While the FDTD approach is very flexible, experience is required to obtain the robust and accurate results necessary for the automatic evaluation of bandgap properties.

To analyze the difficulties of band diagram generation when using FDTD, we focus on a canonical PhC consisting of a square lattice of dielectric rods in air. Specifically, we look at rods with permittivity $\varepsilon = 8.9$, and radius to lattice constant ratio $r/a = 0.2$. This crystal has a well understood bandgap, is simple to simulate with multiple tools, and can be used as an example to demonstrate the approach for more complex crystals. FDTD is by no means the optimal tool for this simple problem, but it is a useful tool for more difficult ones. We describe a similar approach for triangular lattices in [32].

### 2.1.1 Mode detection algorithm and simulation settings

To compute a band diagram with FDTD, we use the ‘Order-N’ method listed in Algorithm 2.1. It was first proposed in [31] as an alternative to the planewave expansion method with improved scalability with respect to the number of grid cells.

**Algorithm 2.1 FDTD band diagram generation**

Create a computation domain consisting of a single unit-cell

for all wavevectors $k$ in the band diagram (along IBZ edges) do

Apply Bloch boundary conditions $F(r + L) = e^{jkL}F(r)$, where $F$ is a complex field quantity $E$ or $H$

Excite the computation domain

Measure a field component for some time $T$

Determine harmonic mode frequencies from the recorded data

end for

Algorithm 2.1 masks implementation subtleties that can greatly impact the performance of the algorithm. Insufficient resolution, measurement time $T$, or failure to excite a mode of interest will all give poor results. Errors due to grid resolution are common, and techniques for mitigating are discussed in [18, 19, 33]. For our simulations, we apply a combination of these techniques to get the best results when possible, and to ensure that elements such as resolution or measurement time are not limiting agents in our simulations. Specifically, we use subpixel smoothing (also called anisotropic averaging), and perform convergence analyses over simulation run time and grid resolution.
To analyze the effect of the source and detector positions, we rely on Algorithm 2.2 to compare the FDTD generated band diagrams to high-accuracy reference results generated by the MPB program. Here, \( \text{TEST}_k = t_1 \ldots t_N \) is the set of test frequencies found for a given \( k \)-vector using FDTD. \( \text{REF}_k = r_1 \ldots r_M \) is the set of reference modes found by MPB. \( u_{\text{min}} \) and \( u_{\text{max}} \) define the range of angular frequencies over which results are considered. \text{matched_modes} \text{ and } \text{missed_modes} \text{ are counters for a single } k \text{-vector that are aggregated after all } k \text{-vectors are analyzed. Finally, } err_{\text{avg}} \text{ and } err_{\text{max}} \text{ show how well found modes match up with reference ones.}

\begin{algorithm}
\textbf{Algorithm 2.2} Computing missed modes and errors for a given wavevector \( k \)
\begin{verbatim}
matched_modes = 0
for \( r_i \in \text{REF}_k \) do
    if \( u_{\text{min}} \leq r_i \leq u_{\text{max}} \) then
        find the nearest test mode \( t_j \in \text{TEST}_k \)
        if \( |r_i - t_j| > \text{Threshold} \) then
            increment \text{missed_modes}
            remove \( r_i \) from \( \text{REF}_k \)
        else
            increment \text{matched_modes}
            compute \( err_m \)
            remove \( r_i \) from \( \text{REF}_k \)
            remove \( t_j \) from \( \text{TEST}_k \)
        end if
    end if
end for
\( err_{\text{avg}} = \langle err_m \rangle \)
\( err_{\text{max}} = \max(\text{err}_m) \)
\end{verbatim}
\end{algorithm}

Using Algorithm 2.2, we first perform a series of initial tests to check which FDTD settings will be ideal for running a large set of simulations. Figure 2.1 shows the error convergence as the FDTD resolution is increased from 40 to 200 grid cells per lattice width. The use of subpixel smoothing makes a large difference in the error convergence. By smoothing the staircased boundary between materials, it smoothes out large fluctuations in the error convergence caused by staircasing effects. This smoothness simplifies the determination of whether resolution convergence has been satisfactorily met. Second, it makes the simulation statistically more accurate for a given resolution, especially for coarser meshes.

Because these FDTD simulations work by obtaining harmonic information from a set of time data, it is also necessary to acquire a sufficient amount of steady-state data to accurately state the angular frequency of a given mode. One approach is to take the Fourier transform and identify resonant peaks, but a better alternative (especially for highly harmonic periodic or resonant systems) is to use the harmonic inversion method (also known as filter-diagonalization) \[34]\.

Figure 2.2 demonstrates the dramatic speedup that is possible by avoiding the discrete
Figure 2.1: Error convergence for matched modes as a function of grid resolution. FDTD simulations are compared to a reference band diagram computed by planewave expansion. Simulations are run with and without subpixel smoothing.

Fourier transform (DFT), which is limited by the uncertainty principle. This defines an inverse relationship between the frequency resolution and the time duration (and sample rate) of a signal. Harmonic inversion benefits from the assumption that the time signal is composed of only harmonic modes \[34, 35\]. The disadvantage is that it is less suitable for determining the spectral characteristics of broadband, non-harmonic signals.

This benefit is also evident in the simulation’s ability to reliably detect modes. Figure 2.3 shows the number of unmatched reference points (missed/undetected modes) as the measurement time increases. Again, harmonic inversion mode detection drastically outperforms conventional DFT. That the number of unmatched modes in this plot converges to a non-zero value is a trivial artifact of the comparison. The remaining five unmatched modes correspond to two uncounted zero-frequency points and three degenerate points at band crossovers.

2.1.2 Effect of source and sensor position

A sensor placed at every point of the Yee-grid would ensure the success of detecting all modes in the band diagram, but would be prohibitively expensive in terms of cost and storage. Typically, a few quasi-randomly placed sensor points suffice. Our results demonstrate that single detector and excitation points are often insufficient. A sensor placed at or near a node (where a mode field amplitude has a zero crossing) will not be able to detect the mode. Similarly, an excitation placed at a certain position will have difficulty exciting modes that have nodes at or near that position.
2.1 Reliable band diagram computation using FDTD

Figure 2.2: Error versus time convergence plot for FDTD simulations, comparing the harmonic inversion and DFT approaches for mode detection. The harmonic inversion approach converges in a fraction of the time required by conventional DFT.

Figure 2.3: Unmatched reference points with respect to measurement time for harmonic inversion and conventional DFT algorithms.

To illustrate these effects when using single detector-excitation pairs, we run Algorithm 2.2 to generate a full band diagram and performance statistics for every pixel of the computation domain (100 × 100 pixel matrix → 10,000 full bandgap diagrams, and 400,000 individual FDTD simulations). Figures 2.4 and 2.5 map the percentage of detected modes as a function of position for transverse electric (TE) and transverse magnetic (TM) modes, respectively, for reduced frequencies 0 ≤ \( u \) ≤ 0.8 and 0 ≤ \( u \) ≤ 1.0. Each of these plots shows a sort of Rorschach ink-blot pattern that follows symmetry lines for the crystal. Along symmetry
Figure 2.4: Sensormaps of the PhC unit-cell for TE modes. Each pixel represents the percentage of modes found in the range $0 \leq u \leq 0.8$ (left) and $0 \leq u \leq 1.0$ (right) at the position of the pixel. The black contour indicates the dielectric rod boundary. The smaller white circle indicates the location of the band diagram shown in Figure 2.6.

lines themselves exists the largest number of missed modes.

We randomly sample several points where the missed mode count is high. For all of the sampled modes, we confirm the existence of a node at the detector position. For the purpose of illustration, we present two such band diagrams in Figure 2.6, corresponding to a detector position on the diagonal line of symmetry for the TE sensor map, and Figure 2.7 for the horizontal line of symmetry on the TM sensor map.

In Figure 2.7, a string of modes is missing from the third and sixth lowest frequency bands, between the $\Gamma$ and X points, or the horizontal leg of the irreducible Brillouin zone (IBZ). The field plot below the band diagram shows a mode pattern corresponding to one of the missed modes in the string of missing modes of the third lowest frequency band. These missed modes have nodes that are coincident with the sensor position. A similar case is shown in Figure 2.6 for the TE polarization.

The points along the symmetry lines confirm that symmetry points miss modes. Another observation is a small deviation of the sensor point from the node position can improve detection significantly. Next to the symmetry lines, a ring of missed points is present close to the dielectric boundary for both polarizations. This arises from modes where the bulk of the field energy is localized within the dielectric. It is therefore also advantageous to set the source and sensor positions apart from dielectric interfaces. As can be seen from the plots however, nodal patterns depend on the upper frequency limit chosen for considering missed modes.

The algorithms presented here are useful for calculating the reliability and accuracy of
2.1 Reliable band diagram computation using FDTD

Figure 2.5: Sensormaps of the PhC unit-cell for TM modes. Each pixel represents the percentage of modes found in the range $0 \leq u \leq 0.8$ (left) and $0 \leq u \leq 1.0$ (right) at the position of the pixel. The black contour indicates the dielectric rod boundary. The smaller white circle indicates the location of the band diagram shown in Figure 2.7.

FDTD simulations for the generation of band diagrams. They can also be used to map the node density of crystal modes. For complete band diagrams, the best approach is to use multiple randomly placed excitation and sensor points. For multiple sensor points, boolean ‘OR’ logic may be used such that if one detector misses a mode and another does not, the mode will be considered as present. Coinciding modes (with close angular frequency) can be resolved by means of averaging.
Figure 2.6: TE bands for the sensor marked by the white circle in Figure 2.4. Reference points are marked with an ‘×’, and test points computed by FDTD with an ‘◦’. The line at $u = 0.8$ marks a limit frequency used for the performance analysis. The field plot below shows the mode pattern of an undetected TE mode from the third band in a three by one section of the crystal. Its node coincides (along the Γ-X horizontal) with the measurement position.
Figure 2.7: TM bands for the sensor marked by the white circle in Figure 2.5. Reference points are marked with an ‘×’, and test points computed by FDTD with an ‘◦’. The line at \( u = 0.8 \) marks a limit frequency used for the performance analysis. The field plot below shows the mode pattern of an undetected TM mode from the third band in a three by one section of the crystal. Its node (along the \( \Gamma \)-M diagonal) coincides with the measurement position.
2.2 Computation of broadband power scattering spectra

In this section we present an alternative approach to the analytic solution for slab scatterers, derived in Appendix A. This approach, using the FDTD algorithm, has been used before for other scattering problems [36]. Although the analytic solution is much faster for the flat slab problem, it cannot solve arbitrary geometries such as curved slabs or rough slabs (discussed in Chapter 4). FDTD provides this flexibility, in addition to the numerous other advantages that come with time-domain methods.

FDTD is convenient for studying antireflective coatings and metamaterial problems. Because it is possible to specify arbitrary geometries composed of lossy and nonlinear materials, there are many realistic situations FDTD can model that analytic techniques cannot. For the thin-film antireflective coating problems discussed here, it is possible to incorporate losses in the analytic solution by specifying complex indices of refraction, but only for an entire layer (as opposed to lossy inclusions, which may be present in metamaterials). Nonlinearities such as the Kerr and Pockels effects where the refractive index varies according to the fields present are readily available with FDTD. Finally, FDTD can be used to examine the time evolution of fields, which can offer additional design insights.

Losses can be realized in fabrication by doping dielectric materials with lossy particles. Usually it is easy to find lossy materials or add losses by doping. It is more difficult, and more desirable for some applications to find broadband loss-free materials [37].

As a grid-based numerical approach, the most significant drawback to FDTD is that computation times can scale rapidly with problem size and resolution. This often results in an attempt to find a balance between accuracy and speed. There are measures which help improve accuracy without increasing computation costs, such as subpixel-smoothing techniques which reduce staircasing errors [18]. Further, it is easy to encounter special situations where a numerical instability resulting from meshing or material properties causes field values to explode [12, 38, 39]. For simple configurations, FDTD can provide robust, accurate and fast results.

2.2.1 Numerical approach for obtaining scattering parameters

A general description of a typical computation domain is shown in Figure 2.8. In the center of the domain is the scatterer to be studied. This could be a single object such as a plasmonic antenna [17], or an element in a unit-cell of a periodic grating structure. Because we focus on metamaterial simulations we will describe a scattering simulation for the latter. The approach for the former is related, but has some differences with respect to the arrangement of perfectly matched layers (PMLs) and source excitation, resulting in a total-field scattered-field (TFSF) simulation [12].

The computation domain consists of some scatterer, flux planes for computing the power reflection coefficients, and PML layers for domain truncation [40, 41].
Figure 2.8: Setup of the computation domain for a two dimensional scattering simulation. Each of the six numbered domain segments should be initially set to one wavelength (the longest wavelength excited) in thickness.

We set the left and right boundaries of the computation cell to have Bloch boundary conditions, where the fields at one boundary are updated as phase shifted copies of fields at the opposite boundary [42]. If the excitation planewave has a non-normal angle of incidence for some single frequency, the phase shift between boundaries is set accordingly. The top and bottom boundary conditions are irrelevant since the PML absorbs waves incident upon those boundaries.

The excitation used should turn on and turn off, as opposed to a continuous wave which is always on. This allows for a one-to-one comparison of the flux integrals. A typical solution is to apply a broadband Gaussian pulse. These have a short excitation time, while exciting several frequencies simultaneously, yielding broadband scattering coefficients. The shape of the pulse is however unimportant, so long as the forward propagating fields die down to zero as \( t \to \infty \).

At the lower boundary of the top PML, an array of phase shifted current sources is used to excite a planewave. We then use two separate FDTD simulations to compute the reflection coefficients. In a first run, without any scatterer, we compute the incident power flux from the planewave excitation. First, we accumulate the Fourier transforms for each point in the flux plane, for the electric and magnetic fields [43], according Equation 2.1 (for the electric field).

\[
E(\omega) = \frac{1}{\sqrt{2\pi}} \sum_n e^{i\omega n \Delta t} E(n \Delta t) \Delta t \approx \frac{1}{\sqrt{2\pi}} \int e^{i\omega t} E(t) dt \quad (2.1)
\]
For a given frequency, the flux power through each flux plane is then found by integrating along the plane according to Equation 2.2

\[ P(\omega) = \text{Re} \mathbf{\hat{n}} \cdot \int \mathbf{E}_\omega^*(x) \times \mathbf{H}_\omega(x) \, d^2x \]  

(2.2)

In the second simulation, with a scatterer, we subtract out stored copies of the Fourier-transformed incident fields from the reflected flux plane, as in 2.3. We then compute the transmitted and reflected power flux, normalizing these to the incident power flux computed in the first run. For optimization, where only geometric and material properties of the scatterer are modified, only a single run without any scatterer is necessary for an entire optimization.

\[ P(\omega) = \text{Re} \mathbf{\hat{n}} \cdot \int [\mathbf{E}_\omega(x) - \mathbf{E}_\omega(0)(x)]^* \times [\mathbf{H}_\omega(x) - \mathbf{H}_\omega(0)(x)] \, d^2x \]  

(2.3)

In the case of a three dimensional simulation, the simulation domain is quite similar. The PML becomes a volume instead of an area, the source plane and transmission and reflection flux integrals occur over planes instead of lines, and two additional boundary conditions are added for the added dimension. These may be periodic boundaries if the system is two-dimensionally periodic.

### 2.2.2 Oblique scattering with FDTD

One advantage to the periodic FDTD technique is that we can acquire transmission coefficients over a range of angles and wavelengths with a single scattering simulation. If the boundary conditions are specified for non-normal incidence, then we can retrieve a broadband, multi-angle sweep of reflection coefficients, where each frequency specifies a unique incidence angle according to the boundary condition relation\(^1\)

\[ k_x = \frac{\omega \sin(\theta_{\text{cen},0})}{\mu_0} \]

\(\theta_{\text{cen},0}\) is the angle corresponding to the center frequency of simulation. To obtain a particular angle of incidence \(\theta_p\) for a frequency \(\omega_p\), we use the relation in Equation 2.4.

\[ \theta_p = \arcsin \left( \frac{k_x}{\omega_p} \right) = \arcsin \left( \frac{\omega_{\text{cen},0} \sin(\theta_{\text{cen},0})}{\omega_p} \right) \]  

(2.4)

With a few simulations, we can obtain a map of the scattering coefficients over the entire \(\lambda-\theta\) plane. To illustrate this, Figure 2.9 shows the scattering map for an optimized multilayer thin-film coating (see Chapter 4). Each line of dots represents a single simulation consisting of a planewave and a scattering run. Values between these lines may be interpolated, but are not displayed in the figure for clarity.

