INFRARED FILTERS AND METAMATERIALS
BASED ON FREQUENCY SELECTIVE SURFACES

A Dissertation in
Electrical Engineering

by
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Recently, frequency selective surface (FSS) technology that has historically been used in various microwave systems has been adapted to infrared applications by scaling the device dimensions with micro- and nano-fabrication techniques. In addition, FSS technology has been investigated for synthesizing a variety of metamaterials, including artificial magnetic conductors, electromagnetic bandgap structures, metaferrites, and low index metamaterials. However, previous design efforts in the infrared have been limited to using intuitive geometries in the FSS structure. In order to improve the state of the art, genetic algorithm optimization methods incorporating fabrication constraints are introduced in this dissertation that enable the synthesis of infrared FSS with user-defined performance criteria and which are ready for accurate fabrication and characterization using micro- or nanofabrication methods. Synthesis procedures are described and demonstrated for metallodielectric FSS and all-dielectric FSS filters. Additionally, liquid crystal is incorporated into several designs and optimized to have a narrow stop band that is tunable across frequency. Synthesis procedures for realizing negative and zero index metamaterials (NIMs/ZIMs) from single or multi-screen FSS are also introduced in this dissertation. These techniques advance the state of the art by optimizing simultaneously for a desired refractive index, minimum absorption loss, and an impedance match to the surrounding medium. Furthermore, optimizing FSS stacks with many metal layers has revealed that thicker, more practical metamaterials can be realized with low losses and metamaterial properties approaching those of a bulk medium.
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I dedicate this thesis to

my father and my mother

for their constant support and love.

I hope to continue to make you proud.
Chapter 1

Introduction

This chapter introduces the topic of the dissertation, which is the development of thin film filters and metamaterials that operate across the infrared spectrum. The technical approach is discussed along with the current state of the art. Finally, the original contributions of the work are outlined.

1.1 Statement of Problem

In recent years the Terahertz and infrared (IR) spectra have garnered increased research interest for a wide variety of applications ranging from remote sensing to solar cells [3,4]. The interaction of infrared light with metallic or dielectric nanostructures embedded in a host dielectric medium gives rise to optical properties that can be utilized to fabricate photonic devices for use in beam-splitters, polarizers, filters, nanoresonators, biosensors, surface-enhanced Raman spectroscopy and zero and negative index metamaterials [5,6,7]. Atmospheric windows also exist in the mid-infrared (mid-IR) wavelength range (roughly 2 to 10 µm), making satellite and terrestrial communications links possible and providing a need for infrared filters.

Early approaches to IR filters included 2-dimensional dielectric gratings or dielectric stacks with many layers [8,9]. These approaches provide a photonic bandgap at the desired infrared wavelength, but are limited with respect to polarization selectivity
and/or costly fabrication. Several groups have investigated using metallodielectric photonic crystals (MDPC), also known as metallodielectric frequency selective surfaces (FSS) [10,11,12,13] in order to achieve a photonic bandgap with one or several planar metallic screens sandwiched together. The Previous research conducted by the author has produced high performance, low-cost, multi-band MDPC filters from a single metallic screen using fractal and genetic algorithm techniques in the far-infrared (far-IR) wavelength range (10 to 100 µm) [14]. However, such synthesis approaches possessed drawbacks leading to limited flexibility in positioning stop bands and requiring the need for geometry adjustment prior to fabrication. Therefore, a primary goal of this research is to develop powerful and versatile synthesis techniques for realizing planar filters for the far-IR and mid-IR that can be accurately fabricated.

Frequency tuning is also desirable for channel selection in communications systems. Research has previously been conducted to develop tunable [15,17] and reconfigurable [14,17] metallodielectric FSS filters. Such approaches to introducing tunability are cumbersome and difficult to implement. A secondary goal of this research is to investigate liquid crystal as a method for tuning the frequency response of FSS filters in the infrared.

A final goal of this research is to advance the field of metamaterials in the infrared. Metamaterials with a zero and negative refractive index are vital for applications such as electromagnetic cloaking, transformational optics, and the ‘perfect lens’ [18,19]. However, previous metamaterial approaches at RF, infrared, and optical wavelengths suffer from high absorption and impedance mismatch losses and are typically unsuitable for applications requiring high transmission through the metamaterial. At optical
wavelengths, another limitation has been device thickness, as most optical metamaterial experiments have been for thin films. Thus, a final focus of this research is to develop low loss zero index metamaterials (ZIM) and negative index metamaterials (NIM) using single or multi-layer metallodielectric FSS. The following section introduces the technical approach used to achieve these goals.

1.2 Technical Approach

It is often useful in engineering to approach a new class of design problems by adapting and merging existing, proven technologies with novel ideas to make things work. In the case of developing IR filters and metamaterials this is no different. The primary technology considered is frequency selective surfaces (FSS), which have been exploited for several decades in the RF for their resonant behavior [20]. Conventional FSS are comprised of one or more metal screen that is periodic in two dimensions, defined by a unit cell, and supported by dielectric substrates or superstrates. FSS naturally filter impinging electromagnetic plane waves by reflecting waves that couple strongly to the FSS surface. The scattering response is governed by Maxwell’s equations, so that if the dimensions of the device were to be scaled down, the resonant wavelengths would scale proportionately. This scalability is exploited in this work by utilizing micro- and nanofabrication techniques to shrink the metal screen features from the centimeter scale to the micron or nanometer scale. Thus, the stop and pass band filter response will shift to the far-IR or near-IR. Contact lithography and electron beam (E-beam)
lithography are both used in experiment to pattern micron and nanometer sized features, respectively.

In order to optimize an FSS design, which has many parameters including the screen geometry, unit cell dimensions and material properties, it is advantageous to consider a robust optimization tool such as a genetic algorithm [21] in order to tailor the scattering characteristics of the FSS for a desired filter response or metamaterial characteristics. Genetic algorithms lend themselves to electromagnetic design problems that optimize many parameters simultaneously because they are relatively simple to implement and can navigate complex cost functions to arrive at a global best solution. Furthermore, this research introduces fabrication design rules to aid in the design and fabrication process. These rules, including geometry simplification techniques and minimum feature sizes, are implemented within the genetic algorithm so that the synthesized FSS design can be accurately fabricated during experiment.

At mid-IR and shorter wavelengths, the metal losses become larger, causing increased absorption loss lower Q resonances in metallodielectric FSS filters. Meanwhile, for mid-IR and optical wavelengths, dielectric materials are available with extremely small loss tangents. Thus, all-dielectric FSS (DFSS), also known as photonic crystal slabs in the literature, are considered for mid-IR filters with narrow stop bands.

Previous studies have shown that the filter response of an FSS can be tuned in frequency by changing the properties of the dielectric layers surrounding the metal screen [15] or by changing the geometry of the metallic patches [16]. The response can also be shifted or completely changed by incorporating switches into the metal geometry to reconfigure the screen [17]. This research considers using liquid crystal as a dielectric
superstrate in order to facilitate frequency tuning of a stop band. At mid-IR wavelengths, the metallodielectric FSS must be designed specifically for narrow bandwidth in order to maximize the channel selectivity in a tunable filter.

In a metamaterial problem, the scattering parameters from the FSS are inverted [22] to obtain the effective permittivity $\varepsilon$ and permeability $\mu$ of a uniform slab with equivalent thickness. For the case of a metallodielectric FSS comprised of a single metal screen sandwiched between dielectric slabs, the metal geometry will typically produce a Drude shaped electric response, $\varepsilon$, for a fully connected screen, or a Lorentz shaped $\varepsilon$ for isolated metal elements at their resonance wavelength. When $\varepsilon$ goes to 0, then also the refractive index $n$ will approach zero, resulting in a ZIM.