\(^1\)In this section we use the dimensionless units of MEEP, where \(\varepsilon_0, \mu_0,\) and \(c\) are all unity.
This map comes from an example that we discuss in more detail in Chapter 4. To illustrate the meaning of slices of this map, we refer to the corresponding figures in Section 4.1. A horizontal cut of the map corresponds to a $\theta$-slice. The $\theta = 0$ slice at the bottom of the map corresponds to the data shown in Figure 4.4. Vertical cuts correspond to $\lambda$-slices, as seen in Figs. 4.5, 4.6, and 4.7. A top down view of the map is shown in Figure 2.10, indicating the location of data points obtained from each FDTD simulation.

Care should be taken to tailor the range of frequencies simulated for larger values of the center frequency angle $\theta_{cen,0}$. The ‘corner angle’ $\theta_{\text{corner}}$ defines the point at which the long wavelength planewaves begin extend past the $90^\circ$ incidence line. For $\theta_{cen,0}$ larger than the corner angle $\theta_{\text{corner}}$, the range of frequencies excited and measured must be reduced to prevent outlying planewaves from propagating with complex angle. The range of frequencies (or wavelengths) is determined by the calculation

$$
\lambda_{\text{max}}(\theta_{cen}) = \begin{cases} 
\lambda_{\text{max,0}} & ; \quad 0 \leq \theta_{cen} < \theta_{\text{corner}}, \\
\sin(\theta_{\text{max}}) \cdot \lambda_{\text{min,0}} \left( \frac{2}{\sin(\theta_{cen})} - 1 \right) & ; \quad \theta_{\text{corner}} \leq \theta_{cen}.
\end{cases}
$$

The corner angle is found as

$$
\theta_{\text{corner}} = \arcsin \left( \sin(\theta_{\text{max}}) \cdot \frac{\lambda_{\text{cen,0}}}{\lambda_{\text{max,0}}} \right).
$$

We can then set the center wavelength of the simulation accordingly:

$$
\lambda_{cen} = \left( \frac{1}{\lambda_{\text{min}}} + \frac{1}{\lambda_{\text{max}}(\theta_{cen})} \right)^{-1}.
$$

A plot of the maximum wavelength $\lambda_{\text{max}}$ as a function of center-frequency planewave angle is shown in Figure 2.11. Between 0 and $\theta_{\text{corner}}$, the wavelength range is maximum. After the corner angle, this range starts to limit as in Equation 2.5.

Because planewaves with shallow angles of incidence (above $70^\circ$) have a small $k_y$ wavenumber, the $y$-propagation of the wave will be slow. As a result, simulations with many shallowly incident planewaves will require more time steps for a pulse to completely traverse the system. Because of this, it is faster to generate the $\lambda-\theta$ map with an analytic solution for flat slab coatings. For complicated coatings however, the FDTD technique is possible and convenient.

Speed limitations are dictated by a number of factors. The most influential of these is the size of the computation domain. For the unit-cell shown in Figure 2.8, the unit-cell width is set by the lattice constant. Each marked region in the unit-cell is ideally a minimum of one wavelength in height, allowing sufficient room for waves to propagate between or decay within layers. Cutting corners is possible but should be done carefully, especially in the case
Figure 2.9: An isometric view of the reflectivity in the $\lambda$-$\theta$ plane of the optimized low-index thin-film metamaterial. Reflectivity values for points between the plotted data can be found by interpolation. The slice $\theta = 0$ corresponds to the optimized loss-free curve of Figure 4.4. $\lambda$ slices represent information the broad angle behavior of a given wavelength. A top-down view of this plot can be seen in Figure 2.10.

of oblique incidence. PML layers for example, can satisfactorily be shorter than a wavelength in thickness for normal incidence, but may need to be thicker for oblique incidence.

In terms of simulation duration, doubling the area or volume of the computation domain doubles the time required for time-stepping. Doubling the grid resolution on the other hand multiplies this time by a factor of $2^N$, where $N$ is the dimensionality of the computation domain.

The scattering simulation duration also depends on the scatterer itself. Metallo-dielectric metamaterials oftentimes have structural features much smaller than a wavelength. If the FDTD code does not have subgridding or non-uniform gridding, sufficient meshing of these small features mean an overmeshing of the computation domain outside of the metamaterial. Further, because metamaterials are generally highly resonant, energy that couples into a metamaterial structure can get stuck inside it, in particular if it is lossless, prolonging the simulation time or requiring multiple narrowband runs.

The technique discussed in this section can also be applied to systems containing dispersive materials. For time domain codes like FDTD, it is not possible to simply input frequency dependent material parameters. The conventional approach is to specify the material properties using Drude, Debye, or Lorentzian material models. These define a time domain susceptibility function that is based on the inverse Fourier transform of a frequency dependent susceptibility.
2.2 Computation of broadband power scattering spectra

Figure 2.10: Top-down view of Figure 2.9, indicating the wavelength and angle positions of data points obtained from simulations. Each string of points corresponds to a separate simulation. For oblique planewave boundary conditions, each frequency represents a planewave with a unique angle.

Figure 2.11: $\lambda_{\text{max}}$ is the maximum wavelength for each FDTD simulation, and corresponds to the wavelength of the rightmost (or upper-rightmost) point in each curve of Figure 2.10. To prevent propagation of waves with imaginary incidence, we limit $\lambda_{\text{max}}$ according to Equation 2.5, plotted here.

Usually, one takes published or measured frequency dependent complex material data and attempts to fit it with one of these models. This is not always simple to accomplish, and takes a certain amount of practice. We use non-linear optimization techniques to perform weighted fits (necessary since the imaginary parts of permittivities are generally small compared to the real parts) of material models containing several resonance terms. As with Fourier series, more terms yield a better fit. They also however increase the
computation and storage requirements for the FDTD algorithm, so a compromise must be chosen between accuracy and speed.
Chapter 3

Effective medium approximations

Photonic crystals, or more generally, mixed media, are an important subset of metamaterials. One dimensional crystals are useful for thin-film optics, similar to structures presented in Chapter 4. Two and three dimensional crystals are used in optical communication [44] and quantum optics [45] applications.

The combination of crystals into multilayer structures creates a difficult design problem. We often need to determine the optimal thicknesses and porosity or doping levels for each layer, requiring many iterative simulations. Since each layer can long with respect to an operating wavelength, the computation domain can be quite large and therefore costly for such structures.

The problem of light propagation in photonic crystals can however be considerably simplified if we investigate it as a problem of light propagation in some effective medium. This is possible if the operating frequency is below that of any photonic bandgap. To define an effective medium, we find suitable approximations for the permittivity, $\varepsilon_{\text{eff}}$, and the permeability, $\mu_{\text{eff}}$.

These approximations are normally valid under certain conditions. First, the filling fraction of inclusions should be small, and their material properties should not differ too much from those of the background material. Further, they are only valid for wavelengths $\lambda$ which are long in comparison with the lattice constant $a$ of the crystal.

In this chapter, we present a numerical approach for examining the validity of effective media approximations for inclusions of varying sizes and index contrast. We focus on the performance of the Maxwell-Garnett (MG) formula for a canonical problem of spherical inclusions in a body-centered cubic (BCC) lattice.

We additionally examine a way to improve the effective media approximations for intermediate wavelengths where the normal long-wavelength assumptions are no longer valid.

3.1 Maxwell-Garnett Accuracy

There are several mixing formulas available for providing the effective permittivities or conductivities of inhomogeneous materials [46]. Of these, one of the better known is the MG formula. This is perhaps a result of its straightforward derivation [47–49], but also because it is well suited to well-separated inclusion mixtures which occur frequently in nature as
well as in human-engineered materials [46].

One requirement when applying the MG approximation is that the size of inclusions must be small with respect to the wavelengths of interest. Additionally, it works best for small filling fractions and low material contrasts.

These requirements are frequently stated in literature, but are numerous and highly context dependent. It is useful to have a visualization of the accuracy of these approximations before using them. In this section we present an approach for comparing the MG approximation to a high accuracy eigenvalue computation of the effective permittivity in order to visualize the deviation between the two. Additionally, we include a third technique using an approximation to an exact analytic solution to confirm our computational approach. We focus on the problem of finding the effective permittivity for a BCC lattice of spheres, but this technique can easily be applied to other lattice structures and inclusion shapes.

### 3.1.1 Effective permittivity computations from the PhC band diagram

The computational approach is based directly on the eigenvalue problem described in [46] where the effective permittivity of a mixture is determined from the slope of the dispersion relation for the first band of the infinite periodic crystal describing that mixture.

For non-dispersive constituent materials, this slope can be determined using the MPB software package [50]. The eigenvalues \(\omega\) are symmetric with respect to the origin, and the eigenvalue at wavenumber zero is zero (\(\omega(k = 0) = 0\)). We can then compute the effective permittivity of a mixture \(\varepsilon_{\text{eff}}\) with second order accuracy \(O(h^2)\) using a single eigenvalue, or a fourth order accuracy \(O(h^4)\) using two.

\[
\varepsilon_{\text{eff}} = \frac{2}{\partial^2 \omega^2(0)}
\]

(3.1)

This comes from an asymptotic analysis of Maxwell’s equations in a periodic domain, and is given in full derivation in [51, 52]. A simplified version is explained in [46].

The second derivatives computed from the eigenvalues of MPB and plugged into (3.1) can be found according to Equations (3.3,3.5), whose derivations are provided in Appendix B.

\[
f''(0) = \frac{2f(h)}{h^2} - O(h^2)
\]

(3.2)

\[
\frac{\partial^2 \omega^2(0)}{\partial k^2} = \frac{2\omega^2(h)}{h^2} - O(h^2)
\]

(3.3)
3.1 Maxwell-Garnett Accuracy

Figure 3.1: Convergence of the permittivity computation when using the second derivative computed from a single eigenvalue. Finer $k$-vector factors $h$ correspond to eigenvalues closer to the (0,0) point of the band diagram.

\[
f''(0) = \frac{16f(h) - f(2h)}{6h^2} + O(h^4) \quad (3.4)
\]

\[
\frac{\partial^2 \omega^2(0)}{\partial k^2} = \frac{16\omega^2(h) - \omega^2(2h)}{6h^2} + O(h^4) \quad (3.5)
\]

In the limit as the wavenumber used to compute the slope approaches zero, the result becomes more accurate. For the fourth order derivative we should expect a fourth order convergence with wavenumber. In a first check, we can examine the convergence of both computations. Figure 3.1 shows this convergence for the second order approach, and Figure 3.2 shows the same for the fourth order one. It is apparent from the curves shown that the converged values have already been reached and that any decrease in wavenumber brings no accuracy benefit for the given combinations of inclusion radius and permittivity contrast. The $n^{th}$-order convergence may become apparent for higher filling fractions.

The resolution (pixels per unit length) used plays a much more significant role in the accuracy of the computation. In MPB, eigenvalues are solved for using a hermitian positive definite matrix. The number of degrees of freedom is equal to the number of grid points for a given polarization. In the isotropic case we only need to consider one polarization. For a cubic unit-cell with edge length equal to 1.0, the corresponding number of degrees of freedom is then equal to the cube of the resolution.

Figure 3.3 shows the convergence of permittivity values as a function of the resolution. It is
Figure 3.2: Convergence of the permittivity computation when using the second derivative computed from two eigenvalues, corresponding to a fourth order convergence.

Figure 3.3: Convergence of effective permittivity values for four permittivity contrasts as a function of MPB resolution. The radius of the spheres was fixed at 0.1 for a unit-cell of size 1.0.

apparent that the resolution can still be raised to obtain a more accurate computation. In this case, the next step up in resolution would be 512, corresponding to $1.34 \times 10^8$ degrees of freedom, which is computationally challenging. For our comparison to MG we juxtapose
3.1 Maxwell-Garnett Accuracy

![Figure 3.4: Effective permittivities for the BCC spherical inclusion problem as obtained by the MG formula for inclusion contrasts ranging from 1 to 128, and radii from 0.0 to 0.45.](image)

results for resolutions of 256 and 512 pixels per unit-cell dimension.

For any approach, we can visualize the permittivities as a three dimensional surface plot where the permittivity is the dependent variable, and the index contrast and the inclusion radius are the two independent variables. The contrast-radius space visualization of the MG formula is shown in Figure 3.4. It can be seen that the permittivity function is smooth and monotonic over this space. We now use the technique described above to compute the same function, albeit over a coarser sample space, shown in Figure 3.5. For values in-between sample points, we rely on bi-cubic interpolation. This is a potential source of error since the interpolation method chosen will influence the shape of our final result. This should be acknowledged and considered when comparing the final results of different resolutions.

Figures 3.6 and 3.7 show the percent error between the computed effective permittivity and the MG formula. The sign is chosen such that the MPB result is the reference. That means that a value of -8 percent on the plot indicates that the MG formula is 8 percent lower than the MPB result.

The main conclusion that we can draw from these plots is that the MG formula deviates from the computation especially at large radii. Higher material contrasts also bring about more error, but this effect is small when compared to that of the inclusion radius. The contour plot view shows for example, little increase in the error for high contrasts and small radii, at the top left of the plot.

We now perform the same analysis for the resolution of 512. Figure 3.8 shows the sample points computed, and the corresponding interpolated surface.
3 Effective medium approximations

Figure 3.5: Computed points for the BCC spherical inclusion permittivity problem. 63 sample points were computed, each corresponding to a simulation with a resolution of 256 pixels per unit length. 17 additional points are available for the trivial problems of zero radius or unity contrast. Values between sample points are interpolated using a bi-cubic interpolation scheme.

Figure 3.6: Percent error between the MG formula and the interpolated computation for a resolution of 256, surface view.
3.1 Maxwell-Garnett Accuracy

Figure 3.7: Percent error between the MG formula and the interpolated computation for a resolution of 256, top-down contour view.

Figure 3.8: Computed points for the BCC spherical inclusion permittivity problem at a resolution of 512 pixels per unit length. Values between sample points are interpolated using a bi-cubic interpolation scheme.

Figures 3.9 and 3.10 show the percent error relative to the MG formula. The similarity with the analogous 256 resolution plots confirms that the resolution is fine enough that it doesn’t play a dominant role in the error calculation.
3 Effective medium approximations

Figure 3.9: Percent error between the MG formula and the interpolated computation for a resolution of 512, surface view. The appearance is similar to the lower resolution version of Figure 3.6.

Figure 3.10: Percent error between the MG formula and the interpolated computation for a resolution of 512, top-down contour view.
3.1 Maxwell-Garnett Accuracy

3.1.2 Comparison with Kristensson formula

Finally, we consider a third approach which we can take advantage of for the particular problem of spherical inclusions. Kristensson derives a formula for the exact solution to the spherical inclusion problem as a matrix summation in [53]. Because its convergence is conditional, and the matrix computation can be difficult, an small volume fraction approximation is also provided. The effective permittivity formula is given as correction term (the last term) to the MG formula:

\[
\varepsilon_{\text{eff}}(r, c_\varepsilon) = 1 + \frac{34\pi^3}{r^3} \cdot (c_\varepsilon - 1) + \frac{2}{c_\varepsilon + 2} \cdot \frac{4\pi^3}{r^3} \cdot (c_\varepsilon - 1) - \frac{155}{3} \cdot \frac{(c_\varepsilon - 1)^3 r^{10}}{(3c_\varepsilon + 4) [c_\varepsilon + 2] - \frac{4\pi^3}{3} (c_\varepsilon - 1)^3 r^{10}}
\]

(3.6)

where \( r \) is the inclusion radius and \( c_\varepsilon \) is the permittivity contrast given by \( \varepsilon_i / \varepsilon_b \), the quotient of the inclusion and background permittivities.

The first comparison we make is between the MG and the Kristensson formulas. The surface in Figure 3.11 shows a similar contour to the comparisons shown above. The rough shape is similar, though it doesn’t have the same ‘waves’ present in the comparisons between the MG formula and computed permittivity surfaces. This may be an artifact of the bi-cubic interpolation that would disappear with a more advanced surface fitting approach. We see from a direct comparison between the 512 resolution surface and the Kristensson formula in Figure 3.12 a peak error of less than 2 percent for large radii and permittivity contrast. This gives us faith in our application of the computational approach, in particular for problems where no analytic solution or acceptable approximation exists.
3 Effective medium approximations

Figure 3.11: A comparison between the Kristensson small volume fraction approximation formula and the MG formula. A percent error of −5 percent indicates that the MG result finds a permittivity which is 5 percent less than that of the Kristensson formula.

Figure 3.12: A comparison between the Kristensson small volume fraction approximation formula and the band diagram computation at a resolution of 512. A percent error of −2 percent indicates that the Kristensson result finds a permittivity which is 2 percent less than that of the band diagram computation.