For the case of an FSS with multiple metal screens, the coupling between screens enables magnetic $\mu$ resonances, or Lorentz shaped $\mu$ profiles. Such a multilayer FSS metamaterial can be optimized for impedance matching where $\varepsilon = \mu$ or a negative refractive index, when $\varepsilon$ and $\mu$ are simultaneously negative. The FSS structure has a lot of flexibility for tailoring the metamaterial profiles to minimize loss and achieve a good impedance match at a ZIM or a NIM band.

Finally, the optimization of metamaterials with many metal screens is studied in this research. In the literature, optical metamaterials typically only have a couple layers [23], meaning that when another layer is added to the structure, the coupling from the new layer may drastically alter the metamaterial properties. Metamaterial stacks are optimized in order to obtain thicker low loss NIMs and ZIMs that have properties approaching those of a bulk metamaterial.
1.3 Original Contributions

The research that I have performed during my Ph.D. studies at Penn State has led to several new developments in the field of IR filters and metamaterials.

- Designed and implemented fabrication rules for a GA in order to optimize IR FSS that could be accurately fabricated.
- Synthesized multiband metallodielectric FSS filters for the far-IR using a GA that were accurately fabricated and showed excellent agreement between optimization goals and measurement.
- Derived a general surface impedance model for metallic FSS screens and implemented dispersive loss models for Ag, Al, Au, and polyimide into the GA.
- Synthesized single and multiband metallodielectric FSS for the mid-IR using a GA that were fabricated and measured, showing excellent agreement with simulation.
- Synthesized tunable single-band FSS filters with a liquid crystal (LC) superstrate for the mid-IR using a GA.
- Developed an algorithm for calculating the effective constitutive parameters for a metamaterial slab by using the NRW inversion algorithm and enforcing continuity of $n$ from low frequencies.
- Implemented the continuity of $n$ inversion method in the GA for optimizing planar metamaterials with one or more FSS screen.
• Synthesized low-loss zero/low index metamaterial (ZIM) with one metal screen for the far-IR that was fabricated and characterized by variable angle ellipsometry to validate the predicted response.

• Synthesized ZIMs with two metal screens to have low absorption loss and either high impedance or low impedance in the mid-IR.

• Synthesized ZIMs with two and four layers to have low loss and matched impedance to free space.

• Synthesized low-loss negative index metamaterials (NIMs) with two metal screens for the mid-IR.

• Synthesized NIMs with many layers to demonstrate thicker metamaterials with low loss and bulk-like effective properties.

These developments have been contributed to the literature by the publication of several papers in the IEEE Transactions on Antennas and Propagation [1,17,24] and in Applied Physics Letters [7]. A paper on the synthesis of multilayer NIM stacks exhibiting bulk-like effective properties has been also recently been accepted for publication in Optics Express [25].

1.4 Overview

This dissertation introduces several novel approaches for synthesizing filters, tunable filters, and metamaterials for the IR using FSS technology. The section provides an overview of the concepts covered in each of the following chapters of this dissertation. The key concepts introduced in the chapter are also summarized.
Chapter 2 reviews the background for several technologies and methods that are used to conduct the research found in this dissertation. This chapter begins in Section 2.1 with a discussion of metamaterial applications and an overview of previous research in in NIMs and ZIMs. Section 2.2 provides background for FSS technology and covers the state of the art in infrared FSS applications. Section 2.3 describes several methods that are integral in performing the optimizations and analyses presented throughout the dissertation. In Section 2.3.1 and Section 2.3.2 two periodic full-wave simulation techniques are described that are used to calculate the scattering from FSS. The metamaterial inversion technique is described in section 2.3.3, and background on GAs is discussed in Section 2.3.4.

Chapter 3 discusses the design, fabrication, and characterization of infrared filters. Section 3.1 focuses on metallodielectric FSS filters designed by a GA incorporating fabrication rules for the far-IR and for the mid-IR. Section 3.2 presents the design and experiment for all-dielectric FSS. Section 3.2.1 describes a dual-band DFSS optimized by hand, whereas Section 3.2.2 describes the GA optimization of a DFSS for the mid-IR with larger angular tolerance. Section 3.3 discusses tuning of metallodielectric FSS using a liquid crystal superstrate.

Chapter 4 describes the design of a single-layer metallodielectric ZIM. Section 4.1 presents several design examples for the far-IR and mid-IR. The design, fabrication, and characterization are discussed for a ZIM that operates in the far-IR is described in Section 4.2.

Chapter 5 discusses the optimization of metamaterials containing more than one metal screen. Section 5.1 describes multilayer FSS ZIMs designed to have a matched
impedance to free space. Examples with two and four screens are presented. Section 5.2 focuses on low loss NIMs with two metal screens, whereas Section 5.3 discusses the optimization of larger NIM stacks. The loss characteristics for larger stacks as well as the bulk characteristics of NIM stacks are analyzed. The final chapter, Chapter 6, provides a summary of this dissertation as well as suggestions for future work.
Chapter 2

Background

The basis for this research is the concept of frequency selective surfaces (FSS) and their applications in the infrared (IR). Several tools are required to analyze and synthesize FSS for the IR, including full-wave electromagnetic solvers, material models, and stochastic optimizers. Furthermore, the concept of metamaterials opens up a broad range of applications for IR FSS and serves to focus the design goals for this research. The following sections expand upon the background of metamaterials, including negative index metamaterials (NIM) and low/zero index metamaterials (LIM/ZIM). Section 2.2 describes the background of metallodielectric and all-dielectric FSS as applied to IR applications. Section 2.3 covers several tools and methods used throughout the rest of the dissertation.

2.1 Metamaterials

Metamaterials are engineered composites that have electromagnetic properties not readily found in nature but arising from inclusions embedded within the host material on a scale smaller than the wavelength of interest [25]. Previous experiments have shown infrared and optical metamaterials with negative, zero, and low refractive indices [25,26,27,28] needed for devices such as flat near- and far-field lenses [19,27,28,30], low-index mirrors [31], and electromagnetic cloaks [32,33,34]. However, realizing these
practical devices also requires that the metamaterials have low absorption losses and well-defined impedance [30] over the operating wavelength range.

Research in both negative index materials (NIMs) [35,36] and the closely related zero index materials (ZIMs) [30,37] has been very active over the past few years. The origin of this excitement can be succinctly summarized in the schematic diagrams shown in Figure 2.1, where the response to a nearby or embedded radiation source of NIMs and ZIMs, respectively, are contrasted to that of conventional positive index materials (PIMs). Section 2.1.1 discusses in further detail NIMs, and Section 2.1.2 presents details on ZIMs.

![Figure 2.1: Electromagnetic properties of PIM, ZIM and NIM. (a) A source radiating in the presence of a conventional PIM, (b) far-field focusing of the radiation from a source (antenna) embedded in a ZIM, (c) a ZIM as a perfect mirror ($\Gamma = \pm 1$, where the plus sign is used if $\mu_{\text{eff}} = 0$ and the minus sign is used if $\varepsilon_{\text{eff}} = 0$), (d) a NIM as a flat near-field focusing lens [1].](image)

### 2.1.1 Negative-Index Metamaterials

Metamaterials with a negative refractive index have become an exciting reality in the last few years. In 1968, Veselago first postulated the possibility of left-handed media with a simultaneously negative permeability and permittivity, along with several
interesting properties associated with such a material, including backward-propagating waves, reversed Doppler shift, a modified Snell’s law, and near-field focusing [38]. The more recent observation that a material with \( n = -1 \) could be formed into a planar “perfect lens” sparked widespread interest in the development and demonstration of negative index metamaterials (NIMs) [19]. NIMs can potentially be used for a great many important applications, such as high gain and directional microwave devices, super-resolving and focusing lenses, magnetic resonance imaging (MRI), novel antennas (including small antennas), series-fed antenna arrays with reduced beam squinting, and backward leaky-wave antennas [35,36].