3.2 Using mixing formulas with revised boundary conditions

We now consider the problem of multilayered crystal systems, where two or more separate photonic crystal slabs form a stack. If the light wavelength is comparable with the lattice constant, then so-called envelope function approximations (EFAs) can be used as in [54–59]. These are analogous to a similar theory taken from semiconductor physics, and are based on the periodicity of crystals, where the dielectric and magnetic constants are functions of wavelength. It has been shown that this dependence is insignificant for the lowest band of the crystal, as long as $\varepsilon_{\text{eff}}$ is not too large, and that wavelength dependence only arises in close vicinity of the band gap. The EFAs can be used for phononic crystals, where wavelengths of interest are on the order of the lattice constant.

The problem becomes more complicated if we study the reflection and refraction of light at the surface boundary of a photonic crystal, or at the boundary between two distinct crystals. To study this problem for real crystals, the well-known Maxwellian boundary conditions (MBCs) are usually applied (continuity of the tangential components of the electric and magnetic fields). The MBCs lead to the well-known Fresnel equations for the reflection and refraction coefficients.

To obtain the MBCs, it is assumed that field wavelengths are large in comparison with the crystal lattice constant $a$. This approximation is often satisfactory for typical photonic crystals, where $\lambda \sim 100 - 1000$ nm and $a \sim 1$ nm.

The problem of the light scattering between two distinct photonic crystals is considered in [60], where the so-called crystal interface impedance is introduced and discussed. This approach significantly simplifies estimations of light propagation through multilayered photonic structures, because impedance values can be calculated separately for each interface. To calculate the impedance, Bloch functions of the contacting crystals are connected at the boundary. This is possible if both crystals are of the same symmetry and the lattice constants are close to one another.

The boundary conditions proposed in [61] are a generalization of the MBCs for photonic crystals. It is shown that an additional term arises for shorter wavelengths. Its value is on the order of $a/\lambda$, and can be interpreted as an influence of some effective layer at the boundary. Simulations using these generalized boundary conditions demonstrate good agreement with experiments on dielectric colloid photonic crystals.

In this section we demonstrate the applicability of the generalized boundary conditions for shorter photonic wavelengths. We use the FDTD method to calculate the reflection coefficients at the boundaries of 2D photonic crystal layers and compare the results with analytic solutions generated by effective media approximations. We show that short wavelengths require a correction to the standard MBCs, followed by additional correction terms representing effective changes in the crystal thickness for even shorter wavelengths.
Figure 3.13: A sample photonic crystal considered for modeling. Plane waves incident from air impinge on an infinite half space of the photonic crystal, comprised of a periodic arrangement of dielectric rods. We consider the region surrounding the $z = 0$ interface with size $2\delta$.

### 3.2.1 Boundary conditions for effective fields in photonic crystals

Consider the illumination of the boundary $z = 0$ of the photonic crystal shown in Figure 3.13. It shows a crystal with inclusions whose diameter $d$ equals the lattice constant $a$. Though we focus on this example of a percolated crystal, the analysis is also applicable to crystals with non-touching inclusions.

Suppose a wave propagates along the $z$ axis, and its electric field $\mathbf{E}$ is polarized in the $y$ direction, so that $\mathbf{E} = (0, E, 0)$. In the effective media approximation, the electric field of the wave obeys the wave equation of 3.7

$$\frac{\partial^2 E}{\partial z^2} + \frac{\omega^2 \varepsilon}{c^2} E = 0.$$  \hspace{1cm} (3.7)

This equation holds in regions far from the interface $z = 0$ such that $\varepsilon = 1$ for $z \ll -\delta$, and $\varepsilon = \varepsilon_{\text{eff}}$ for $z \gg +\delta$. To estimate the reflection coefficient, the MBCs for the effective fields (continuity of $E$ and continuity of $dE/dz \propto H_z$) are usually written at the boundary $z = 0$. Figure 3.13 shows $\delta$ to be approximately $a/2$, or half the lattice constant. This choice is somewhat arbitrary. It would also be reasonable to choose a thicker boundary region for matching purposes, but it is often desirable to apply this technique to finite crystals consisting of only a few lattice constant thicknesses. $\delta$ should however be large enough that the effective media approximation holds outside the region $|z| < \delta$.

The wave equation does not hold in the interface region $|z| < \delta \simeq a$. This makes it
impossible to write the simple MBCs. Instead, we can try to match analytic extensions of the effective fields from $z\ll -\delta$ and $z\gg +\delta$ to the interface region $|z|<\delta$ as shown in Figure 3.14. These boundary conditions are however not simple. In general, they can be written as

$$
\begin{pmatrix}
E(\delta) \\
E'(\delta)
\end{pmatrix}
= 
\begin{pmatrix}
t_{11} & t_{12} \\
t_{21} & t_{22}
\end{pmatrix}
\begin{pmatrix}
E(-\delta) \\
E'(-\delta)
\end{pmatrix},
$$

(3.8)

Here $E'=dE/dz$, and $t_{ik}$ are the frequency dependent transfer parameters. These depend on the position of the assumed crystal boundary with respect to the $z=0$ plane. This position can be chosen arbitrarily inside the $|z|<\delta$ region. The matrix $||t_{ik}||$ must be unimodular (det $||t_{ik}||=1$) to maintain the continuity of the Poynting vector across the interface.

Simple MBCs correspond to the identity matrix $t_{11}=t_{22}=1$, $t_{12}=t_{21}=0$. The boundary conditions proposed in [61] assume $t_{11}=t_{22}=1$, $t_{12}=0$, and $t_{21}=\omega^2\alpha/c^2$, where $\alpha$ is a frequency independent fitting coefficient. A more general form for these parameters is derived in [62], leading to the $t_{ik}$ parameters shown in Equation 3.9

$$
\begin{pmatrix}
E(\delta) \\
E'(\delta)
\end{pmatrix}
= 
\begin{pmatrix}
1 + \beta \frac{\omega^2}{c^2} & 0 \\
\alpha \frac{\omega^2}{c^2} & (1 + \beta \frac{\omega^2}{c^2})^{-1}
\end{pmatrix}
\begin{pmatrix}
E(-\delta) \\
E'(-\delta)
\end{pmatrix}.
$$

(3.9)

Here, $\alpha$ and $\beta$ are some interface parameters that must be found for each unique pair of neighboring layers. The usual approach is to simply determine their values by fitting results using the model to reflection computations generated by a full wave solver for the complete crystal structure. It is however also possible to give these parameters a physical interpretation that links them to the thickness and permittivity of intermediate layers, as described in [62]. There, in a special case, it is shown that $|\alpha|=2(\varepsilon-1)\delta$ and $|\beta|=(\varepsilon^2-1)\delta^2$. 
We apply the boundary conditions in (3.9) to compute the plane wave reflection coefficients of two dimensional finite photonic crystal slabs. These consist of stacks of dielectric rods of various permittivities, in a geometry similar to the one shown in Figure 3.13. Instead of semi-infinite periodicity in the vertical dimension, we tested our approach with finite stacks of three, five, and seven rod layers.

Consider the normal incidence of waves whose electric field is polarized parallel to the cylinders (the y axis in Figure 3.13). This polarization allows an exact analytic solution for the effective permittivity. The electric field has to be continuous across the cylinder boundary. The value of the Poynting vector does not change, in this case, when we replace the photonic crystal with an effective homogeneous media with the simple averaging formula of Equation 3.10

$$\varepsilon_{\text{eff}} = v\varepsilon_1 + (1-v)\varepsilon_2.$$  \hspace{1cm} (3.10)

Here $\varepsilon_1$ and $\varepsilon_2$ are the dielectric permittivities of the cylinders and of air (or other background material), respectively, and $v = \pi r^2/(4r^2) = \pi/4$ is the volume fraction occupied by the cylinders in the square lattice of Figure 3.13. For simplicity, in the following tests we assume the background material to be air, with relative dielectric permittivity equal to one.

The approximation in Equation 3.10 holds only for long wavelengths of $y$-polarized light,
shown as small values of $k$ in Figure 3.15. Our modeling should give a good result over the linear region of the dispersion curve, but not outside it, close to the band edge. In general, $\varepsilon_{\text{eff}}$ can be estimated from photonic band calculations. These estimates are found from the slope of the lowest band in the regime where the dispersion behaves linearly. Otherwise, the dispersion of the dielectric permittivity $\varepsilon_{\text{eff}}(k)$ has to be taken into account.

To determine the parameters $\alpha$ and $\beta$, we compare the estimate of the reflectivity from the model to reference numerical FDTD calculations. We use a two-dimensional semi-periodic model and illuminate it with normally incident plane waves. The boundaries in the propagation direction are truncated using perfectly matched layers. In planes parallel to the crystal interface, the reflection and transmission flux power is accumulated and compared to a normalization simulation containing no scatterer. Figure 3.16 presents these results for several structures. We see that the conventional MBCs ($t_{11} = t_{22} = 1$, $t_{12} = t_{21} = 0$) hold only for small frequencies (or long wavelengths, $\lambda/\sqrt{\varepsilon_{\text{eff}}} \geq 10a$), whereas the improved boundary conditions of (3.9) hold for $\lambda/\sqrt{\varepsilon_{\text{eff}}}$ greater than approximately $2a$. It is important that the parameters $\alpha$ and $\beta$ are independent of frequency and demonstrate at most a weak dependence on the slab thickness. When these conditions are met, $\alpha$ and $\beta$ can be used as characteristic parameters for the boundary.

The large variations of the reflectivity seen as ‘humps’ are due to interference of the waves reflected from each boundary of the slab (i.e. Fabry-Perot resonances). These humps have a constant maximum for all frequencies for curves obtained using the simple MBCs. The boundary conditions of (3.9) result in reflection coefficients with non-constant peak amplitude. This results in a better estimation of the curves obtained via simulations of the full crystal structure.

We choose the frequency unit in the figures so that $\omega = 1$ corresponds to the easily-computed approximate position of the photonic mid-gap $\omega_g = \pi c/(a \sqrt{\varepsilon_{\text{eff}}})$. Its exact position can be estimated as the nearest maximum of the reflectivity in the FDTD calculations, as indicated by arrows on Figures 3.16(a,d). The difference between the exact and approximate mid-gap positions gives us a rough estimate of the non-linear region of the photonic dispersion characteristic. Outside this region, we obtain a good estimate of the reflectivity spectra, and within it the assumption used in the analytical modeling does not hold.

It is also possible to demonstrate that the revised model works for interfaces between two photonic crystals, and not only air-crystal interfaces. We perform several tests to show this. First we examine a structure with a step change in cylinder diameter (several cylinder layers of one diameter followed by several cylinder layers of another). Then we check the model behavior for a structure with a step change in cylinder permittivity.

Figure 3.17 presents reflectivity results for two structures; (a) for cylinders with $\varepsilon = 2$, and (b) for cylinders with $\varepsilon = 10$. Each is composed of 4 cylinder layers with diameter $d = 1 \ \mu m$ above 6 cylinder layers with $d = 0.5 \ \mu m$. The total stack-up thickness is 7 $\mu m$. The red curves represent the reflectivity of 7 cylinders of diameter $d = 1.0 \ \mu m$. It should be emphasized that the parameters $\alpha$ and $\beta$ of the improved boundary condition on the
3 Effective medium approximations

Figure 3.16: Reflectivity of the three (a, d), five (b, e), and seven (c, f) layer photonic crystal slabs (Figure 3.13). The relative permittivity of the cylinders is $\varepsilon = 2$ for (a, b, c) and $\varepsilon = 10$ for (d, e, f). Solid black lines represent the exact numerical results from FDTD simulations. Red and blue dashed lines indicate approximations from our model (3.9) and the conventional MBCs model, respectively. The light frequency is in the units of the approximate mid-gap position $\omega_g = \pi c/a\sqrt{\varepsilon_{\text{eff}}}$. Its exact position marked with arrows in plots (a) and (d).
3.2 Using mixing formulas with revised boundary conditions

Figure 3.17: Reflectivity of the double layer slabs of cylinders of different diameters with \( \varepsilon = 2 \) (a) and \( \varepsilon = 10 \) (b).

The external boundary of the smaller cylinders must be reduced from the original parameters according to scaling considerations. Specifically, \( \alpha \rightarrow \alpha/2, \beta \rightarrow \beta/4 \).

The plots in Figure 3.18 present the reflectivities of structures consisting of stack-ups of \( n \in \{3, 5, 7\} \) layers of cylindrical rods of permittivity \( \varepsilon = 2 \) above a stack of \( n \) more rod layers of permittivity \( \varepsilon = 10 \).

We denote the parameters \( \alpha \) and \( \beta \) of the internal boundary as \( \alpha_{32} \) and \( \beta_{32} \). To estimate them, we assumed the parameters of the external boundaries to be the same as those for the single crystal structure approximation. We observe a slow variation of the values of \( \alpha_{32} \) and \( \beta_{32} \) with increased layer thickness. The variation disappears entirely for the thicker layers. Independence of \( \alpha_{32} \) and \( \beta_{32} \) from the thickness of each layer means that we can estimate these values for the boundary between two photonic crystals.

As a final test of the method, Figure 3.19 shows reflectivity curves for the H-polarization. Note that the effective dielectric permittivities are different for these waves due to different polarization of the electric field. These values were estimated from the best fit of the curves at long wavelengths, where the effect of the boundary shape can be neglected (\( \alpha \rightarrow 0, \beta \rightarrow 0 \)).

The parameters of these boundary conditions are independent of the light wavelength over a long interval. This allows us to consider them as material properties, or more precisely, as properties of the particular boundary, which can be either calculated or measured. These parameters allow one significantly simplify the simulation of the light propagation in multilayered photonic structures.

Specifically, full wave simulations of a crystal stack-ups that might take minutes or hours to compute can be reduced to simple matrix computations. These are fast and accurate approximations for wavelengths that are intermediate and long with respect to the lattice.
3 Effective medium approximations

Figure 3.18: Reflectivity of the composite $\varepsilon = 2, \varepsilon = 10$ structures for $3+3$ layers, $5+5$ layers, and $7+7$ layers. $\omega_g$ corresponds to $\varepsilon = 10$ (nearest gap position).

Figure 3.19: H-polarized reflectivity of the seven layer structure with $\varepsilon = 2$ and $\varepsilon = 10$.

constants present in the stack-up. The corresponding computational cost is dominated only by the overhead computation of the interface parameters $\alpha$ and $\beta$. These must be computed for each unique pairing of two crystals. While a separate full wave simulation is necessary for each of these unique pairings, they can be faster than simulating a complete
crystal structure that is much thicker than the minimalist structure necessary to compute the interface parameters.

The physical boundaries of photonic crystals are usually imperfect, making it difficult to suggest any reliable model of the boundary structure. It is however apparent that a distortion of the crystal structure in the narrow region near the boundary can be considered in terms of the boundary conditions. In this model such a distortion would simply alter the parameters of the boundary conditions $\alpha$ and $\beta$. 

3.2 Using mixing formulas with revised boundary conditions
Chapter 4

Antireflective coatings

One very practical application of metamaterial technology is antireflective coating design. Such coatings are commonly used in a variety of industries. Because they can be highly periodic, it is easy to apply field solvers to analyze their grating properties.

In this chapter we examine three antireflective coatings. We use the FDTD method to study all three. They each present however, a unique facet to the metamaterial design problem.

The first problem deals with a simple, one dimensional nanorod thin-film coating. We show how coupling the reflectivity computation with a numerical optimizer can yield a metamaterial with highly desirable optical properties. The second problem deals with a thin-film solar cell roughness morphology design. We examine how grating effects play a role in the reflection behavior for cells where the random roughness is approximated using periodic models. For the final problem we examine a three dimensional antireflective coating for infrared receivers, and compare FDTD results with those from frequency domain methods.

4.1 High performance nanorod coatings

Graded dielectric materials promise excellent antireflective properties and have been the subject of scientific analysis and investigation \cite{63, 64}. Recent advances in fabrication techniques promise a high degree of control over extremely low-index optical thin-films. By means of oblique deposition of \text{SiO}_2 and \text{TiO}_2 nanorods, indices of refraction as low as 1.05 have been reported \cite{65, 66}. The density of a nanorod layer can be fine tuned by varying the deposition angle. Sub-unity filling fractions reduce the effective permittivity of the layer in the same way that dielectric foams do so on a macroscopic scale. Further, while the geometry of staggered deposition angle results in asymmetry, anisotropic effects have been stated to be negligible for low effective indices due to high porosities and small layer thicknesses \cite{67}.

Low-index thin-films are very practical for antireflective coatings because they can be used to achieve a good match between air and underlying optical elements. Quarter-wave thick monolayer coatings with index equal to the geometric average of the indices of surrounding media can minimize reflection at a single wavelength. Multilayer coatings are capable of reducing reflection over a wide range of wavelengths. Low-index nanorod multilayer thin-films have been shown to function as broadband and broad angle antireflective coatings.
4 Antireflective coatings

Figure 4.1: 5-layer oblique nanorod thin-film antireflective coating consisting of layers of SiO$_2$ and TiO$_2$ nanorods, reproduced from [65]. The length, radius, and deposition density of the nanorods is used to tune the permittivity of each layer. Here, the layer stackup is used to approximate a quintic permittivity profile to minimize reflections.