The refractive index \( n \) of a metamaterial is defined by the permittivity \( \varepsilon \) and permeability \( \mu \) of the medium and calculated according to Eq. 2.1, such that if the real parts of \( \varepsilon \) and \( \mu \) are both negative, the real part of \( n \) will also be negative. Likewise, the

![Diagram](image)

Figure 2.2: Simplified parameter space for \( \varepsilon \) and \( \mu \) assuming \( \varepsilon'' = \mu'' = 0 \) [2].
impedance $Z$ of the medium, normalized to the impedance of free space $Z_0$ is given by Eq. 2.2. Figure 2.2 shows a simplified parameter space for $\varepsilon$ and $\mu$, with the imaginary parts of both parameters equal to zero, including a description of naturally occurring materials that would lie in each quadrant. It is notable that in the third quadrant, where we would find a negative refractive index and a propagating mode (i.e., $n'$ is larger than $n''$), there are no naturally occurring materials. Thus, metamaterial composites have been exploited which contain embedded electric and magnetic resonators, giving $\varepsilon < 0$ and $\mu < 0$, respectively. Embedding magnetic resonators, such as the split ring resonator used in RF applications [39], into a medium will produce Lorentz shaped resonance in the permittivity profile, whereas the permittivity can contain either a Lorentz shaped resonance from embedded metallic elements or a Drude shaped profile when an interconnected metallic mesh or metallic wires with an infinite length are embedded in the medium [40].

$$n = \sqrt{\varepsilon\mu} \quad (2.1)$$

$$Z = \frac{1}{Z_0} \sqrt{\frac{\mu}{\varepsilon}} \quad (2.2)$$

Artificial materials with an effective negative refractive index have since been demonstrated from the microwave regime to the edge of the optical spectrum [41,42]. Previous work on NIMs has primarily focused on planar 2-D periodic structures, including the split ring resonator and dipole array [43], gold nanowires [23], perforated gold films [44] and GA optimized FSS structures [45]. Recently, however, some groups have developed concepts for 3-D NIM structures that are based on molecules or...
inclusions in the form of dielectric spheres, for example magneto-dielectric spheres [46] and coated non-magnetic spheres [47]. In the latter case, these dielectric sphere guests are included into a host substrate to form a 3D non-magnetic metamaterial that can be used for applications with target frequencies in the infrared.

A well known problem associated with passive NIMs is high losses including absorption loss and sometimes significant mismatch loss. Such losses are unacceptable for transmissive applications, such as planar lensing. Furthermore, fabricating bulk metamaterials for infrared/optical devices presents a difficult problem due to the limitations of nano-fabrication techniques that are time-consuming and expensive to use in a layer by layer fashion. Only very recently has a multilayer magnetic metamaterial been demonstrated for infrared/optical wavelengths, using advanced alignment techniques between layers of split ring resonators [48]. Section 5.2 addresses efforts to overcome the inherent losses in NIMs, and Section 5.3 discusses the optimization of thicker, bulk-like NIMs that would be useful for practical applications at IR wavelengths.

2.1.2 Zero-Index Metamaterials

While NIMs have garnered much attention in recent years following Pendry’s postulation of a flat NIM lens overcoming the diffraction limit [19], far less research has focused on the perhaps more important class of low/zero index metamaterials, a necessary component in electromagnetic cloaks [32,33,34], flat far-field lenses [28,29,30], and low-index mirrors [31]. The earliest investigations into realizing LIMs/ZIMs used volumetric arrays of wires [31] or metallic meshes [29] to achieve a
negative permittivity $\varepsilon_{\text{eff}}$ and corresponding low effective index $n_{\text{eff}}$. More recently, a frequency selective surface screen [37] and a rotationally stacked Drude-dielectric checkerboard [49], both of which rely on a zero or negative permittivity for their low index properties, have also been theoretically explored as ZIM candidates. Two other theoretical studies suggest that incorporation of a magnetic resonator into the metamaterial design allows for the possibility of the permittivity and permeability both approaching zero together, giving a zero index and matched impedance (i.e., $n \approx 0$ and $Z \approx 1$) [30,50].

Table 2.1: Constitutive parameter conditions leading to ZIM behaviour.

<table>
<thead>
<tr>
<th>case</th>
<th>Medium Property</th>
<th>Metamaterial Impedance</th>
<th>Reflection Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\varepsilon \rightarrow 0$</td>
<td>$Z \rightarrow \infty$</td>
<td>$\Gamma \rightarrow +1$(PMC)</td>
</tr>
<tr>
<td>2</td>
<td>$\mu \rightarrow 0$</td>
<td>$Z \rightarrow 0$</td>
<td>$\Gamma \rightarrow -1$(PEC)</td>
</tr>
<tr>
<td>3</td>
<td>$\varepsilon \rightarrow 0, \mu \rightarrow 0$</td>
<td>$Z \rightarrow 1$</td>
<td>$\Gamma \rightarrow 0$</td>
</tr>
</tbody>
</table>

If we consider a wave normally incident upon a half space of metamaterial, then the reflection coefficient would be given by Eq. 2.3. Examining the parameter chart in Figure 2.2 reveals three cases outlined in Table 2.1 for $\varepsilon$ and $\mu$ that would produce a zero or low refractive index. These three regions are highlighted in Figure 2.2 by silver bars and a silver circle. The first case, when $\varepsilon$ approaches zero along the vertical silver bar in Figure 2.2, results in a reflection coefficient of +1, meaning that the reflected wave is in phase with the incident wave. This boundary condition is indicative of a perfect magnetic conductor (PMC) or artificial magnetic conductor (AMC). Thus, one application for a ZIM is an AMC ground plane. The second case, when $\mu$ approaches zero along the
horizontal silver bar in Figure 2.2, results in a reflection coefficient of -1, which is the same boundary condition as a perfect electric conductor (PEC). Either case 1 or case 2 can be used in a perfect mirror application, where all of the incident radiation is reflected. The final case, when \( \varepsilon \) and \( \mu \) approach zero at the same rate as shown by the silver circle at the origin in Figure 2.2, gives a matched impedance, equal to that of free space (i.e., \( Z = 1 \)). This condition is useful for the transmissive applications mentioned earlier, including electromagnetic cloaking.

\[
\Gamma = \frac{Z - 1}{Z + 1}
\]

Furthermore, ZIMs produce parallel waves irrespective of the angle of incidence of the radiation at the boundary of the material. This unique characteristic can be utilized in many applications, such as flat superstrate lenses to focus the far-field radiation patterns of embedded antennas, signal phase manipulation and equalization devices, extremely convergent microlenses and other imaging applications [30,51]. Chapter 4 considers how a single screen FSS can be used to achieve a ZIM. Section 5.1 examines the use of multi-screen FSS for achieving ZIMs with matched impedance.

### 2.2 Frequency Selective Surfaces

Frequency selective surfaces (FSSs) are planar devices comprised of a doubly-periodic array of metallic elements backed by a thin dielectric substrate [20]. An example of a FSS is shown in Figure 2.3 with cross-dipole patches as the metallic
elements. The dielectric substrate and/or superstrate layers are typically thin compared to a wavelength at the operating frequency.

In simulation, a FSS of infinite extent is illuminated by a plane wave with either transverse electric (TE) or transverse magnetic (TM) polarization as shown in Figure 2.4. In this diagram, the angle from the normal to the surface of the FSS is $\theta$, and the azimuth angle, measured from the horizontal axis of the FSS, is $\phi$. For normal incidence ($\theta = \phi = 0^\circ$) TE indicates that the electric field is polarized vertically along the FSS screen geometry, and TM polarization indicates that the electric field is aligned with the horizontal axis.

Figure 2.3: Diagram of a FSS with cross-dipole shaped elements on a substrate.
FSSs have long been used at radio frequencies (RF) as filtering devices in radomes and reflector antennas because the periodic metallic screen has the electromagnetic effect of reflective or transmitting incident radiation depending on the frequency. Section 2.2.1 provides further background regarding metalldielectric FSS and their applications in the IR, and Section 2.2.2 discusses all-dielectric FSS (DFSS).
2.2.1 Metallodielectric Frequency Selective Surfaces

Frequency Selective Surfaces are well known in the literature for their filtering characteristics at microwave and millimeter wave frequencies [20,52]. FSSs have also been used extensively in the microwave regime as metamaterials such as artificial magnetic conducting (AMC) surfaces [53], metaferrites [54], and ZIMs [37]. This section will provide a background for FSS applications as spatial filters in the IR. Synthesis and experimental results for IR FSS filters will be presented in Chapter 3, and the use of FSS in NIM and ZIM applications will be examined in Chapter 4 and Chapter 5.

An FSS screen naturally acts as a spatial filter by producing a strong reflection band, or stop band, at resonance. The simple FSS geometry shown in Figure 2.3 is comprised of a periodic array of cross dipole elements. From antenna theory one would expect that these individual cross dipoles would couple well with incident electromagnetic radiation when the wavelength of the illuminating wave is approximately twice the length of the cross-dipole \( (i.e., \) when the scatterer resembles a half-wave dipole. At this wavelength, a current will be induced along the cross dipole, which will, in turn, re-radiate as a strong back-scattered field. Considering again the array of cross-dipoles, each of these elements will couple with the incident plane wave and together re-radiate a strong reflected wave in the specular direction at their resonant wavelength. In addition to the resonant properties of the individual scatterers, the resonance frequency of the FSS screen is also affected by the coupling between neighboring scatterers (periodicity) as well as dielectric loading from substrates or superstrates supporting the FSS screen.
FSS have been investigated for use as IR band-reject and band-pass filters with application to low-cost, high-performance devices including beam-splitters, filters, radomes, and polarizers [55]. FSS are also referred to in the IR as metallodielectric photonic crystals (MDPCs), which in the past have often been fabricated by stacking several dielectric layers with screens of metallic patch elements to achieve a single strong stop band (>10 dB) [10,11]. Currently, there is increasing interest in extending the filtering capabilities of single layer MDPCs to achieve multiband responses [12,13].

There has been interest in pushing FSS technology to infrared frequencies for filtering applications for several decades. Work in the far-IR (wavelengths from 10 µm to 100 µm) has demonstrated a range of filtering capabilities using sub-mm scale metallic meshes and grids to achieve high-pass, low-pass, band-pass, and band-stop responses in the far-IR spectrum [10,11,12,56,57,58,59]. The performance and flexibility of these far-IR filters is significantly improved by stacking multiple metallic grids and meshes [10,11,56]. One study demonstrated multiband filtering in the mid-IR and far-IR using a metallic screen with fractal H slits [12]. However, the performance of this multiband FSS filter was poor, demonstrating passbands with only 14% to 36% transmission [12].

In the mid-IR (wavelengths from 2 µm to 10 µm), many studies have been performed on single-layer FSS filters with a variety of relatively simple metallic patch and aperture elements that possess single stop-bands or pass-bands [4,55,60,61,62,63,64,65]. Measured filter performance from most of these examples is unacceptably poor. However, strong stop bands with rejection up to 20 dB have been achieved in the mid-IR using multiple FSS screens [65]. Stacked FSS screens were also used to achieve dual stopbands in the mid-IR [13]. A study in the near-IR (wavelengths
shorter than 2 µm) with sub-micron circular patch elements demonstrated that, when working in this band, it is important to optimize the metal film thickness for desired filter performance [66].

FSS filters operating at near-IR and mid-IR frequencies have been suggested for incorporation into thermophotovoltaic (TPV) conversion devices to increase their efficiency. A theoretical study on the absorption in FSS at near-IR and mid-IR wavelengths underscores the need for taking into account ohmic loss when designing efficient FSS filters at these wavelengths [67]. Further theoretical and experimental evidence suggests that absorption in current FSS technology is prohibitively high for TPV applications when compared with alternate technology [68].

Another interesting application for IR FSS has recently been studied using a FSS screen of packed micron scale conducting square loops that resonate in the mid-IR [69]. Instead of a good conductor, a lossy metal is chosen for the FSS screen, so that at resonance, the FSS absorbs incident radiation. The emissive properties of such an FSS absorber are equivalent to its absorbing properties, so this IR FSS is ideal for constructing an IR emitter with custom spectral characteristics. It has been shown that the emission spectrum can be adjusted by designing the FSS appropriately.

2.2.2 All-Dielectric Frequency Selective Surfaces

The use of inhomogeneous all-dielectric periodic structures in filtering applications has been an area of interest for several years [8,70,71,72,73,74,75]. A typical all-dielectric frequency selective surface (DFSS) consists of two or more different
dielectric materials distributed periodically throughout an inhomogeneous slab. At infrared (IR) frequencies, DFSS offer the advantage of low absorption loss as compared with metallic FSS [70,24]. The one dimensional version of the DFSS, which is sometimes called a dielectric grating waveguide, was proposed by Bertoni et al. as early as the 1970’s [8,70]. The resonance properties of such dielectric waveguide gratings were examined at millimeter-wave frequencies. Sharp resonance features were predicted theoretically and observed experimentally in [71], and bandstop filters were designed in [72]. A major disadvantage of employing one-dimensional dielectric gratings in frequency selective filter design is that the response of the structure is strongly dependent on the polarization of the excitation plane wave. By extending the periodicity of the DFSS to two dimensions, polarization independent filter designs can be obtained. A design methodology using genetic algorithms (GA) has been proposed for synthesizing 2D periodic DFSS with polarization dependent [73] and independent [74] responses. Simulations in [75] suggest that a DFSS filter for the mid-IR can also be tuned with a liquid crystal substrate or superstrate. The results in [74] use a single inhomogeneous dielectric layer to achieve a strong stopband in the mid-IR (2 μm < λ < 10 μm) regime. Design and experiment results presented in Chapter 3 of this dissertation seek to demonstrate that a multiband DFSS filter with polarization insensitivity can be achieved with a single inhomogeneous dielectric layer.
2.3 Analysis and Synthesis Methods

Several simulation and synthesis techniques are utilized in achieving the results presented in this dissertation. Two full-wave electromagnetic analysis techniques, a periodic moment method (PMM) and a periodic finite element-boundary integral (PFE-BI) method were used to calculate the scattering from FSS screens and are discussed in Section 2.3.1 and Section 2.3.2, respectively. The metal screens in FSS are represented in the models by impedance surfaces, and several methods for calculating the surface impedance of metals at IR wavelengths were used in this work. These models are discussed in Section 2.3.3. The Nicholson, Ross, and Weir (NRW) inversion technique is used to calculate the effective properties of planar metamaterials. This inversion technique along with logic for determining the root of $n$ is presented in Section 2.3.4. Finally, genetic algorithms (GA) are used throughout the work to synthesis filters and metamaterials and are discussed in Section 2.3.5.