To attain a broadband, broad angle behavior, different multilayer index profiles have been studied and fabricated. For the nanorod films, theoretical continuously-graded coatings were considered, where the index of the coating varied with a linear, cubic, and quintic relation with respect to height. It was shown that the quintic profile exhibited the best performance [65]. An approximation of the quintic profile was then fabricated by using a discrete five layer system composed of nanorod thin-films.

While the quintic profile may be close to optimal for continuously graded coatings [68, 69], we show that there are solutions which attain better broadband, broad angle behavior for the five discrete-layer thin-film system. Additionally, we present a numerical approach for discovering the optimal profile for discrete film systems. While the analytic solution for Fresnel reflection coefficients can be used for fast calculations of simple layered linear systems, the numerical FDTD approach we present can be used to solve arbitrary geometries composed of nonlinear, lossy materials. We finally demonstrate that losses can be used to further drive down reflectivity levels in systems where good transmission is not necessary, such as in radar applications.

4.1.1 Fresnel reflection design and optimization

Transmission and reflection coefficients for loss-free multilayer systems can be solved by obtaining the solutions to a linear system of equations [70]. These equations are obtained by representing complex valued incident and reflected fields in each layer, and relating fields in neighboring layers according to Snell’s law, as well as boundary conditions enforcing the continuity of tangential electric and magnetic fields. For non-normal angles of incidence,
we apply separate boundary conditions for TE and TM polarizations. For larger problems with many layers, these systems can be quickly solved numerically by using a matrix representation, provided in Appendix A.

For antireflective coatings, two straightforward design parameters which we can adjust for each layer are thickness and index of refraction. In an $N$ layer system, we can optimize $2N$ real-valued parameters to determine which configurations are best. Fitness functions for evaluating a given configuration can be tailored to what is desired. Two standard goals for this problem would be to minimize reflectivity over a broad range of wavelengths, and over a broad range of incident angles for a fixed frequency.

We undertook such an optimization to determine if obliquely deposited nanorods in a quintic approximation layering offered the best performance antireflective coating. It is fastest to evaluate individuals using the analytic matrix approach, however we ran our optimizations using the flexible FDTD technique described in Chapter 2. We then confirmed our results using the matrix approach. This process, while more time consuming, allowed us to confirm the reliability of the FDTD technique when used with the optimizer.

We found that there are other nanorod configurations which do perform better than the approximated quintic profile, and lie within the same fabrication boundaries (minimum and maximum layer thickness, and minimum and maximum index). Thus, with the assumption that thickness and index of refraction can by fabricated in a decoupled manner, it is possible to achieve lower reflectivities, broader bandwidths, and broader angle behavior over a higher range of wavelengths.

For the optimization, we used a simple evolutionary strategy (SES) code. SES has shown fast convergence to global maxima for similar problems [71]. Other strategies may also be applied. Table 4.1 shows the best parameters found for the layers of Figure 4.2. A comparison of the quintic and optimized layer stackups is provided in Figure 4.3.

### 4.1.2 Optimized nanorod thin-film results

Figure 4.4 illustrates the results. The first curve represents the baseline published result [65] of percent reflectivity for normal incidence, between 300 and 2000 nm. There is a single null where the reflectivity becomes very small at 780 nm. The 0.1% bandwidth is between 632 and 933 nm, corresponding to a fractional bandwidth of 38.5%. The optimized loss-free curve of the same plot shows multiple nulls at 555, 745, 1105, and 1673 nm. The spacing of these nulls is spread out in such a way that the 0.1% bandwidth is increased by a factor of 2.94 to 113%, ranging from 526 to 1895 nm.

The optimizer configures the layer parameters in a way that interference frequencies are spread out over the bandwidth of interest. Accordingly, we have also found it possible to obtain even lower reflectivities for narrower bandwidths, by moving the reflectivity nulls closer together.
Figure 4.2: Geometry and material parameters of the five layer model for an antireflective coating. Each layer consists of a dielectric with constant permittivity, equal to the effective (measured) permittivity of the fabricated nanorod equivalent. Planewaves of wavelength $\lambda$ are incident with angle $\theta$ from some medium, here we assume free space. The thin-films are matched to a substrate with fixed permittivity.

<table>
<thead>
<tr>
<th>layer</th>
<th>thickness (nm)</th>
<th>index of refraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>192.197</td>
<td>1.080</td>
</tr>
<tr>
<td>2</td>
<td>161.876</td>
<td>1.241</td>
</tr>
<tr>
<td>3</td>
<td>133.729</td>
<td>1.488</td>
</tr>
<tr>
<td>4</td>
<td>112.403</td>
<td>1.761</td>
</tr>
<tr>
<td>5</td>
<td>78.475</td>
<td>1.958</td>
</tr>
</tbody>
</table>

Loss parameters (layer 3):
- $\omega_n = 5 \cdot 10^{-3} \rightarrow \lambda_n = 200$ nm
- $\gamma_n = 5 \cdot 10^{-3}$
- $\Delta \varepsilon_n = 5 \cdot 10^{-3}$

Table 4.1: Parameters for optimized layer thickness and index of refraction for a 5 layer thin film system. Layer 1 corresponds to the first layer upon which fields are incident. Normal incidence broadband antireflection using a 5 layer system composed of these parameters is shown as the second curve in Figure 4.4. Additional loss parameters at the bottom of the table are used to demonstrate additional performance by means of absorption. These parameters do not correspond to an actual material, and are only used for illustration. Parameter units are dimensionless as specified in MEEP. The location of the Lorentzian resonance corresponding to the $\omega_n$ parameter is at 200 nm.

The performance of the optimized structure is also enhanced with respect to angle of incidence. For certain wavelengths, such as the wavelength for which measured results were published in the baseline study (632.8 nm), broad angle behavior is similar, as shown in Figure 4.5 for TE and TM illumination. For other wavelengths however, the optimized
Figure 4.3: Comparison of the quintic profile proposed in [65] (left), and the optimized profile with layer thicknesses given in Table 4.1 (right). The aluminum nitride substrate is shown with a index of refraction of 2.05. The quintic profile has a total thickness of 624.9 µm, and the optimized profile has a total thickness of 678.68 µm.

structure has much lower reflectivities over a wide range of angles, as can be seen in Figures 4.6 and 4.7. The two wavelengths chosen correspond to one normal incidence null wavelength (1104 nm), and one crest wavelength (1370 nm).

The FDTD technique allows us to visualize the three dimensional scattering behavior, shown previously for the optimized structure in Figure 2.9. A horizontal cut of the map corresponds to a θ-slice. The θ = 0 slice at the bottom of the map corresponds to the data shown in Figure 4.4. Vertical cuts correspond to λ-slices, as seen in Figures 4.5, 4.6, and 4.7.

The three dimensional view offers a better demonstration of how the broadband scattering evolves with increased incidence angle than individual uniangular slices would. A top down view of the map is shown in Figure 2.10, indicating the location of data points obtained from each FDTD simulation.

The FDTD approach also allows us to consider the additional benefits that material losses may confer. As a demonstration, we set the material parameter of the center slab to have loss parameters according to a standard Lorentz media model with a single resonance term given by the following relation:

\[
\varepsilon(\omega) = \varepsilon_\infty + \frac{\omega_n^2 \Delta \varepsilon_n}{\omega_n^2 - \omega^2 - j\omega \gamma_n},
\]

where the loss parameter values are given in Table 4.1. \(\varepsilon_\infty\), the bulk part of the real permittivity, remained a tunable optimization parameter. By adding slight losses to a single layer of the system, we can further reduce the attenuation in the stop band as can be seen by the third curve in Figure 4.4, obtaining even better antireflective properties. Losses can be increased, or added to multiple layers to further attenuate reflections.
Figure 4.4: Broadband reflectivity for various layer configurations and normal incidence illumination. The first curve shows results presented in the Schubert publication [65]. The second curve is for the five layer thin-film system, with parameters as in Table 4.1, as determined by an evolutionary optimization. The optimized result provides a much larger 0.1% bandwidth, between 526 nm and 1895 nm. Even better performance is possible when losses are included in one layer, as shown in the third curve, which has a slightly larger 0.1% bandwidth and better attenuation over the entire band.

According to these results, newly fabricated low-index nanorod thin-film systems can be optimized to provide better antireflective coatings. A bandwidth improvement by almost a factor of three is obtainable by separating interference wavelengths using a multi-parameter evolutionary optimizer. Additionally, broad angle behavior is enhanced with respect to previously published results. Lossy coatings can further improve results, as demonstrated using an FDTD periodic planewave approach.
4.1 High performance nanorod coatings

Figure 4.5: Broad angle behavior of the previously published \[65\] and optimized thin-film coatings at a wavelength of 632.8 nm. The broad angle behavior is comparable at this particular wavelength. For TE polarization, it can be seen that the optimized coating performs better for angles below 47°, and worse thereafter. For TM polarization, the previously published coating performs better in midrange angles of incidence.

Figure 4.6: Broad angle behavior at 1104 nm, corresponding to a null location in the normal incidence reflectivity of Figure 4.4. The optimized coating exhibits lower reflectivity for all angles of incidence, and for lower angles by more than two orders of magnitude.
Figure 4.7: Broad angle behavior at 1370 nm, corresponding to a crest location in the normal incidence reflectivity of Figure 4.4. A dip centered at 40° allows for very low midrange oblique reflectivities with the optimized coating. Even at a crest wavelength in the stop band, the optimized coating has lower reflectivities for all angles of incidence.
4.2 Thin-film roughness simulations for solar applications

Finite energy resources have spurred new interest and investment in alternative energy technologies. Solar energy is a particularly promising area for research because available technologies are expensive to manufacture and inefficient in converting solar energy into electricity. Figure 4.8 shows how research has helped improve solar output since 1976 [72].

While recent improvements in multi-junction concentrators have raised solar cell efficiencies to over 40%, such cells require the deposition of many layers, each finely tuned for a separate portion of the solar spectrum. This makes them prohibitively expensive for large-scale manufacture. Thin-film solar cells are a promising alternative because they do not require the large amounts of silicon of conventional silicon cells, or the many layers of multi-junction photovoltaic cells [73]. Industrial manufacturers are currently looking to combine low cost thin-film devices with new processing and design capabilities to create a photovoltaic cell that is viable for the mass market.

One effective way to accomplish this goal is to create models that predict the light scattering in solar cells. Using lossy materials that are representative of the layer structure of a thin-film cell, simulations can predict unknown variables such as optimal layer thicknesses, roughness geometries, and doping quantities. Conventional design-by-trial manufacturing
is slow and costly. A simulation model can accelerate the convergence to an optimal design or an increased understanding of underlying design principles.

We focus on the analysis of a single design aspect – the internal roughness morphology – of one type of thin-film solar cell. Its photovoltaic layers are comprised of both amorphous (\textit{aSi}) and microcrystalline (\textit{mcSi}) Silicon. The layer topology for this type of cell is shown in Figure 4.9. Incident light comes from a protective glass layer through a low-loss Zinc oxide layer (\textit{ZnO}) whose main role is to establish the internal roughness morphology. A scanning electron microscope (\textit{SEM}) image of such a surface is shown in Figure 4.10. This roughness defines how well incoming light is scattered into the photovoltaic layers, with more scattering corresponding to more absorption and therefore higher efficiency. The amorphous silicon (\textit{aSi}) and microcrystalline silicon (\textit{mcSi}) layers are followed by an insulating zinc oxide (\textit{ZnO}) layer, and a Lambertian (uniform reflection brightness independent of observation angle) back-scatterer.

The peaks in the \textit{SEM} image appear to have some random properties, such as shape and size. Our numerical models attempt to capture some of this randomness so as to imitate the behavior of the real structure. It should be noted however that the actual structure is not entirely random. The roughness peaks for example tend to grow according to the crystalline properties of Zinc oxide, and by the deposition process. These properties should be considered when modeling the problem numerically. We use three models to consider randomness in the roughness. The first is a regular triangular grating which has zero randomness. The second is a hand-randomized periodic grating with multiple roughness peaks in one unit-cell. The final one is a numerically randomized grating (using truncated gaussians) with multiple random properties, including peak sizes, positions, and peak skews. It is by iteratively increasing the ‘randomness’ in our models that we approach results that are plausibly comparable to published measurements.

In our simulations we focus on two metrics for evaluating the performance of a given structure, namely the reflectivity spectra and the total absorption. For both we use the \textit{FDTD} approach described previously in Section 2.2. The current \textit{MEEP FDTD} code implementation limits us to integrating absorption power over a box shaped volume. For a corrugated layer structure, this makes it difficult to compute the absorption in a given layer of contiguous material. Instead, we examine the total absorption over the entire structure.

\subsection{Material models}

To model lossy materials and the absorption within them, we use a five term Lorentzian model as is common in time-domain codes, shown in (4.1). Better fits would be possible with more terms, but large numbers of terms significantly increases the amount of memory consumed. Each Lorentzian term adds a polarization field to be kept track of. The time evolution of these polarization fields is then used to compute loss.
4.2 Thin-film roughness simulations for solar applications

Figure 4.9: Model of a thin-film solar cell consisting of a glass superstrate, a Zinc oxide layer, a p-i-n amorphous Silicon layer, a p-i-n microcrystalline Silicon layer, a second Zinc oxide layer, and a back reflector. Scattering at the ZnO-aSi interface has a strong bearing on energy conversion.

Figure 4.10: Scanning electron microscope image of Zinc oxide thin-film surface morphology, provided by Oerlikon Solar. Length scale indicator is 1 µm.

\[
\varepsilon = \varepsilon_\infty + \sum_{n=1}^{5} \frac{\omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n}
\]  \hspace{1cm} (4.1)
4 Antireflective coatings

The fits for the three lossy materials we used are shown in Figures 4.11, 4.12, and 4.13. The measurement data was provided by Oerlikon Solar. The fitting region under consideration is between 600 and 800 nanometers, for all materials. The aSi and mcSi fits tend to overestimate the losses for longer wavelengths, but are otherwise qualitatively good. Because of the low losses for ZnO, it was easier to obtain a qualitatively excellent fit. We use an evolution strategy optimizer to obtain complex fits. It is necessary to weight the imaginary parts of these datasets when computing the least squares error for the fitness computation. This is because a relatively small deviation in the imaginary term amounts to a significant difference in the loss properties of the material. Because the available dataset is preliminary, we use these fits consistently for all simulations regardless of quality as a demonstration of the approach. When higher quality data is available, in particular at shorter wavelengths for all materials, we can repeat the procedure shown here.

4.2.2 Comparison between FDTD and analytic solution

To check the FDTD approach and the material fits we obtained, we first examine a simple problem that has an analytic solution. The geometry consists of a flat slab scatterer that approximates the geometry of Figure 4.9, only with no internal roughness. Specifically, light is normally incident from an infinite space of glass (\( \varepsilon = 2.25 \)), and approaches flat slabs of ZnO (2 \( \mu \)m thick), aSi (300 nm), mcSi (2 \( \mu \)m), a second ZnO layer (2 \( \mu \)m), and finally a perfect electric conductor (PEC) back reflector.
4.2 Thin-film roughness simulations for solar applications

Figure 4.12: Complex permittivity data and a 5-term Lorentzian model fit for microcrystalline Silicon. The fit region is between 600 and 800 nm.

Figure 4.13: Complex permittivity data and a 5-term Lorentzian model fit for Zinc oxide. The fit region is between 600 and 800 nm.

The analytic solution is computed as described in Appendix A. In Figure 4.14 we compare the analytic result to the FDTD computation, run at a resolution of 600 cells per \( \mu \)m. On the same vertical scaling but on a secondary axis of the same plot, we show the relative
Figure 4.14: Reflectivity for a test structure consisting of flat slabs. Analytic and FDTD solutions (resolution of 600 cells per $\mu$m) are plotted, in addition to the relative error.