2.3.1 Periodic Moment Method

A full-wave PMM analysis technique was employed in this work to perform the electromagnetic simulations of metallodielectric FSS. This analysis technique follows the well-established procedure of solving the Electric Field Integral Equation (EFIE) for the current distribution on the conducting patches, derived by enforcing the Floquet’s periodicity condition in an elementary unit cell [52,76]. Consider a screen lying in the $x$-$y$
plane, with cell periodicities $T_x$ and $T_y$ along the x- and y-directions, respectively. Under these conditions, the EFIE may be cast in the form:

$$
\begin{bmatrix}
E_x^{inc}(x,y) \\
E_y^{inc}(x,y)
\end{bmatrix} = \frac{2\pi}{j\omega \epsilon_0 T_x T_y} \sum_m \sum_n \left[ k_0^2 - \alpha^2_m - \alpha_m \beta_n \right] \tilde{G}(\alpha_m, \beta_n) \begin{bmatrix}
\tilde{J}_x(\alpha_m, \beta_n) \\
\tilde{J}_y(\alpha_m, \beta_n)
\end{bmatrix} e^{j\alpha_m x \pi \epsilon_{\alpha m}} e^{j\beta_n y} - Z_e \begin{bmatrix}
\tilde{J}_x \\
\tilde{J}_y
\end{bmatrix}
$$

(2.4)

where $E_x^{inc}$ and $E_y^{inc}$ represent the x- and y-components, respectively, of the electric field incident on the FSS screen. The parameters $\alpha_m$ and $\beta_n$ in Eq. 2.4 may be expressed in terms of the periodicity of the screen and the incident wavenumber as

$$
\alpha_m = \left( \frac{2m\pi}{T_x} \right) + k_x^{inc}
$$

(2.5)

$$
\beta_n = \left( \frac{2n\pi}{T_y} \right) + k_y^{inc}
$$

(2.6)

where $k_x^{inc}$ and $k_y^{inc}$ are the projections of the incident plane-wave wave vector $k_0$ along the x- and y-directions, respectively. Finally, $\tilde{G}(\alpha_m, \beta_n)$ is the dyadic spectral Green’s function that accounts for the presence of the lossy dielectric substrate of thickness $t$ upon which the metallic patches of the FSS are printed. Eq. 2.4 must be solved for the unknown current distributions $\tilde{J}_x$ and $\tilde{J}_y$, after imposing the proper boundary condition on the surface of the conductor. If the patch material has a finite conductivity, the tangential components of the total electric field must satisfy an impedance boundary condition, where the total electric field on the surface is equal to the product of the surface impedance and the surface current density [77]. This boundary condition can be written as:
where $Z_s$ is the impedance of the metallic screen.

At this point the current distribution is expressed in terms of a set of basis functions on the sub-domain of the periodic cell, which are commonly referred to as “rooftops” [78]. The next step is to derive a matrix equation from Eq. 2.4 by applying the Galerkin’s procedure and to solve it for the unknown current distribution. The final steps are to compute the FSS response from the knowledge of this current distribution.

The PMM code has several key capabilities that are essential to FSS synthesis in the IR. The use of “rooftop” subdomain basis functions to represent the currents induced on the metal screen allow us to pixelize the screen geometry for optimization by a genetic algorithm. Additionally, any arbitrary screen geometry can be simulated by the code. The code can also simulate lossy dielectrics and metals. At IR wavelengths, losses play a significant roll in the FSS filter and metamaterial response, so measured dispersive dielectric values and metal models based on measurement are used in the simulation.
2.3.2 Periodic Finite Element-Boundary Integral Method

A second PFE-BI method is used to calculate the scattering from FSS with multiple metallic screens or with inhomogeneous dielectric layers. The PFE-BI method, a hybridization of the traditional MoM with the finite element method (FEM), is a powerful and efficient full-wave numerical method for handling inhomogeneous problems [79,80]. For periodic structures, the method begins with a functional description of the field problem where only a single unit cell of the periodic structure is considered. Figure 2.5 illustrates the generic problem geometry. The structure is assumed to be planar, periodic in $x$-$y$ plane, with cell periodicities $D_x$ and $D_y$ along the $x$- and $y$- directions, respectively. The four vertical walls of the unit cell are designated as $\Gamma_L$, $\Gamma_R$, $\Gamma_F$ and $\Gamma_B$, where $\Gamma_L$ and $\Gamma_F$ are assumed to be the sidewalls opposite to $\Gamma_R$ and $\Gamma_B$, respectively. A standard FEM technique described in [79] is employed to solve the field inside the unit cell, and the FEM computation domain is terminated in the $z$- direction by applying the mixed potential integral equation (MPIE) [81] on the top and bottom planar surfaces of the unit.
Under these conditions, the pertinent finite element functional may be cast in the form

\[
\int_V \left[ -\frac{1}{\mu} (\nabla \times \bar{W}) \cdot (\nabla \times \bar{E}) - k_0^2 \epsilon_0 \bar{W} \cdot \bar{E} \right] dv - 2k_0^2 \int_S \int_S G_p(\vec{r}, \vec{r}') (\hat{n} \times \bar{W}) \cdot (n \times \bar{E}) ds'ds \\
- 2\int_S \int_S G_p(\vec{r}, \vec{r}') \nabla_s \cdot (\hat{n} \times \bar{W}) \nabla_s' \cdot (\hat{n} \times \bar{E}) ds'ds = -jk_0Z_0 \int_S (\hat{n} \times \bar{W}) \cdot \vec{H}^w ds 
\]

where \( \bar{W} \) is the weighting function, \( V \) represents the finite element domain, which is the volume of the unit cell, \( S \) represents the top and bottom surfaces of the unit cell, \( \hat{n} \) is the normal vector of surface \( S \), directed out of the finite element domain, \( k_0 \) and \( Z_0 \) are the wave number and wave impedance of the free-space, respectively, and \( G_p(\vec{r}, \vec{r}') \) is the periodic Green’s function. The slowly converging series in the spatial domain periodic Green’s function are converted into two rapidly converging series by using the Ewald transformation [81]. To relate the fields on the opposing walls of the unit cell in the finite element problem, the phase boundary conditions (PBC), which can be expressed as

\[
e_{\Gamma_x/\Gamma_y} = e_{\Gamma_x/\Gamma_y} \exp(-jk_0 \sin \theta_0 \cos \varphi_0 x + k_0 \sin \theta_0 \sin \varphi_0 y)) \]

are employed on the vertical walls of the unit cell. In Eq. 2.9, \( e_{\Gamma_x/\Gamma_y} \) represents the unknown field at an edge on one of the vertical walls and \( \theta_0 \) and \( \varphi_0 \) are the angle of the excitation planewave. For the discretization of the unit cell volume integrals in Eq. 2.8 we employ edge-based basis functions on three-dimensional cubic elements. The matrix equation is solved by using the bi-conjugate gradient method (Bi-CG), which yields the coefficients of the basis functions. The electric field on the top and bottom surfaces of the unit cell is then constructed through the basis functions to find the scattering parameters of the periodic structure.
2.3.3 Material Loss Models

At infrared wavelengths, the loss characteristics of dielectrics and metals are dispersive and play a significant role in determining the scattering from IR FSS. For dielectric materials used in this work, thin film samples generated by our fabrication methods have been characterized using infrared variable angle spectroscopic ellipsometry (IR-VASE). Plots showing the dispersive permittivity $\varepsilon_r$ for these materials are presented in the Appendix. The metal metals used in this work are Lorentz-Drude models fitted to experimental data and are found in the literature [82]. In the PMM and FE-BI codes, metals are represented by impedance surfaces and described by the metal surface impedance $Z_s$. Three surface impedance calculations were considered throughout the course of the work and are described in the following paragraphs.

The first surface impedance model assumes that the thickness of the metal sheet is much larger than the skin depth. If the measured optical properties of the metal are the complex permittivity represented by the complex permittivity $\varepsilon_r = \varepsilon' - j\varepsilon''$, then the surface impedance at the boundary of the metal can be calculated as

$$Z_s = \sqrt{\frac{\mu_r}{\varepsilon' - j\varepsilon''}} = \frac{Z_0}{\sqrt{\varepsilon' - j\varepsilon''}} \quad (2.10)$$

where $\mu_r = 1$ is the permeability of the metal and $Z_0 = 377\Omega$ is the impedance of free space [67]. This model is useful for filter designs in the far-IR, where the metal permittivity of the metal is large, shrinking the skin depth of the metal to much smaller than the thickness of the metal film.
The second impedance model is derived using the volume equivalence theorem. If we consider the geometry shown in Figure 2.6, we can represent the equivalent volume current $\vec{J}_{eq}$ inside the layer by

$$\vec{J}_{eq} = j\sigma(\varepsilon_r - \varepsilon_0)[\vec{E}^i + \vec{E}^s],$$

(2.11)

where $\varepsilon_r$ is the complex permittivity inside the layer. The wave will attenuate in the layer according to $\vec{E} \sim e^{-jkz}$, where $k = \sigma\mu\sqrt{\varepsilon\mu} = \frac{\omega}{c}$ is the complex propagation constant in the layer. Neglecting reflections, the equivalent volume current as a function of the layer depth $z$ can be written approximately as

$$\vec{J}_{eq}(z) = j\omega(\varepsilon - \varepsilon_0)[\vec{E}^i + \vec{E}^s] \bigg|_{z=0} e^{-jkz} = \vec{J}_0 e^{-jkz},$$

(2.12)

where $\vec{J}_0$ is the equivalent volume current at the top of the layer. The surface current can then be determined by integrating the volume current over the thickness $d$ of the layer:

$$\vec{J}_s = \int_0^d \vec{J}_{eq}(z)dz = \int_0^d \vec{J}_0 e^{-jkz}dz = -\frac{\vec{J}_0}{jk} e^{-jkz} \bigg|_0^d = \frac{\vec{J}_0}{jk} \left(1 - e^{-jkd}\right).$$

(2.13)

The surface impedance is then given by
Substituting for $k$ leads to

$$Z_s = \frac{\sqrt{\varepsilon_r \mu_r \varepsilon_0}}{\alpha \varepsilon_0 (\varepsilon_r - 1) \left( 1 - e^{-j\sqrt{\varepsilon_r \mu_r \varepsilon_0 d}} \right)} = \frac{Z_0}{\left( \sqrt{\varepsilon_r - 1} \varepsilon_0 \right) \left( 1 - e^{-j\sqrt{\varepsilon_r \mu_r \varepsilon_0 d}} \right)}. \quad (2.15)$$

For the case where $d$ is much larger than the skin depth and the permittivity is large, Eq. 2.15 simplifies to the first surface impedance model given by Eq. 2.10.

---

**Region 1**

$e_1, \mu_1, \eta_1$

$\vec{E}^1$

$\vec{H}^{1\parallel}$

$\vec{H}^{1\perp}$

$\vec{E}^{r1}$

$\vec{B}_1$

---

**Region 2**

$e_2, \mu_2, \eta_2$

$\vec{E}^2$

$\vec{H}^{2\parallel}$

$\vec{H}^{2\perp}$

$\vec{E}^{r2}$

$\vec{B}_2$

---

**Region 3**

$e_3, \mu_3, \eta_3$

$\vec{E}^3$

$\vec{H}^{3\parallel}$

$\vec{H}^{3\perp}$

$\vec{E}^{r3}$

$\vec{B}_3$

---

Figure 2.7: Geometry for surface impedance derivation calculated from the scattering from a slab.
The third impedance model is derived from the geometry shown in Figure 2.7. The impedance for this geometry is given by the ratio of the total electric field to the total magnetic field

\[ Z_{\text{in}}(z) = \frac{E_{\text{total}}(z)}{H_{\text{total}}(z)}. \]  

(2.16)

Calculating the surface impedance at the first interface gives

\[ Z_{\text{in}}(z = -d^+) = \eta_2 \left( \frac{1 + \Gamma_{\text{in}}(z = 0^-) e^{-2\gamma_d d}}{1 - \Gamma_{\text{in}}(z = 0^-) e^{-2\gamma_d d}} \right) = Z_{\text{in}}(z = -d^-) \]  

(2.17)

where

\[ \gamma_2 = j \omega \sqrt{\mu_r \varepsilon_r} \sqrt{\varepsilon_r' - j \varepsilon_r''} \]  

(2.18)

and

\[ \Gamma_{\text{in}}(z = 0^-) = \frac{Z_{\text{in}}(z = 0^+) - \eta_2}{Z_{\text{in}}(z = 0^+) + \eta_2} = \frac{\eta_3 - \eta_2}{\eta_3 - \eta_2} \]  

(2.19)

Substituting the impedances all three regions and simplifying gives the final expression for the surface impedance:

\[ Z_s = Z_{\text{in}}(z = d) = \frac{Z_o}{\sqrt{\varepsilon_r' - j \varepsilon_r''}} \left( \frac{\sqrt{\varepsilon_r' - j \varepsilon_r''} + 1 + \left( \frac{\varepsilon_r' - j \varepsilon_r''}{\varepsilon_r' - j \varepsilon_r''} \right) e^{-2\gamma_d d}}{\sqrt{\varepsilon_r' - j \varepsilon_r''} + 1 - \left( \frac{\varepsilon_r' - j \varepsilon_r''}{\varepsilon_r' - j \varepsilon_r''} \right) e^{-2\gamma_d d}} \right). \]  

(2.20)

This expression also simplifies to Eq. 2.10 when \( d \) becomes much larger than the skin depth. The final surface impedance calculation is considered to be the most accurate because reflections from the bottom of the layer are taken into account. Plots comparing the calculated \( Z_s \) from these three models in the infrared for Al, Ag, and Au metals are presented in the Appendix.
2.3.4 Metamaterial Inversion Techniques

When analyzing and synthesizing FSS based metamaterials, the scattering parameters obtained from PMM or PFE-BI codes must be inverted to obtain the refractive index and impedance or permittivity and permeability of a slab of equivalent thickness. Figure 2.8 conceptually illustrates how a single or multilayer FSS metamaterial would produce the same scattering parameters $S_{11}$ and $S_{21}$ as a slab with the same thickness and inverted constitutive parameters.

The inversion algorithm for a normally incident wave used in this work is credited to Nicolson, Ross, and Weir (NRW) [22,83], however equivalent algorithms have emerged recently in metamaterials literature [39]. The NRW procedure begins by calculating the S-parameters from the metamaterial when illuminated at normal incidence. The scattering parameters are then manipulated as follows.

Figure 2.8: Metamaterial structure and slab with equivalent constitutive parameters will produce the same S-parameters.
are used to calculate

\[ X = \frac{1 - V_1 V_2}{V_1 - V_2} \]  

(2.23)

\[ Y = \frac{1 + V_1 V_2}{V_1 + V_2}, \]  

(2.24)

which are then used to determine the parameters \( \Gamma \) and \( P \) from

\[ \Gamma = X \pm \sqrt{X^2 - 1} \]  

(2.25)

\[ P = Y \pm \sqrt{Y^2 - 1} \]  

(2.26)

The signs in Eq. 2.25 and Eq. 2.26 are chosen such that \( |\Gamma| \leq 1 \) and \( |P| \leq 1 \). Finally, the normalized impedance and refractive index for the equivalent slab can be obtained from

\[ Z = \frac{1 + \Gamma}{1 - \Gamma} \]  

(2.27)

\[ n = \left( \frac{jc}{\alpha d} \right) \left[ \ln(P) + j2\pi m \right], \quad m = \pm 0, 1, 2, \ldots, \]  

(2.28)

where \( \omega \) is the angular frequency and \( c \) is the speed of light. It is notable that the solution for \( n \) is multivalued and must be determined using additional information. The constitutive parameters can be calculated from \( n \) and \( Z \) according to
where $Z_0$ is the impedance of free space.