<table>
<thead>
<tr>
<th>Layer</th>
<th>absorption energy</th>
<th>% of total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass ($\infty$)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>ZnO (2.0 $\mu$m)</td>
<td>1.08863380602912e-4</td>
<td>5.4149</td>
</tr>
<tr>
<td>aSi (0.3 $\mu$m)</td>
<td>4.72987588057873e-4</td>
<td>23.5265</td>
</tr>
<tr>
<td>mcSi (2.0 $\mu$m)</td>
<td>1.37229595675781e-3</td>
<td>68.2582</td>
</tr>
<tr>
<td>ZnO (2.0 $\mu$m)</td>
<td>5.63002876699194e-5</td>
<td>2.8004</td>
</tr>
<tr>
<td>PEC back reflector</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4.2: Absorption rates and percentages by layer for a simple flat slab solar cell structure. This is the rate at which energy is lost to absorption, integrated over the entire simulation bandwidth.

error between the two results. The good agreement follows from the high resolution of
the simulation. A lower resolution gives a similar curve but with a slight frequency shift,
yielding larger errors especially near frequencies where the slope of the reflectivity is high.
In two or three dimensional simulations, we cannot use such a high resolution for practical
reasons. We can however use a lower resolution to make some design conclusions, then run
a higher resolution simulation for more exact results.

The absorption energies (arbitrary units) in the structure are listed in Table 4.2. We see
that most of the energy absorbed goes into the Silicon layers, and a little more than 8% is
absorbed by ZnO losses. For optimal efficiency, it is desirable to maximize the absorption
rate over the entire cell while minimizing the percentage lost in the non-photovoltaic layers.
4.2 Thin-film roughness simulations for solar applications

We attempt to model the light scattering problem using an iterative approach. First we model the internal roughness as a simple two dimensional triangular-ridge grating with adjustable lattice width $sx$ and base angle $\alpha$, as shown in Figure 4.15. We then examine more complex models with more irregular triangular peaks to draw additional conclusions about the structure’s performance.

All of our solar cell models are two dimensional ones. Although the problem of Figure 4.10 is a three dimensional one, there are several arguments that favor a simplification. The first is that the three dimensional problem is intractably large. The second is that the two dimensional models are sufficient. The two dimensional models are physically anisotropic, meaning the reflection will depend on the excitation polarization. A realistic three dimensional structure will combine the behaviors of both polarizations. We can therefore try to draw conclusions for the full three dimensional structure by simulating both polarizations of the two dimensional one. Another argument is that we are trying to discern general trends for these problems, and not focus on the detailed spectral variations that might arise from a particular geometry. A good three dimensional model may help mask those anomalies, but the overall trends can still be derived from a series of two dimensional models, as we will show.

Figure 4.15: 2d triangular grating structure with adjustable parameters $\alpha$, the peak angle, and $sx$, the lattice periodicity.

4.2.3 Triangular ridge grating model

We attempt to model the light scattering problem using an iterative approach. First we model the internal roughness as a simple two dimensional triangular-ridge grating with adjustable lattice width $sx$ and base angle $\alpha$, as shown in Figure 4.15. We then examine more complex models with more irregular triangular peaks to draw additional conclusions about the structure’s performance.

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4 Antireflective coatings

<table>
<thead>
<tr>
<th>Lattice width:</th>
<th>sx = 250 nm</th>
<th>sx = 650 nm</th>
<th>sx = 850 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>decay = 1 $\times$ $10^{-07}$</td>
<td>18 min</td>
<td>50 min</td>
<td>74 min</td>
</tr>
<tr>
<td>decay = 1 $\times$ $10^{-12}$</td>
<td>25 min</td>
<td>166 min</td>
<td>115 min</td>
</tr>
</tbody>
</table>

Table 4.3: Computation times for three simulations run to two different field decay parameters.

For the triangular grating model, we ran the problem twice (for two polarizations) for 42 geometries, with $\alpha \in \{10 \, 20 \, 30 \, 40 \, 50 \, 60\}^\circ$, and $sx \in \{0.25 \, 0.35 \, 0.45 \, 0.55 \, 0.65 \, 0.75 \, 0.85\}$ µm. We consider normal incidence illumination for each simulation.

One can expect that a geometry with a wider unit-cell will require more computation because of the larger computation domain. This is generally true, but it depends on the simulation termination condition. Timing results for some of these simulations are shown in Table 4.3, for a resolution of 100 cells per µm. The simulations are terminated when the field component of the chosen polarization reaches a decay factor in magnitude of its peak value. Because field decay is nonlinear, this results in a counterintuitive drop in simulation time from 650 to 850 nm for the low decay factor of $1 \times 10^{-12}$. The timing results shown here are for simulations run on a 2.66 GHz Intel Core 2 Quad computer.

The aggregated results are shown in several plots. Figure 4.16 shows the normalized absorption rate for each geometry, for the $E_z$ polarization. Here $z$ is the dimension normal to the plane drawn in Figure 4.15. To explain the normalization, consider the previous flat slab problem. In that geometry, doubling the lattice width doubles the size of the volume integrated over to compute the absorption rate. It therefore makes sense to normalize unit-cells by their lattice width so as not to bias or disadvantage the absorption rates of geometries with wider or narrower periodicities.

In Figure 4.16, it is evident that larger angles $\alpha$ lead to higher absorption in the scatterer. The horizontal axis trend for a given angle $\alpha$ is not as strong. This is also an indicator that randomness of the surface roughness is not as critical a factor for good absorption. This can be seen more directly in Figure 4.17, where lines of constant sx are plotted on top of each other.

Similar results were obtained for the $H_z$ polarization, shown in Figures 4.18 and 4.19. For this class of gratings, the $H_z$ absorption rate is consistently greater than the $E_z$ one for the corresponding geometry. This can be understood as an analogue to polarization-specific coupling coefficients for waveguide gratings.

As a useful aid in understanding these results, we can plot the reflectivity spectra for any of the geometries computed. We can compare for example the spectra for the points with highest and lowest absorption rates of Figures 4.16 and 4.18. For the $E_z$ polarization, this is shown in Figure 4.20, and for the $H_z$ in Figure 4.21. We see that the geometries of high absorption result in lower reflectivities over most wavelengths. Additionally, the
4.2 Thin-film roughness simulations for solar applications

Figure 4.16: Normalized absorption rates for the $E_z$ polarization for $\alpha \in \{10, 20, \ldots, 60\}$° and $s_x \in \{0.25, 0.35, \ldots, 0.85\}$ µm. Lines represent a constant peak angle $\alpha$.

Figure 4.17: Normalized absorption rates for the $E_z$ polarization. Lines represent a constant lattice width $s_x$.

$H_z$ polarization reflects less, especially at longer wavelengths, as is also evidenced by the absolute values of the respective total absorption rates.

Additionally, we can observe how the spectra evolve as we sweep over geometry angles $\alpha$ for
Figure 4.18: Normalized absorption rates for the $H_z$ polarization for $\alpha \in \{10, 20, \ldots, 60\}^\circ$ and $sx \in \{0.25, 0.35, \ldots, 0.85\} \mu m$. Lines represent a constant peak angle $\alpha$. 

Figure 4.19: Normalized absorption rates for the $H_z$ polarization. Lines represent a constant lattice width sx.

a fixed lattice width. Such sweeps are shown for the $E_z$ polarization in Figure 4.22, and $H_z$ in Figure 4.23. As expected, larger angles $\alpha$ give lower reflectivities over most wavelengths. Individual peaks in the spectra can be traced as the $\alpha$ is increased, with most peaks tending to reduce in size.
4.2 Thin-film roughness simulations for solar applications

Figure 4.20: $E_z$ reflectivity spectra for the highest and lowest absorption results from Figure 4.16.

Figure 4.21: $H_z$ reflectivity spectra for the highest and lowest absorption results from Figure 4.18.

These peaks are however an undesirable artifact that comes with the triangular grating model. Real cell measurements do not have such highly modulated responses, ostensibly because they have a much more random peak structure, as shown in the SEM plot of Figure 4.10.
Figure 4.22: $E_z$ reflectivity spectra swept over peak the six angles for a fixed lattice width $s_x = 0.25 \mu m$.

Figure 4.23: $H_z$ reflectivity spectra swept over peak the six angles for a fixed lattice width $s_x = 0.35 \mu m$. 
4.2 Thin-film roughness simulations for solar applications

Figure 4.24: A more complicated grating structure with a lattice constant of 2.2 µm, consisting of 6 triangular peaks with peak angle $\gamma = 105^\circ$.

4.2.4 Multi-peak unit-cell computations

We now we consider a more difficult structure, one that better approximates the surface roughness of the various solar cell layers. The roughness is approximated by six overlapping peaks of semi-randomly chosen width and position, spread out over a unit-cell of 2.2 µm. These values are not truly random because they were simply chosen by hand in an initial attempt at capturing some of the randomness present in reality. For this surface, the peak angle $\gamma$ is fixed at 105 degrees. This angle corresponds to a large but practically manufacturable peak sharpness used in commercial cells.

On the quad-core processor described above, the 2.2 µm geometry required approximately 12.5 hours per polarization, run to a field decay of $1 \times 10^{-10}$.

For the $H_z$ polarization, we compare this more random structure, labeled ‘full struct’, with a spectrum for a comparable geometry from the triangular grating simulations. That geometry has larger peaks representative of the random structure, and also a peak angle $\alpha = 40^\circ$ ($\gamma = 100^\circ$) close to the 105$^\circ$ of the full structure. The juxtaposed spectra are shown in Figure 4.25 for the $H_z$ polarization.

The compared geometries have similar performance for wavelengths up to about 720 nm. Beyond that value, the triangular ridge grating shows peaks due to grating effects while the
more random structure has improved absorption.

In order to try to destroy the coherence of reflections, we optionally add a shift of the surface roughness of the mcSi/ZnO interface with respect to the aSi layer. We do something similar for the back reflector, while also optionally scaling the peaks of the back reflector by some factor.

For the offset, we shifted the mcSi/ZnO layer right by an arbitrary value of 300 nm, and the back reflector by 450 nm. This offset strategy did not have a profound effect when compared to the structure with aligned layers, as shown in Figure 4.26 for the $H_z$ polarization.

Separately, we scaled the back reflector interface by factors of 0.5 and 2.0, halving or doubling its height, respectively. These results are shown in Figure 4.27 for the $H_z$ polarization. We might expect that a scaled back reflector may reduce modulations in the spectra by removing some of the coherent interferences of reflections in the structure. The plots however indicate that this is not the case, as the best performance comes from the geometry with
4.2 Thin-film roughness simulations for solar applications

Figure 4.27: Spectra comparison for the $H_z$ polarization for the structure of Figure 4.24, and a similar structure with a vertically scaled back reflector. Three cases are compared. $yscale = 1.0$ means the back reflector shape matches that of the other layers in the stack-up, $yscale = 0.5$ means the height of the back reflector topology is halved, and $yscale = 2.0$ means it is doubled.

4.2.5 Randomized roughness layers

In a further iteration, we define larger, ‘more random’ structures using an algorithm that sets triangular peaks to define a surface roughness.

The triangular peaks have a base width between 300 nm and 800 nm, with a truncated Gaussian normal distribution centered at 500 nm and a standard deviation of 100 nm (ignoring truncation).

The peaks may also be ‘skewed’, meaning the peak of the triangle is not aligned with the center of the base. Skews are defined for each triangle as a value between 0.0 and 1.0, where 0.0 means the peak is vertically aligned with the left vertex of the base, and 1.0 the right vertex. We set our algorithm to produce triangles with skews between 0.25 and 0.75, with Gaussian mean of 0.5 and Gaussian standard deviation of 1.0 ignoring truncation.

The altitude of each triangle is assigned based on the base width, such that the peak angle would be 103 degrees if the skew value were 0.5. Any other skew value will reduce the peak angle slightly.

Finally, each triangle overlaps the previous triangle by a fixed value 150 nm. We generate enough triangles to produce a structure 6 $\mu$m wide. Using this algorithm we generated the five roughness geometries shown in Figure 4.28. These are intended to be two dimensional representations of slices of realistic surface roughness, such as the one illustrated in the SEM plot in Figure 4.10.

The $E_z$ reflectivities for the five cell models and the average of the five reflectivity curves are shown in Figure 4.29. For the $H_z$ polarization, the same curves are shown in Figure 4.30.
Figure 4.28: Five surface roughness morphologies. A single unit-cell of width 6 µm is shown for each structure. Each peak has a randomly chosen height and skew angle.

Figure 4.29: $E_z$ reflectivity spectra for the five structures shown in Figure 4.28. The bold curve shows the averaged spectrum.

While the convergence of results generated from random structures can be expected to be slow, we can already get a sense of an evolving pattern by looking at the average over five results.

Finally, we consider the case where unpolarized light is incident upon the solar cell. In this case, we assume the total reflectivity is the simple arithmetic mean of the reflectivities of the $E_z$ and $H_z$ polarizations. These results are shown in Figure 4.31, in addition to the average over the five curves.

We can imagine that the modulations or humps in the reflectivity curves could be averaged away if we took many more geometry samples. The result would be four larger humps that are more spread out in frequency (wavelength). This may then match previously published measurements for solar cells (keeping in mind that our structures are not identical), shown in Figure 4.32.
4.2 Thin-film roughness simulations for solar applications

Figure 4.30: $H_z$ reflectivity spectra for the five structures shown in Figure 4.28. The bold curve shows the averaged spectrum.

Figure 4.31: Unpolarized reflectivity spectra for the five structures shown in Figure 4.28. The total reflectivity for each curve is the average of the corresponding $H_z$ and $E_z$ curves from Figures 4.30 and 4.31. The bold curve shows the average over of all five unpolarized spectra. In the average we can start to recognize four major humps.

4.2.6 Summary of findings

The three solar cell models show that analysis using FDTD simulations is a feasible alternative to the cumbersome design-by-manufacturing approach. The simple triangular ridge grating model confirms the industry knowledge that sharper roughness peaks generally create higher efficiency solar cells. Modulations in the reflection spectra of these gratings indicate however that the model is insufficient in describing the actual behavior of solar cells. The semi-random model gives much better results in this regard, but still has some periodicity artifacts not present in manufactured panels. The third iteration of the model with randomized peak sizes and shapes shows that more complexity can bring additional improvements.

A next iteration using a more complex model is simply a question of computation power. Additional degrees of freedom in the surface roughness definition, three dimensional rough-
Figure 4.32: Quantum efficiency measurement for a thin-film solar cell, from [74]. The QE is inversely related to the absorbance in the cell. The four humps in the absorbance curve could correspond to trends that emerged in Figure 4.31.

These simulation results offer a host of options for further work. Because thin-film solar panels are a low cost alternative to more efficient variants, they are generally not installed on one- or two-axis sun-following mounts. As a result, it would be useful to optimize thin-film layers for all-day efficiency. FDTD would be suitable for computing the angular incidence performance. For an optimization, it may be possible to use a single broad angle, broadband simulation to compute a fitness for any one structure.

Layer specific absorption rates are also interesting for design purposes. In the FDTD implementation we use, it is only possible to integrate polarization energies over a rectangular volume. Implementing arbitrary volume integrations would allow for layer specific loss computations in solar cells with internal roughness.

Additional material data with suitable fits for shorter wavelengths would allow a better comparison to published results and measurements. The simulations could be rerun using better material models, not only to search for better agreement, but to also compare to the above results to check how sensitive the simulated structures are to the material properties.

Finally, it may also be possible to link light scattering simulations to semiconductor models of the photovoltaic layers. This would open a new avenue for comparing simulated results with measured ones, lending credence to the approach of design-by-simulation for the solar cell problem. Additionally, the engineer designing a cell is more interested in its electrical performance and less its light scattering properties. A link between the two would facilitate that end.
4.3 Scattering properties of a 3D textured antireflective surface

Antireflective coatings are also an important technology for sensitive infrared receivers, such as those used for deep-space astronomy. These receivers require special cooling systems to minimize their noise temperatures, highly sensitive sensor elements to pick up low signals from distant sources, and antireflective coatings to help maximize signal-to-noise ratios.

In this section we examine one such infrared antireflective coating designed for a receiver operating in the mid-wave infrared region (3 to 5 \( \mu \text{m} \)). This coating presents an interesting test case for FDTD analysis because it is two dimensional in periodicity and three dimensional in shape. In this section, we discuss how to analyze this problem using FDTD, and compare the results with those generated by two other methods, namely finite element (FE) and rigorous coupled wave analysis (RCWA).

4.3.1 FDTD analysis

The problem is defined by the pyramidal grating structure shown in Figure 4.33. A lossless Silicon pyramid (\( n = 3.42 \)) sits atop a Silicon substrate not pictured, and is infinitely repeating in two dimensions. The geometry parameters given for this problem are \( a_b = 1.2 \ \mu \text{m}, a_t = 0.25 \ \mu \text{m}, \) and \( h = 1.25 \ \mu \text{m}. \)

The FDTD analysis is analogous to the one presented in Section 4.1 and Chapter 2, only expanded to three dimensions. For the three dimensional case, a source plane is used to generate incident waves (as opposed to a line for the two dimensional problem). Likewise, transmission and reflection flux integrations take place over planes parallel to the scatterer.
Figure 4.34: Normal incidence reflectivity for the pyramidal roughness antireflective coating on an infinite layer of silicon. Doubling the resolution from 40 nm to 20 nm shows a slight change in the grid size.