The root for $n$ is determined by enforcing $n'$ to be continuous across frequency and tracing $n'$ from a known point. For the FSS based metamaterials presented in Chapter 4 and Chapter 5, we recognize that because the constituent materials for the designs are not magnetic that in the low frequency limit, the permeability should approach unity:

$$\lim_{f \to 0^+} \mu = 1 - 0j$$

Thus, the S-parameters are collected from low frequencies up to the frequency range of interest, choosing $m$ such that $n'$ remains continuous.

### 2.3.5 Genetic Algorithm Optimization

A genetic algorithm (GA) optimization technique has been employed throughout this work to synthesis filters and metamaterials. GAs are a robust class of optimizers based off the Darwinian notions of natural selection. They lend themselves to FSS design because they are, capable of searching a large parameter space for a solution that simultaneously meets multiple constraints [21,84,85,86,87,88]. GAs have been used extensively in the microwave regime to synthesize FSS devices [89,90]. GAs mimic the evolutionary process, where a population of possible designs is iteratively mated, weeding out poor designs and keeping the best designs, until a design that meets the
specified requirements is found. In addition to being robust search algorithms, GAs are relatively simple to implement, requiring only that the design parameters be encoded into a binary chromosome and a fitness function be defined.

A flowchart detailing the configuration of the GA used in this work is shown in Figure 2.9. The optimization begins by generating a random population of candidate FSS designs. Because each candidate design is represented by a binary string, called a chromosome. The initial population is comprised simply of an array of random binary strings. Each string is, in turn, passed to the fitness function, which translates the chromosome into a FSS design and evaluates its performance using the PMM or PFEBI

Figure 2.9: Flowchart showing the GA optimization procedure used in this work.

A flowchart detailing the configuration of the GA used in this work is shown in Figure 2.9. The optimization begins by generating a random population of candidate FSS designs. Because each candidate design is represented by a binary string, called a chromosome. The initial population is comprised simply of an array of random binary strings. Each string is, in turn, passed to the fitness function, which translates the chromosome into a FSS design and evaluates its performance using the PMM or PFEBI
codes. Every chromosome is assigned a fitness value and subsequently they are ranked according to fitness. If the best fit member does not yet meet the design goal, a new generation is created using the genetic data from the existing population. Tournament selection is used to choose parents for each new offspring. Several potential parents are randomly selected, and then a ‘tournament’ picks the two fittest parents from the random cluster to mate. During mating a single point in the chromosome is chosen and the data is swapped between the parents before and after the crossover point to produce two new offspring. This selection and mating process continues until a new generation is filled. Then, a small (typically less than 1%) percentage of the population is selected for random mutation, where a bit in the chromosome is randomly chosen and flipped. Finally, elitism is enforced at each generation, so the member with the best fitness is copied into the new generation, unaltered. Then, the new generation is evaluated for fitness, and the mating process starts over again. The stopping criterion for the optimizations performed in this work was to end the optimization when the fitness did not improve for many generations.

The parameters defining the FSS structure, including the cell geometry, dimensions, and material properties, are encoded into a binary chromosome. In order to attain polarization insensitivity for a normally incident wave, the cell geometry is divided into 8 mirrored triangular folds, only one of which is encoded into the chromosome. The genes in the chromosome for metallodielectric FSS would then be ‘1’ for conductive pixels and ‘0’ for non-conductive pixels. Other parameters, such as the unit cell size, substrate thickness, dielectric constant of the substrate, and so on can be specified in the chromosome as variables to be optimized.
The fitness function must also be determined prior to each optimization. Because the fitness function varies depending on the particular optimization goals, a fitness function will be presented for each application in the following chapters of the dissertation.

In order to make accurate fabrication of designs possible, fabrication rules have been introduced into the GA synthesis process. These fabrication constraints eliminate single, isolated pixels from a chromosome’s geometry before simulation. Diagonal connections between patches are also eliminated, creating a minimum 1 pixel gap between neighboring patches of metal. Finally, an appropriate minimum pixel size is enforced on the geometry, corresponding to the resolution limit of the fabrication method.
Chapter 3
Planar Infrared Filters

The use of Frequency Selective Surfaces (FSS) for filtering applications at infrared (IR) wavelengths has become an area of increasing interest over the past few years [24,66,69,91]. While originally developed for applications at microwave frequencies, FSS technology can be utilized for IR applications by reducing the geometry dimensions from the cm scale to the micron or nm scale and by accounting for the material properties at IR wavelengths. This chapter focuses on the application of metallodielectric and all-dielectric FSS as filters for far-IR and mid-IR wavelengths. Section 3.1 discusses examples of metallodielectric FSS filters, and section 3.2 discusses all-dielectric structures. Section 3.3 examines the use of liquid crystal (LC) for tuning the response of metallodielectric FSS filters in the mid-IR.

3.1 Metallodielectric Frequency Selective Surfaces

Traditional metallodielectric FSS are comprised of metallic screens that are periodic in two dimensions and supported by one or more dielectric substrates and superstrates. Several experimental efforts have been made to demonstrate FSS technology in the near-IR (λ < 2 µm) for filters to be used in photovoltaic systems [66,91] and for custom absorbers or emitters [69]. In the far-IR (10 µm < λ < 100 µm) multiband FSS filters with stopband attenuation > 10 dB have been achieved with a single FSS screen by using fractal and GA synthesis techniques [24]. In this work the incorporation of fabrication constraints in GA
optimization of FSS filters is proposed to ease fabrication efforts. Section 3.1.1 presents the
design, fabrication, and characterization of multiband filters for the far-IR using a GA with
fabrication constraints. Section 3.1.2 discusses multiband filters for the mid-IR.

3.1.1 Far-Infrared Filter Design, Fabrication and Characterization

In this section metallodielectric FSS filter designs for the far-IR are considered. Optical contact lithography was chosen as the method for fabricating far-IR FSS in this work because it is a mature technology, and it is a parallel write process which can achieve feature sizes as small as one micron line-widths and spacing. A feature resolution of 1 µm is small enough to provide sufficient flexibility in the pixelized geometry that the GA can exploit for multiband resonances. Polyimide was selected as the FSS substrate because it is flexible, it can be spun to sub-micron thicknesses, and it is transmissive in the far-IR. The metallic features are 75 nm thick aluminum deposited by thermal evaporation. Two polyimide substrate thicknesses, 4 µm and 0.5 µm, were studied in the designs presented in this section.

Because the substrate thickness and substrate dielectric material for each FSS design were chosen a priori, the only parameters represented in the chromosome were the metallic screen geometry and the unit cell size. The unit cell is comprised of a 16x16 pixel grid of binary values indicating the presence (“1”) or absence (“0”) of metal on a given pixel. Eight-fold symmetry is applied to the unit cell to achieve polarization independence. Thus, only one triangular fold of the unit cell is encoded into the chromosome. The unit cell size is also encoded into the chromosome as an eight bit
string. The pixel size is constrained to be larger than the minimum resolution of 1 μm set by the targeted contact lithography fabrication method.

The fitness of each candidate FSS filter design is measured against a desired filter response. Several pass band and stop band frequencies are chosen over the desired band of operation. Then, each design is simulated at the specified frequencies and penalized for energy transmitted at stop band frequencies and energy reflected at pass band frequencies. The minimizing fitness function used for the optimizations in this work is given in Eq. 3.1, where $R$ is the reflectance at each specified pass band frequency and $T$ is the transmittance at each specified stop band frequency.

$$Fitness = \sum_{\text{pass}} R + 3 \sum_{\text{stop}} T$$  \hspace{1cm} (3.1)

A weighting coefficient of 3 is generally used to achieve greater attenuation at the specified stop bands.