As with two dimensional problems, the periodic boundary conditions enforce unique excitation angles for each excitation frequency. To obtain spectra for a particular incidence angle, it is therefore necessary to run multiple simulations. For increased accuracy, we make these simulations narrowband ones (center wavelength, ±10%). The angles covered by plane waves over these wavelengths are defined by the relationship of Equation 4.2 and are in the range
4.3 Scattering properties of a 3D textured antireflective surface

![Diagram](image)

Figure 4.35: Top-down view of the simulation results shown in Figures 4.36 and 4.37. Each simulation results in a line of points in the $\lambda$-$\theta$ plane. Because the simulations are narrowband, these are straight lines. Broadband simulations yield a different shape, shown in Figure 2.10.

\[
\arcsin \left( \frac{1}{1.1} \sin 30^\circ \right) \leq \theta_i \leq \arcsin \left( \frac{1}{0.9} \sin 30^\circ \right) \quad (4.2)
\]

\[
27.036^\circ \leq \theta_i \leq 33.749^\circ \quad (4.3)
\]

for $\theta_{cen} = 30^\circ$. This yields a $\lambda$-$\theta$ plane pattern shown in Figure 4.35, for center wavelengths $\lambda_{cen} \in \{3.1, 3.2, 3.3, \ldots 5.0\}$ $\mu$m. Each simulation is visible as a line of points. Were they not as narrowband, the results would appear less as lines and more as curves, as in Figure 2.10.

An isometric perspective shows these results as a three dimensional surface in Figure 4.36 for the $E_y$ polarization and in Figure 4.37 for $H_y$. This perspective allows us to observe the ridges present in the reflectivity spectra. The highlighted points indicate those of the center wavelength of each simulation, corresponding to an incident angle of $\theta_i = 30^\circ$.

These points undersample the ridge peak present in the plot. Figures 4.38 and 4.39 show these points on a two dimensional plot, fit with curves of cubic interpolation. As is visible in the isometric perspective however, we can resolve the ridge better (and the maximum level of the peaks present at $30^\circ$) by using a surface interpolation and then taking a slice of that surface. This possibility is an additional benefit of the FDTD approach. An alternative, also suitable for frequency domain methods, would be to use model-based parameter estimation (MBPE) to run additional simulations to increase the sampling close to the ridge.
4 Antireflective coatings

Figure 4.36: Three dimensional plot of the $E_y$ reflectivity results from 21 narrowband, multi-angle FDTD simulations. Points on the cut plane for $\theta = 30^\circ$ are shown. This view helps accentuate that the reflectivity ridge maximum is not resolved well by fixed frequency sampling.

Figure 4.37: Three dimensional plot of the $H_y$ reflectivity results from 21 narrowband, multi-angle FDTD simulations. Points on the cut plane for $\theta = 30^\circ$ are shown.

4.3.2 Comparison with other methods

We now perform a qualitative comparison with results of two alternative methods. One is an FE method using a software package called JCMsuite [75, 76], and the other is an
4.3 Scattering properties of a 3D textured antireflective surface

Figure 4.38: $E_y$ reflectivity spectrum for the pyramid grating at 30° incidence. The points correspond to values simulated by separate FDTD simulations, while the line connecting them is a cubic polynomial fit.

Figure 4.39: $H_y$ reflectivity spectrum for the pyramid grating at 30° incidence. The points correspond to values simulated by separate FDTD simulations, while the line connecting them is a cubic polynomial fit.

RCWA [77] implementation run on MATLAB.
For normal incidence, the results of each method are shown in Figure 4.40. The agreement of the three curves affords us confidence that the different techniques can find the correct result within some error bound. The FDTD technique, highlighted by the bold curve for the resolution of 20 nm, is able to get a much finer frequency resolution in a single simulation through the Fourier transform described in Chapter 2. This resolution is beneficial in resolving the peak, where the two frequency domain methods noticeably undersample. This is not a guarantee of increased accuracy, but is rather useful for attaining many sample points for resolving resonances. The RCWA curve deviates from the rest for shorter wavelengths because those simulations were undermeshed.

The oblique incidence comparisons are shown in Figures 4.41 and 4.42. For these plots, each point of the FDTD curve was found by a separate simulation, similar to the frequency domain approaches. The differences are comparable to those for the normal incidence comparison, but indicate the need for a further convergence study. A coarser grid resolution was used for the FDTD simulations, possibly decreasing the accuracy.

While there are some advantages to the FDTD approach, speed is not one of them. The 40 nm resolution curve of Figure 4.40 took 7.5 hours to compute on a 2.66 GHz Intel Core 2 Quad computer, distributed over the four processors. This time can be reduced by a factor of 4 for the normal incidence results by taking symmetries into account. For oblique incidence simulations, symmetries cannot be used. Oblique simulations are also slower because of the forward propagation speed of oblique waves, and because the computation domain is necessarily larger (to ensure the success of PML layers, for example). A single run required slightly less than 8 hours using 16 processors (2.5 GHz AMD Opteron 8380) on a cluster.
4.3 Scattering properties of a 3D textured antireflective surface

Figure 4.41: Oblique incidence (30°) $E_y$ reflectivity spectra as computed by three different numerical methods.

Figure 4.42: Oblique incidence (30°) $H_y$ reflectivity spectra as computed by three different numerical methods.

(about 1 week per polarization, including 21 separate simulations). Both polarizations were computed in under 4 days using 128 processors.

JCMwave is able to perform much faster because it uses higher order finite elements and can therefore compute to a satisfactory accuracy on a coarse meshing. In an unoptimized
trial, it only required about 100 seconds per frequency point for each angle of incidence and polarization (about 30 minutes for a 20 point frequency sweep). Simulations were run on a 2.8 GHz Opteron 8220 using four threads.

The RCWA MATLAB script required a fixed time of 130 seconds per frequency for each incidence angle and polarization. While this is slightly longer than the time needed by JCMwave, it was only run on a single core 1.6 GHz Itanium II processor. This impressive timing is possible because the approach is semi-analytic. It can still be improved using a faster non-interpreted implementation of the RCWA algorithm.
In this chapter we examine a type of metallo-dielectric metamaterial known in literature as Sievenpiper structures, named after Daniel Sievenpiper who first published results on their applications as high-impedance surfaces (HISs). They are also known as mushroom-like structures because of their metal geometry, consisting of a post (the stem), supporting a patch (the cap).

Because of their useful electromagnetic properties, Sievenpiper structures have applications in antenna design \[78\] as well as switching noise reduction in high-speed digital circuit power planes \([79, 80]\). By a process of experimentation, we discover that they are also useful for the sealing of microwave radiation.

Early microwave ovens had several bolts to secure the oven door to the oven body. Because this was inconvenient for readily accessing the oven cavity, doors were modified so they could freely be opened and closed, leaving only a small air gap between the door and the door frame. A quarter-wave choke (QWC) fitted close to this gap then uses half-wave cancellation to minimize the amount of microwave radiation that escapes the oven.

A QWC for a combination microwave/convention oven is shown in Figure 5.1. It consists of folded fins (with ribs for mechanical strength) and slots between fins to prevent the formation of standing waves. A computer-aided design (CAD) model in Figure 5.2 reveals some of the hidden complexity required for mounting the QWC to the oven door.

This chapter focuses on the use of a Sievenpiper structure based EBG waveguide filter to replace conventional, costly QWC seals. A cartoon top-down cross section of the conventional QWC seal and the replacement seal are presented in Figure 5.3. We first discuss the simulation approach and design of these structures, then present simulation results and measurements for a prototype EBG microwave seal.

5.1 Modeling and simulation

There are several models available in the literature for analyzing Sievenpiper structures using simple circuit or transmission line approximations \([6, 78, 80]\). The most basic model defines the center bandgap frequency for an infinite crystal, or central stop band frequency for a finite one. It is defined by a capacitance between two neighboring plate edges and an inductive path formed by the loop between those edges, as shown in Figure 5.4.
Figure 5.1: Photograph of the inside of an oven door and the conventional QWC. The QWC consists of fins that are 3 cm long, corresponding to a quarter wavelength for a frequency of operation of 2.45 GHz. Slots between the fins prevent the buildup of heat-inducing standing waves.

Figure 5.2: A CAD model showing the complexity of the oven door construction. The bottom piece is the main section of door steel, the top left piece is the cavity door frame, and the top piece is the QWC. The QWC is joined with the door steel by an elaborate process involving many screws (one screw head is visible in figure) and welds.

The characteristic resonance frequency is defined by the parallel LC resonance \( \omega_{res} = \frac{1}{\sqrt{LC}} \). The resonator bandwidth is found by using surface impedance considerations defined in [81]. There, the fractional bandwidth is approximated to be
5.1 Modeling and simulation

Figure 5.3: A cartoon schematic that illustrates the placement of the conventional QWC seal and the EBG seal replacement.

Figure 5.4: A simple model equating the gap capacitance of a Sievenpiper array and the post/plate inductive path to a parallel LC resonator.

\[ \frac{\Delta \omega}{\omega_0} = \frac{Z_0}{\eta} = \frac{\sqrt{L/C}}{\sqrt{\mu_0/\varepsilon_0}} \]  

(5.1)

where \( Z_0 \) is the characteristic impedance of the HIS, defined by the impedance of a parallel LC resonator, and \( \eta \) is the impedance of free space. These relations, in conjunction with the model shown in Figure 5.4 provide design rules shown in Table 5.1.

This simple model does not consider the many resonances present in an EBG material made of Sievenpiper structures, but it does provide a tool that overcomes the brunt of the design work. For example, if we have a structure design that has a stop band at 10 GHz but need a new design that operates at 5 GHz, we can simply double the loop inductances and inter-gap capacitances by multiplying all geometric dimensions by a factor of two. If we then

<table>
<thead>
<tr>
<th>Tighter bandwidth</th>
<th>Smaller L, larger C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower frequency</td>
<td>Larger L, larger C</td>
</tr>
<tr>
<td>Larger L</td>
<td>Larger plates, longer posts</td>
</tr>
<tr>
<td>Larger C</td>
<td>Larger plates</td>
</tr>
</tbody>
</table>

Table 5.1: EBG design rules for mushroom-like structures based on the simple parallel LC resonator model.
Figure 5.5: A lumped element circuit model for the Sievenpiper structure. Metallic paths correspond to inductive elements at microwave frequencies, and air gaps function capacitively.

require a wider bandwidth at that frequency, we can increase the inductance and decrease the capacitance while keeping their product constant.

More accurate circuit models exist, such as the ABCD transmission line model presented in [80]. It can accurately predict the position and bandwidth of the stop band for a semi-finite Sievenpiper structure waveguide filter. Because it is a one dimensional model however, it fails to predict the multiple nulls present in the stop band, replacing these with a single system resonance.

Two dimensional lumped circuit and transmission line models attempt to overcome these deficiencies. One such model is shown in Figures 5.5. Depending on the model chosen, the lumped elements will have different parameter values. The model for each unit-cell is then combined to form a larger two dimensional network, shown in Figure 5.6, depicting the external circuit connections for a five-by-five network of the two-port unit-cell models of Figure 5.5. There, a waveguide mode is approximated by using voltage sources with amplitudes that sample those of a waveguide mode. Alternatively, for a transverse electromagnetic (TEM) system, only one voltage source and one column of unit-cells is necessary, with matched ports embodying the periodicity of the system.

The main inadequacy of these models is that it is difficult to predict what lumped parameter values will yield a suitable result (such as an $S_{21}$ spectrum) for a given geometry. This can be seen in comparisons of two dimensional circuit models to FEM simulations [80]. Several lumped element formulas are summarized in [82], but they are at best rough approximations. For the inter-gap capacitance problem, there are several microstrip technology papers available, including a notable series of papers by Wheeler on a conformal mapping approach [83–88]. There are however no simple explicit laws that govern equivalent gap capacitances. Less literature is available for computing the inductance of vias. More complex models are available that may provide insight for a new analysis [89].
5.1 Modeling and simulation

Figure 5.6: A circuit model for analyzing two-port units of Figure 5.5. The model shown can be used to approximate the seal behavior in a PEC waveguide. The choice of termination elements depends on whether the waveguide opens to free space, has PEC walls, or infinitely periodic in the transverse direction. This example shows a 5 port by 5 port system. For a TEM waveguide, only one input and output port and one column of unit-cells is sufficient.

5.1.1 Band diagram computation for EBG metamaterials

Numerous methods are available for computing band diagrams of infinitely periodic metallo-dielectric EBG materials. These diagrams are useful from a design perspective because they can be used to quickly isolate the start and stop frequency of the bandgap. They can also identify the frequency and wave vector of all periodic field solutions. Some noteworthy work on the computation of dispersion diagrams for shielded Sievenpiper structures considers a closed form analytic solution [90], as well as a numerical multiconductor transmission line (MTL) theory approach [92].

Consider as an example the application of the FDTD method to compute the dispersion curves for a mushroom-like EBG structure in a waveguide with geometry parameters shown in Figure 5.7. Using the approach described in Chapter 2, we can generate the band diagram of Figure 5.8, which identifies a bandgap between 9.58 and 18.8 GHz. Results from sixty separate FDTD simulations are plotted, with each simulation corresponding to a single wave vector.

Other computational methods that yield similar results for Sievenpiper type structures include FEM [81] and the transmission line matrix (TLM) method [93]. While band diagram generation is computationally demanding for all methods, it is usually unnecessary to compute the entire diagram for the purpose of gap frequency extraction. In our example of

\[1\] Clayton wrote the ‘bible’ on MTL analysis, including both time- and frequency-domain approaches. It starts with simple two conductor lines, but then generalizes to multiconductor ones [91].
Figure 5.7: Unit-cell model of a mushroom-like EBG structure in a waveguide. The geometric parameters are the lattice width $a$, the waveguide height $b$, the substrate height $h$, the patch width $w$, the patch thickness $d$, and the via diameter $v$. For the FDTD computation of the dispersion curves, a point source is placed in a random location to excite all harmonic modes.

Figure 5.8: Band diagram of the structure of Figure 5.7 with parameters $a = 2.4$ mm, $w = 2.25$ mm, $h = 1.5$ mm, $v = 0.35$ mm, $d = 0.1$ mm, $b = 3.1$ mm, and $\varepsilon_r = 2.2$. Computations were performed using an FDTD resolution of 20 pixels/mm. Vertical lines represent IBZ corners, while horizontal lines represent the bandgap edge frequencies.

Figure 5.8, the gap start frequency is defined at the first band edge by a single wave vector in the first IBZ leg. The stop frequency is defined by the intersection of the second mode with the light cone. A simple search algorithm can be used to identify these minima and maxima over a small number of wave vectors.
5.2 Microwave radiation seal using an EBG metamaterial

5.2.1 FDTD scattering simulations

For the microwave design of finite EBG structures, it is usually necessary to compute the scattering parameters (more specifically, the power reflectance and transmittance spectra).

We investigate finite and semi-finite EBG seals for a microwave application at 2.45 GHz. The goal of such a seal is to achieve a high attenuation (low $S_{21}$) over a bandwidth large enough to accommodate fabrication tolerances. Such a design for closed waveguide filtering is shown in Figure 5.9. By optimization, this example achieves a filter attenuation of over -80 dB over a bandwidth greater than 250 MHz. Physical constraints may however limit the stop band performance of a real design, such as the one discussed in the following section. There, it is not possible to have an arbitrarily thick substrate, for example.

Semi-finite EBG filters require a similar FDTD analysis. An infinitely wide parallel plate waveguide has a finite number of rows of EBG elements in the depth dimension of the waveguide (where a normally-incident TEM mode propagates in the depth dimension). These simulations run faster than their closed waveguide counterparts because we can take advantage
Figure 5.10: A series of parallel plate waveguide simulations where number of rows of patches is increased from 1 to 20. Significant $S_{21}$ attenuation becomes available with five or more rows, for this geometry. A large enough row count and a simulation run to a low enough energy drop would indicate a filter characteristic that matches the band edges (vertical lines) for the crystal whose band diagram is shown in Figure 5.8.

of periodic boundary conditions to reduce the computation domain size. The domain then contains a single column of patch/post structures. If we increase the row count, we should have better filter behavior. The more rows there are, the more the filter approximates the bandgap of an infinite structure. This is demonstrated in Figure 5.10, where the number of EBG rows is increased from 1 to 20. An infinite number of rows would result in a filter with a stop band corresponding to the bandgap of Figure 5.8.
5.3 Radiation seal

In this section we describe the design approach and fabrication of a microwave oven radiation seal. We first examine a few design aspects, then present results from one of several tested designs.

5.3.1 Design

There are several plate shape possibilities. Fork and ‘F-shaped’ plates were proposed in [94]. We show the fork variants in Figure 5.11, along with hexagonal patches proposed by Sievenpiper [78, 95], as well as a Helvetic cross variant with passive inter-cross patches for increased capacitive coupling. While an infinite number of variations are possible, there is no great variation in performance or electromagnetic properties. This is partially due to the fact that forbidden EBG frequencies are defined by lattice interactions, and not higher frequency resonances that may occur on the patch itself. Rectangular shaped patches offer enough degrees of freedom to provide for compact high attenuation seals, so we focus on these types for our design.

Next to the patch shape, some other degrees of freedom include substrate thickness (and post length), inter-plate gap sizes, air gap size, and post geometry. Because individual simulations run too long to allow for numerical optimization of the many degrees of freedom available, we must rely on simple single parameter sweeps to understand the role of each parameter.

For a fixed operation frequency and patch row count, there is a tradeoff between substrate thickness and total filter width (Figure 5.12). This can also be seen from the LC model discussed above. The seal, which sits like a frame around a painting (in this case, the oven

Figure 5.11: An assortment of patch geometries. The fork shape patches were proposed to control the interaction between neighboring elements. While an infinite number of patch shapes is possible, the bandgap of an EBG crystal is defined mainly by the patch area, gap size, and substrate thickness. The hexagonal patches use a triangular lattice, but do not differ extremely in bandgap behavior from square lattice EBG designs.
Figure 5.12: Geometry parameters for substrate thickness $t$ and segment width $w$. For a desired attenuation, there exists a tradeoff between these two parameters.

<table>
<thead>
<tr>
<th>$t$ (mm)</th>
<th>$w$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>90.7</td>
</tr>
<tr>
<td>8</td>
<td>73.0</td>
</tr>
<tr>
<td>10</td>
<td>65.0</td>
</tr>
<tr>
<td>17</td>
<td>43.0</td>
</tr>
</tbody>
</table>

Table 5.2: Final dimensions for the substrate thickness $t$ and total width $w$ for several EBG designs that provide -80 dB of attenuation over a minimum of 100 MHz bandwidth.

cavity opening), must satisfy some geometry constraints. A frame segment may not for example be so wide as to block the oven viewing window or prevent the oven from fitting inside the allotted cabinet space. Material constraints, on the other hand, such as available substrate thicknesses, preclude an arbitrarily thick seal.

To understand this trade off, we simulate several geometries where we adjust the lattice size, patch width, and substrate thickness. We search for geometries that provide -80 dB of attenuation in a stop band with a minimum of 100 MHz bandwidth. Table 5.2 shows the final dimensions for a segment width $w$ for several substrate thicknesses $t$. For this example the substrate permittivity is fixed at $\varepsilon_r = 2.7$, but for the actual design we use a permittivity of $\varepsilon_r = 4.5$ which suitably models the FR4 substrates available.

The air gap between the patches and the top face of the waveguide (shown in figure 5.13) also plays a role in the filter performance. One analysis considers the propagation modes in an inhomogenously filled parallel plate waveguide, but this excludes the presence of EBG structures [96]. The simplest approach is to perform a parameter sweep over the air gap spacing. Figure 5.14 shows the evolution of the stop band as the air gap is adjusted between 2 and 5 mm. The start and stop frequencies of the stop band vary considerably, along with the attenuation of the stop band. This particular filter design gives the best attenuation over a sufficient bandwidth for an air gap dimension of 3 mm. Filter performance decreases for larger air gaps.
5.3 Radiation seal

Figure 5.13: Sideview of the shielded EBG filter. The filter consists of patches and posts embedded in a substrate, connected through a common ground plane. An air gap and an optional superstrate separate the patches from the top of the waveguide.

![Figure 5.13: Sideview of the shielded EBG filter.](image)

Figure 5.14: $S_{21}$ curves for one EBG waveguide filter as the air gap spacing is varied from 2 to 5 mm. The curve for an air gap of 3 mm has higher attenuation than the other three curves.

![Figure 5.14: S_{21} curves for one EBG waveguide filter as the air gap spacing is varied from 2 to 5 mm.](image)

Additional geometries offer additional degrees of freedom. Some of the geometries we investigate include ones with two posts, patches with passive coupling plates underneath (such as the ones shown in [95]), and folded posts like the one shown in Figure 5.15. These folded style posts allow for simplified manufacturing while creating a similar bandgap effect to the structures with centered cylindrical posts. Adjusting the width of these folded posts has a similar effect to adjusting the radius of centered posts, as can be seen in Figure 5.16, where the flat post width is adjusted between 2 and 4 mm.

![Figure 5.15: Folded posts.](image)

![Figure 5.16: Adjusting the width of these folded posts.](image)

During the design process, it is oftentimes useful to understand how the filter functions by looking at field plots. Figure 5.17 shows an electric field slice and how the fields are
5 Metamaterials for microwave shielding

Figure 5.15: A type of post geometry that offers an alternative to drilling holes through a substrate. This type of design exhibits a similar stop band to conventional Sievenpiper designs with centered, cylindrical posts.

blocked by the patch post configuration at 2.85 GHz. A time stepped animation over the entire phase cycle shows how fields resonate between neighboring structures in order to reject propagating waveguide modes. Surface current visualizations are an alternative way to observe these effects.

For the first seal prototype, we use a seal design with sufficient attenuation and bandwidth. The $S_{21}$ curve for a section of this design in a PEC waveguide is plotted in Figure 5.18.

5.3.2 Fabrication and measurement

Simulations of EBG waveguide filters predict that they are a feasible alternative to conventional QWCs. We fabricate a complete oven seal using the EBG principle to develop a working proof of concept. Initial measurements of first prototypes indicate a favorable outcome.

A perspective view of the seal frame situated on the oven door frame is shown in Figure 5.19. For the prototypes it is necessary to consider the form factor dictated by the oven geometry. Specifically, the frame segment width dimension may be no wider than 45 mm. Because of manufacturing constraints (available substrate thicknesses, and aspect ratio for drilled holes), the thickness of the substrate layer is limited to 10 mm. These two constraints are opposing, as described in Table 5.2. We are able to design a geometry with sufficient attenuation and bandwidth that satisfies these constraints.
5.3 Radiation seal

Figure 5.16: $S_{21}$ parameters for various folded post widths $s$. The frequency shift indicates that it is possible to adjust the operation of the EBG structure without changing the main dimensions of substrate thickness and width, while at the same time not sacrificing bandwidth.

5.3.3 Full seal simulations

Using a commercial FDTD simulation tool (CST Microwave Studio), we check to see if the full three dimensional EBG microwave seal performs as well as the simple waveguide section simulations. A CAD model of the microwave oven cavity and door are used. Instead of modeling the oven magnetron and waveguide channel, we simply use a waveguide mode and a section of the waveguide for the excitation.

Field plots then indicate the performance of a given design. Cut planes of a functioning and a non-functioning seal are shown in Figure 5.20. The non-functioning seal is transparent to microwaves at the frequency of operation, whereas the functioning seal effective blocks waves from escaping the cavity.

The same field plot for the final EBG seal design is shown without the door to illustrate the cavity modes present in Figure 5.21. This design consists of many more patch elements,
Figure 5.17: A slice showing the electric field and its attenuation as waves unsuccessfully attempt to propagate through the waveguide. The excitation is a waveguide mode at the left port, and the direction of propagation is from left to right, leading to a reduction in standing waves along the inner ring of the seal.

Additional field views help illustrate the functionality of the final design. A side cut in Figure 5.22 shows how the electric field strength decreases as waves try to propagate along the door near the top corner of the oven model. In non-functioning models it is evident how waves escape at the same location, as shown in Figure 5.23.

A final post-processing near-field to far-field transform (NTFF) [12] results in the power pattern shown in Figure 5.24. We can judge the performance of the seal with respect to other designs by examining the maximum of the field plot, as well as its symmetry. A good design leaks no more and no less on any side or corner, resulting in a fairly spherical power pattern.

5.3.4 Manufacturing of seal prototypes

Using geometry parameters from simulation models, we then create CAD models for printed circuit board (PCB) layouts. Because of the large numbers of elements (in some designs, over 900 patches and posts for a full seal), it is advantageous to automate the generation layout Gerber files using some scripting language.

For the initial run, we use both in-house and external prototyping to compare manufacturing techniques, and also to study repeatability (resilience to variations within manufacturing
5.3 Radiation seal

Figure 5.18: $S_{21}$ parameters for a microwave seal in a PEC waveguide. The substrate is 10.0 mm thick with $\varepsilon_r = 4.5$. Patches are 6.5 mm square, with 0.1 mm metalization thickness, with 1.0 mm gaps in between. Post diameters are 1.5 mm, and the air gap between the patches and the waveguide roof is 2.0 mm. The $S_{21}$ drop below 1.5 GHz is caused by waveguide cutoff and disappears for TEM simulations of the EBG device in parallel plate waveguides.

tolerances). The in-house prototype is made from sheets of copper-clad FR4 PCB stock. We use 4 layers of 2.5 mm FR4 to arrive at a total substrate thickness of 10.0 mm. The holes for the posts are drilled using a high speed vertical drill press, and the posts are created by using 1.5 mm diameter copper rivets, shown in Figure 5.25.

Because of in-house fabrication limitations, the full frame is assembled using a dovetail fabrication technique. Here, the PCB layout is divided into 4 smaller quadrants that are attached to one another by overlapping or dovetailing copper-free inner layers. These layers are then epoxied together, creating a full frame seal. Seams in the ground plane are short circuited using copper tape. Finally, corners of the seal are cut out to accommodate door hinges. Simulations show that these cutouts result in a minimal performance reduction.

The externally fabricated prototype uses copper plated vias for posts, as seen in cross section in Figure 5.26. For posts with small aspect ratios (height/diameter < 8), we are also able to obtain EBG behavior with samples that use a type of paste that is highly conductive at microwave frequencies. Holes drilled for the posts are coated with this paste by means of vacuum suction.
Figure 5.19: A full three-dimensional oven model with an EBG seal structure mounted on the cavity door frame. The oven door is present in the model but transparent to allow a view of the EBG surface and oven cavity. The waveguide at the top of the oven is illuminated with a \( \text{TE}_{10} \) mode, and is used to form multiple modes inside the oven cavity. The inside of the cavity is marginally simplified to reduce the number of cells necessary to mesh the oven, but the main dimensions and electromagnetically relevant shapes remain unaltered.

Figure 5.20: Electric field plots of functioning and non-functioning microwave EBG seal designs. The non-functioning seal is transparent to waves following the waveguide channel formed between the oven door and the cavity door frame. This results in microwaves that radiate away from the oven. The functioning seal rejects these waves so they stay inside the oven cavity.
5.3 Radiation seal

Figure 5.21: Electric field distribution snapshot for a full oven seal corresponding to the structure described by Figure 5.18. The oven door has been made transparent to illustrate the modes present inside the oven cavity.

Figure 5.22: A side cut showing the field distribution in a plane transverse to the EBG seal patches. Microwave fields decrease toward the outside of the seal.

5.3.5 Seal leakage measurements

Before we record measurements with the oven seals, we measure the complex permittivity of substrate samples. The purpose is first to check that the permittivity assumed during the design process and the permittivity of the delivered substrate do not differ drastically. For simplicity and speed, design simulations are undertaken using a simplified substrate permittivity model that neglects dispersion and losses. In the case of FR4, the losses are significant at microwave frequencies ($\varepsilon'' \approx 0.06$ at 2.45 GHz), but these losses enhance the performance of the filter. For measurements, we place unplated cut-to-fit samples of the FR4 stock in an S-band waveguide (2-4 GHz). A standard measurement uses a Hewlett-Packard (HP) 8753ES S-parameter network analyzer in conjunction with the HP 8507B analysis package for computing complex permittivities from S-parameter measurements. These permittivity measurement procedures are described in detail in [97–99]. Pictures of
5 Metamaterials for microwave shielding

Figure 5.23: A side cut illustrating the field leakage across poorly designed EBG seal. Waves that enter the channel between the microwave oven door and the cavity door frame propagate outside the oven in an unadulterated fashion.

Figure 5.24: NTFF radiation power computed for the seal shown in Figure 5.22. This pattern is fairly symmetric and spherical, indicating good performance. The peak power level of -45.1 dB is on par with the far-field peak for simulations of the oven shielded by the conventional QWC.

the waveguide measurement setup are shown in Figure 5.27.

To measure the sealing behavior of the conventional QWC and the EBG seal, we use the following procedure. First, using the available oven, we remove the magnetron and replace it with a low-power magnetron probe (Toshiba E4435). This has the same end probe of a normal magnetron, and an N-type connector that can be hooked up to a vector network.
5.3 Radiation seal

Figure 5.25: Photographs showing the ground plane side of an EBG seal with copper rivets to be inserted as posts, and the front side of an EBG seal with finished riveting.

Figure 5.26: A sample of the externally produced EBG seal. The cross section bisects the posts, showing the copper plating of the vias used as EBG posts. The substrate shown is FR4, which has an inherently yellow color. A protective solder mask on the top surface gives the sample a greenish appearance.

Measurements are taken at a fixed distance from the oven door (by using a microwave transparent foamboard spacer), at both horizontal and vertical polarizations. Wave components normal to the sensor waveguide aperture are negligible because of the nature of the analyzer. We can then perform controlled frequency sweeps over the frequency band allowed by the S-band waveguide (approximately between 2 GHz and 3 GHz). We then use an open ended S-band waveguide as the sensor connected to the second port of the network analyzer.\(^2\)

\(^2\)Microwave heating and radiation measurements of microwave ovens are described thoroughly in several books, including one by Chan [100], which also covers heating fundamentals and basic numerical simulation methods, and cavity theory. Datta also covers electromagnetic aspects as well as instrumentation and measurement, but continues onto industrial process design [101]. The book by Meredith [102] is a very thorough reference on several topics, including attenuation chokes, microwave sources (tubes, klystrons, magnetrons), as well as high voltage electronics. One conference paper describes oven measurements specifically in the context of specific absorption rate (SAR) biological phantom measurements and safety standards [103].

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5 Metamaterials for microwave shielding

Figure 5.27: Permittivity measurement of FR4 substrate samples. Slabs of known thickness are placed in an S-band waveguide. The S-parameter network analyzer records the S-parameters which are converted into complex permittivities.

Figure 5.28: Low-power leakage measurement using a Toshiba magnetron probe (mounted on top of oven) and an open faced S-band waveguide. Horizontal and vertical polarization sweeps are taken by rotating the open faced waveguide. Measurements are taken at 16 positions around the perimeter of the oven door gap.

channel between the door and the oven door frame. Measurements are taken at 16 positions distributed around the perimeter of the oven door, in various seal configurations. A total of 32 S-parameter sweeps are then recorded for each seal configuration (16 per polarization). Figure 5.28 shows a typical measurement being performed.

Initially, we measure the conventional QWC seal to provide a benchmark against which we can evaluate the performance of the EBG seal. Next, we replace the door with a custom fabricated flat face door that allows us to mount the EBG seal without the QWC. We measure it with the EBG seal mounted on the door (patch tops facing oven), mounted on the opposing door frame with opposite orientation (patch tops facing door, as in Figure 5.29), and finally with no seal whatsoever.

Figures 5.30 and 5.31 show sample measurements for the vertical and horizontal polar-
5.3 Radiation seal

![Photograph showing the EBG seal mounted on the cavity door frame. The conventional QWC on the oven door is in the picture for visual comparison purposes only. A not-pictured flat steel door replaces the one pictured for EBG seal measurements. Elimination of the QWC greatly reduces the effort and number of parts required to construct the oven door.](image)

Figure 5.29: Photograph showing the EBG seal mounted on the cavity door frame. The conventional QWC on the oven door is in the picture for visual comparison purposes only. A not-pictured flat steel door replaces the one pictured for EBG seal measurements. Elimination of the QWC greatly reduces the effort and number of parts required to construct the oven door.

The data shown has been corrected to account for the return loss of the system. The erratic nature of these curves arises from the high number of modes present in the cavity. We are still however able to undertake a qualitative analysis to compare the EBG seal and the conventional choke. For each measurement position, we combine data taken from the vertical and horizontal polarization measurements. For each seal configuration, the maximum power over all measurement positions is used as a metric for the performance of that configuration. Table 5.3 shows these consolidated results. The first design of the EBG seal performs only slightly worse than the conventional QWC (a difference of 3.5 dB).

We confirm these measurements by using a second procedure involving a regulation power meter (Narda radiation monitor, meter model 8211, probe model 8221). These meters are designed to measure radiation leakage from microwave ovens to check that they do not surpass legal radiation limits. Many countries define a legal leakage radiation limit for microwave appliances of 5 mW/cm² at a distance of 5 cm from the device.

This type of measurement is a high-power one, and requires the replacement of the Toshiba microwave probe with the original oven magnetron. The Narda meter shows leakage power fluxes of 350 to 800 μW/cm², depending on the position of the metallic rack within the cavity. This measurement and previous ones indicate the success of the proof-of-concept prototype.
Figure 5.30: A sample measurement in the vertical polarization of the QWC seal, the EBG seal mounted on the door frame, and the EBG seal mounted on the door itself. The noisiness of the measurements can be attributed to the large number modes present in the oven cavity. The EBG seal performs on par with the QWC, in particular over frequencies close to the operating point of 2.45 GHz. The seal is designed to have the center of its stop band at this frequency.

Figure 5.31: Measurement in the horizontal polarization of the QWC seal, the EBG seal mounted on the door frame, and the EBG seal mounted on the door itself. The EBG seal performs on par with the QWC in both the on-door and on-door-frame configurations.
Table 5.3: Leakage power calculations derived from measurements for various seal configurations, evaluated at 16 measurement points distributed around door gap.
Chapter 6

Discussion and outlook

6.1 Completed work

Numerical approaches are vital for the design and analysis of metamaterials. When possible, we use analytic solutions. If none is available, semi-analytic ones are a good alternative because they can quickly compute solutions to a high accuracy. When these are not useful because of geometry or material considerations, we resort to powerful, general tools like FDTD that are slower, but usable for a larger set of problems. Even these solvers however must be operated with finesse. The user must take care not to blindly accept results, and must take certain measures to ensure that they are generated in an efficient manner.

Specifically, we outlined procedures for solving grating problems. Metamaterials can usually be reduced to grating problems because they are periodic in one or more dimensions. We examined the basic setup of such problems in FDTD, and the requirements for generating reliable scattering spectra. We then outlined the generation of scattering spectra surfaces when computing with periodic boundary conditions. Additionally, we developed an algorithm for checking the reliability of FDTD generated band diagrams using tools such as the ‘missed mode map’, presented in Chapter 2.

When FDTD is too cumbersome, as is often the case with optimizations, we have to simplify problems by using effective media approximations. We presented an approach for checking the validity of these approximations using high accuracy solvers. We also presented a way to tune boundary conditions between photonic crystals so that the approximations can be used for wavelengths where they otherwise lose their validity.

We used several practical examples to demonstrate these findings. A useful application of metamaterials is for the deposition of antireflective thin-films. First, we showed an example of layer stack-up optimization for a nanorod thin-film problem. Another seminal result was the light scattering analysis for a thin-film solar cell with lossy layers. Finally, we showed that these methods are also useful for designing three-dimensional antireflective infrared coatings.

The last example studied the complete design cycle for a microwave metamaterial using the FDTD method. For this we needed to examine the dispersion characteristics of an EBG seal, design it in two and three dimensions using a complete microwave oven model, and finally fabricate and measure the device. Without the tools and methods discussed in this dissertation, we would not have the idea or the design capability to invent such a
metamaterial seal.

6.2 Future work

Metamaterials present a new umbrella for a group of electromagnetics problems. These have behaviors that can be exploited for a host of applications. Each individual problem brings new insights and future opportunities for research.

In Chapter 3 we presented ways in which more difficult metamaterial problems can be reduced. One important application for this is in the field of thermal barrier coatings. There we would like to have the opposite behavior of the one presented in the chapter on thin-films, namely maximum reflection over a broad infrared bandwidth. The currently used industrial thermal barrier coatings are hand optimized. It would be beneficial to use numerical simulation to extract manufacturing tuning parameters for these coatings, including porosity gradients for example.

If we simplify these problems using a tangible mixed media approach, we can then use efficient optimizers to handle the design work for us, or to extract clues about what makes a thermal barrier coating successful. This of course must follow constraints set up by the problem from a materials perspective. That is, it would be necessary to take available materials (ones that do not melt) and compatible materials (with respect to thermal expansion, for example) into account. Finally, we would want to fabricate and measure such coatings to confirm that the simulation approach is a suitable one.

The solar cell design results present a promising start into the study of light scattering in thin film solar cells. We were able to show a connection between the photovoltaic roughness morphology and the absorption within the cell. This can be exploited so as to optimize the cell design. We focused on roughness shape, size, and randomness, but many more parameters can be considered. One could for example tune layer thicknesses to enhance the cell efficiency. Better material models and larger, more random cell simulations would allow us to better compare the FDTD approach with published results on the quantum efficiency (QE) and absorption in this type of cell.

Another exciting approach would be to investigate the multiphysics aspect of the solar cell as a semiconductor problem. This would allow an ab initio analysis, from light illumination and absorption, to semiconductor current generation. If we incorporate this with circuit models then we could potentially create a complete numerical model that could be independently tested using measurements from fabricated devices. This by itself is a broad topic with room for lots of new and exciting research. From an industrial perspective this would be a great step towards minimizing development costs while maximizing solar cell efficiencies.

For the microwave EBG seal presented in Chapter 5, we were able to close this design loop and demonstrate the utility of numerical solvers for metamaterial design. The next step would be to accelerate the design process by developing newer, more reliable models.
These would reduce the EBG structure to the fundamental models already presented, and would generate reliable microwave scattering spectra in a fraction of the time necessary for full-wave solvers.

It should be noted that the proof of concept developed is by no means a finished product. Industry needs to develop the product so that it is viable to manufacture, and also satisfies the many product constraints that hold for these appliances. One example is the substrate for the EBG seal. Our prototypes used FR4. This would melt and burn at the high temperatures reached by a combination oven with convection heating. A different substrate means a different dielectric permittivity and therefore a new dimensioning of the mushroom structures used. One could write these problems off as a separate chore for industry to handle, but it is exactly these problems that should influence our thinking and our approach to the numerical design process.

In several problems, we were able to take advantage of parallelization to speed up the computation. Parallelization opens new doors for the future of numerical field theory because it allows us to solve more problems, and larger, more difficult ones at that. This includes problems like the microwave oven one that are non-periodic, have large voids surrounding complex, intricate cavities, and also incorporate losses. It is not simply a question of brute force power, but also the types of problem that one can start to think about solving. Because of parallelization, we can start to think about studying the effect of losses and also heating effects in EBG structures. Thermal expansion of the EBG seal presents a problem because of frequency shifting. These effects can be considered ever more readily.

Another step that additional computing power and memory will provide is the possibility of using higher order FDTD for more accurate, faster analysis of metamaterial problems. Combined with subgridding approaches as in [104], this could be used to study plasmonic metamaterial problems that normally require very high resolutions to achieve a suitable accuracy.
Appendix A

Analytic solution for flat slab structures

In this section we describe the analytic solution for the problem where an oblique plane wave impinges from some medium upon a stack-up of dielectric slabs. Light exiting these slabs continues to infinity with no further reflection, either in free space or in some dielectric medium. For the case where the slabs have a back-reflector, the solution is quite similar to the one shown here. For normal incidence, the electric and magnetic polarization results are identical. Schematics showing these polarizations are in Figure A.1.

![Figure A.1: Plane waves obliquely incident on a dielectric interface, from [105]. The field polarizations allow us to use a sign convention for keeping track of field components. On the left is the incidence, reflection and transmission of a plane wave whose electric field is parallel to the interface. The magnetic polarization is shown on the right.](image)

A.1 Electric field parallel to interface

We begin by describing the complex field amplitudes in each layer. Every layer has an incident and a reflected field, except the final layer which extends to infinity and has no backward traveling waves.

For layer $l$, these fields take the form
A Analytic solution for flat slab structures

\[ E_{li} = \text{Re}[\hat{E}_{li} e^{j(\omega t - k_l \sin \theta_l x - k_l \cos \theta_l z)]} \quad (A.1) \]

\[ H_{li} = \text{Re}[\frac{\hat{E}_{li}}{\eta_l} (-\cos \theta_l \hat{x} + \sin \theta_l \hat{z}) e^{j(\omega t - k_l \sin \theta_l x - k_l \cos \theta_l z)}] \quad (A.2) \]

\[ \hat{E}_{lr} = \text{Re}[\hat{E}_{lr} e^{j(\omega t - k_l \sin \theta_l x + k_l \cos \theta_l z)]} \quad (A.3) \]

\[ \hat{H}_{lr} = \text{Re}[\frac{\hat{E}_{lr}}{\eta_l} (\cos \theta_l \hat{x} + \sin \theta_l \hat{z}) e^{j(\omega t - k_l \sin \theta_l x + k_l \cos \theta_l z)}] \quad (A.4) \]

Working with the complex amplitudes, we can now consider the boundary conditions at each layer interface. These require continuity of the tangential fields at the interface. For an interface boundary with position \( z = d_b \) between two arbitrary layers \( f \) and \( g \), these are manifested in two equalities:

\[ \hat{E}_{fi} e^{-jk_f \cos \theta_f d_b} + \hat{E}_{fr} e^{jk_f \cos \theta_f d_b} = \hat{E}_{gi} e^{-jk_g \cos \theta_g d_b} + \hat{E}_{gr} e^{jk_g \cos \theta_g d_b} \quad (A.5) \]

\[ -\frac{\hat{E}_{fi}}{\eta_f} e^{-jk_f \cos \theta_f d_b} + \frac{\hat{E}_{fr}}{\eta_f} e^{jk_f \cos \theta_f d_b} = -\frac{\hat{E}_{gi}}{\eta_g} e^{-jk_g \cos \theta_g d_b} + \frac{\hat{E}_{gr}}{\eta_g} e^{jk_g \cos \theta_g d_b} \quad (A.6) \]

where the frequency-dependent wavenumber \( k \) is obtained through the simple dispersion equation \( k = \omega \sqrt{\mu/\varepsilon} \), with \( \omega = 2\pi c \lambda^{-1} \). \( \eta \) is the wave impedance given in each material by \( \eta = \sqrt{\mu/\varepsilon} \). The reflection and transmission angles in each layer are found by Snell’s law as a function of the incidence angle of the previous layer, shown in Figure A.1. Thus, by specifying the initial incidence angle, we can determine the reflection and transmission angles for all layers.

For a system consisting of \( n \) media, the number of interface boundaries is \( n - 1 \), and the number of equations is \( 2n - 2 \). The first layer is the one from which light impinges, and is infinite in thickness. The final layer is also infinite and contains only forward travelling plane waves.

As a linear system of equations we can treat the problem as a standard matrix problem, shown in Figure A.2. There, we let the first interface be placed at \( z = 0 \), and the value of the excitation amplitude be 1.
Figure A.2: Matrix problem for electrically polarized oblique plane waves incident upon a layered dielectric slab system.
A Analytic solution for flat slab structures

If we instead apply a back reflector (such as a PEC mirror) to a final layer, instead of allowing waves to travel to infinity in the final medium, we can use a similar solution. Mathematically we set the final incident field $\hat{E}_{n,i}$ to zero. This results in an overdetermined system. Alternatively we can remove the final row and column of the matrices in Figure A.2 (and Figure A.3 for the other polarization), and the final elements of the column vectors, solving the problem with dimension reduced by one.

When solving systems with many (thousands) of layers, the matrix becomes large (but remains sparse). It is fastest to use FORTRAN libraries such as the zgbsv algorithm in the LAPACK set of routines. This is an implementation of a banded-diagonal matrix solver. Specialized solvers like this one run much faster than the more general solvers.

A.2 Magnetic field parallel to interface

The magnetic field polarization follows a similar derivation. For completeness, we write the corresponding boundary conditions and matrix problem here.

We first write the incident and reflected fields as follows.

$$\bar{E}_{li} = \text{Re}[\hat{E}_{li}(\cos \theta_l \hat{x} - \sin \theta_l \hat{z})e^{j(\omega t - k_l \sin \theta_l x - k_l \cos \theta_l z)}]$$  \hspace{1cm} (A.7)
$$\bar{H}_{li} = \text{Re}[\frac{\hat{E}_{li}}{\eta_l}e^{j(\omega t - k_l \sin \theta_l x - k_l \cos \theta_l z)} \hat{y}]$$ \hspace{1cm} (A.8)
$$\bar{E}_{lr} = \text{Re}[\hat{E}_{lr}(-\cos \theta_l \hat{x} - \sin \theta_l \hat{z})e^{j(\omega t - k_l \sin \theta_l x + k_l \cos \theta_l z)}]$$ \hspace{1cm} (A.9)
$$\bar{H}_{lr} = \text{Re}[\frac{\hat{E}_{lr}}{\eta_l}e^{j(\omega t - k_l \sin \theta_l x + k_l \cos \theta_l z)} \hat{y}]$$ \hspace{1cm} (A.10)

We then write the boundary conditions at $z = d_b$ between layers $f$ and $g$.

$$\hat{E}_{fi} e^{-jk_f \cos \theta_f d_b} - \hat{E}_{fr} \cos \theta_f e^{jk_f \cos \theta_f d_b} = \hat{E}_{gi} \cos \theta_g e^{-jk_g \cos \theta_g d_b} + \hat{E}_{gr} \cos \theta_g e^{jk_g \cos \theta_g d_b}$$ \hspace{1cm} (A.11)
$$\frac{\hat{E}_{fi}}{\eta_f} e^{-jk_f \cos \theta_f d_b} + \frac{\hat{E}_{fr}}{\eta_f} e^{jk_f \cos \theta_f d_b} = \frac{\hat{E}_{gi}}{\eta_g} e^{-jk_g \cos \theta_g d_b} + \frac{\hat{E}_{gr}}{\eta_g} e^{jk_g \cos \theta_g d_b}$$ \hspace{1cm} (A.12)

These can then be used to form the matrix problem shown in Figure A.3.
Figure A.3: Matrix problem for magnetically polarized oblique plane waves incident upon a layered dielectric slab system.
Appendix B

Derivatives for effective permittivity approximations

To compute the effective permittivity from the band diagram, we look at the slope of the first dispersion curve. We can take advantage of the $\omega = 0$, $k = 0$ point to reduce the number of points needed to compute this slope. The same applies for the symmetry consideration that $\omega(k) = \omega(-k)$.

First we list the Taylor polynomials for four evenly spaced points (with spacing $h$) in the region of point $x$

\[
\begin{align*}
    f(x + h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \ldots \quad (B.1) \\
    f(x - h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \ldots \quad (B.2) \\
    f(x + 2h) &= f(x) + 2hf'(x) + \frac{4h^2}{2}f''(x) + \frac{8h^3}{6}f'''(x) + \ldots \quad (B.3) \\
    f(x - 2h) &= f(x) - 2hf'(x) + \frac{4h^2}{2}f''(x) - \frac{8h^3}{6}f'''(x) + \ldots \quad (B.4)
\end{align*}
\]

We begin with the second order second derivative.

Adding the $f(x \pm h)$ terms, we obtain

\[
(B.1) + (B.2) \quad f(x + h) + f(x - h) = 2f(x) + h^2f''(x) + O(h^4) \quad (B.5)
\]

\[
f''(x) = \frac{f(x + h) - 2f(x) + f(x - h) - O(h^4)}{h^2} \quad (B.6)
\]

\[
f''(0) = \frac{2f(h)}{h^2} - O(h^2) \quad (B.7)
\]

The fourth order first and second derivatives can be found similarly. For the first derivative, we subtract (B.2) from (B.1), and (B.4) from (B.3), and then linearly recombine their results to cancel out the third derivative term.
\( B \) Derivatives for effective permittivity approximations

\( (B.1) - (B.2) \quad f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3} f''(x) + \ldots \quad (B.8) \)

\( (B.3) - (B.4) \quad f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8h^3}{3} f''(x) + \ldots \quad (B.9) \)

\( 8 \cdot (B.8) - (B.9) \quad 8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h) = 12hf'(x) + O(h^5) \quad (B.10) \)

Rearranging (B.10) we find the fourth order first derivative:

\[
f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4) \quad (B.11)\]

For the fourth order second derivative, we follow a similar procedure

\( (B.1) + (B.2) \quad f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12} f'''(x) + \ldots \quad (B.12) \)

\( (B.3) + (B.4) \quad f(x+2h) + f(x-2h) = 2f(x) + 4h^2 f''(x) + \frac{16h^4}{12} f'''(x) + \ldots \quad (B.13) \)

\( 16 \cdot (B.12) - (B.13) \quad 16f(x+h) + 16f(x-h) - f(x+2h) - f(x-2h) = 30f(x) + 12h^2 f''(x) + O(h^6) \quad (B.14) \)

(B.14) can be rearranged to find the second derivative term

\[
f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + O(h^4) \quad (B.15)\]

Evaluated at \( x = 0 \), and assuming symmetry, this becomes

\[
f''(0) = \frac{16f(h) - f(2h)}{6h^2} + O(h^4) \quad (B.16)\]


BIBLIOGRAPHY