At IR frequencies the loss in the metallic screen begins to affect the performance of FSS filters and should be incorporated into the simulation of the FSS [67,92]. Measured optical and infrared properties of the metals used in this work have been fit to Lorentz-Drude fitting models [82]. The published complex frequency-dependent dielectric function are related to the wave impedance of the metallic screen by the expression described in Eq. 2.10. The dielectric loss in the FSS also plays a significant role in the filter response of the FSS. Because a spectral permittivity model for polyimide was not available in the far-IR, an estimated value of $\varepsilon_r = 3.0 - 0.3j$ was used for all simulations in this section. The real part of this value was estimated by extrapolating published near-IR polyimide measurements [93], while a value for the imaginary part
was chosen to produce simulated stop-band performance that corresponded with levels measured in experiment [24].

Previous work described in [24,94] demonstrated that multiband IR FSS could be achieved by GA synthesis, but an additional step of trimming the GA optimized screen geometry was required for fabrication. Such trimming and the resulting shifts in resonance positions are clearly undesirable. In order to mitigate the need for trimming after a GA optimization, a set of constraints based on fabrication rules were developed and incorporated into the GA. The fabrication rules suppress diagonal connections between metallic pixels as well as single pixel metallic patches. The fabrication rules scan each chromosome for unwanted diagonal connections or single pixel islands. If any are found, a pixel in the geometry is switched from metal (“1”) to no metal (“0”) to eliminate the unwanted metallic pixel.

The first GA synthesized metallodielectric FSS example incorporating fabrication rules was optimized for a 0.5 \( \mu \)m polyimide substrate. Two stop bands were specified at 3.5 THz and 6.5 THz, and pass bands were requested elsewhere over the operating range of 1 THz to 10 THz. For all of the following GA optimizations with fabrication rules presented in this section a population size of 75 was evolved over 300 generations. For this first design, the metallic screen loss in aluminum at 10 THz was included in the fitness evaluation. The optimized geometry is shown in Figure 3.1(a) with a unit cell size of 36.8 \( \mu \)m on a side. There are no diagonally touching pixels in this design geometry, due to the fabrication rules that were incorporated into the GA. The PMM simulated transmission spectrum including metallic and dielectric losses shown in Figure 3.2 indicates that the MDPC meets the design goals of the optimization.
Figure 3.1: GA synthesized IR FSS for stop bands at 3.5 THz and 6.5 THz. Fabrication rules were employed in this optimization. (a) The unit cell geometry and (b) an optical microscope image of the fabricated screen are shown.
Each sample was fabricated on a sacrificial silicon wafer. Samples with a 4 µm polyimide substrate were strong enough to be peeled off the silicon wafer and mounted on an aluminum slide for characterization as shown in Figure 3.3. The aperture in the aluminum slide through which the characterization beam could pass is approximately 5 mm x 5 mm. Samples with a 0.5 µm polyimide substrate did not possess enough tensile strength to be removed from the wafer. Hence, an aperture with a diameter of 1 mm was etched in the silicon wafer beneath the sample by potassium hydroxide (KOH) meniscus interface etching. Characterization of the fabricated MDPCs was performed using Figure 3.2: Simulated and measured transmission spectra for the GA synthesized design shown in Figure 3.1.
Fourier transform infrared (FTIR) spectroscopy to measure the transmission spectrum of each sample at normal incidence. For samples with 0.5 μm polyimide substrates the characterization beam was cropped to match the cross-section of the aperture etched through the silicon wafer. The transmission spectrum of each metallodielectric FSS sample is ratioed to that of a blank polyimide substrate with the same thickness to remove the effects of absorption bands that appear in the polyimide spectrum.

An optical microscope image of the fabricated MDPC is shown in Figure 3.1(b) and demonstrates an accurate representation of the GA designed screen geometry. There
is some blooming, or swelling of the metallic features, that was introduced during fabrication. However, the measured transmission spectrum is in excellent agreement with the original simulated response as seen in Figure 3.2. Slight discrepancies between the measured and simulated responses can most likely be attributed to the effects of blooming during fabrication.

Figure 3.4: IR FSS synthesized via GA for stop bands at 3.8 THz and 7 THz. (a) The cell geometry and (b) an optical microscope image of the fabricated screen are shown.
A second GA synthesized metallodielectric FSS design is shown in Figure 3.4. This design was optimized on a 0.5 µm polyimide substrate for two stop bands at 3.8 THz and 7 THz and pass bands elsewhere over the range from 1 THz to 10 THz. Metallic loss from aluminum at 10 THz was included in the fitness evaluation. The resulting geometry shown in Figure 3.4(a) has a unit cell size of 36.9 µm on a side and does not contain any diagonally connecting pixels. An optical microscope image of the fabricated structure in Figure 3.4(b) reveals an accurately fabricated screen geometry with some slight blooming.
around the metallic patches. The simulated and measured transmission spectra for this design are shown in Figure 3.5. Once again we have very good agreement between simulation and measurement. Slight differences can be explained by the blooming of metallic patches that occurred during fabrication.

Figure 3.6: GA synthesized IR FSS on a 4 μm polyimide substrate with stop bands at 2.7 THz and 5.9 THz. The (a) unit cell geometry and (b) an optical microscope image of the fabricated screen are shown.
The next GA synthesized metallodielectric FSS example was designed on a 4 µm polyimide substrate to demonstrate GA synthesis of IR FSS with thicker substrates. Here the GA searched for a design with two stop bands at 2.7 THz and 5.9 THz and pass bands elsewhere from 1 THz to 10 THz. Because the substrate is thicker, the substrate loss can play a more significant role in degrading the stop band performance. Thus, both metallic and dielectric losses were included in the fitness evaluation. The resulting geometry is shown in Figure 3.6(a) with a cell size of 35.9 µm on a side. The optical microscope image of the fabricated metallodielectric FSS shows an accurate representation of the

Figure 3.7: Simulated and measured transmission spectra for the GA synthesized IR FSS shown in Figure 3.6.
designed structure with some blooming. The simulated and measured transmission spectra in Figure 3.7 show excellent agreement between the design goals and the response of the fabricated structure.

Figure 3.8: GA synthesized IR FSS optimized for stop bands at 3 THz and 7 THz with a 0.5 μm polyimide substrate. The (a) unit cell geometry is shown along with optical microscope images of (b) the fabricated screen and (c) the fabricated inverse or dual screen.
The last GA designed metallodielectric FSS example with fabrication rules was synthesized on a 0.5 µm polyimide substrate. Stop bands were specified at 3 THz and 7 THz and pass bands were requested elsewhere over the range from 1 THz to 10 THz. Metallic loss was included in the fitness evaluation. The optimized unit cell geometry is shown in Figure 3.8(a) with a cell size of 38.3 µm on a side. An optical microscope image of the fabricated structure is shown in Figure 3.8(b). Blooming is evident,
especially on the central patch structure. However, the simulated and measured transmission responses show excellent agreement as seen in Figure 3.9.

![Graph showing simulated and measured transmission spectra](image)

Figure 3.10: Simulated and measured transmission spectra for the inverse or dual GA IR FSS shown in Figure 3.8(c).

For this last example, the inverse, or dual, structure was also fabricated and is shown in Figure 3.8(c). In this example, metal pixels were changed to no metal, and pixels with no metal were replaced with metal pixels. Comparing Figure 3.8(b) and Figure 3.8(c), the blooming that occurs during fabrication can be clearly seen. For the inverse structure, we expect the transmission and reflection spectra to be reversed. As expected, by examining the response of the dual structure in Figure 3.10, we find pass
bands in both measured and simulated transmission spectra at 3 THz and 7 THz, where we saw stop bands in the original structure. We also find stop bands over the remainder of the operating range from 1 THz to 10 THz.

3.1.2 Mid-Infrared Filter Design, Fabrication and Characterization

The design procedure for realizing multiband mid-IR FSS filters borrows some techniques from the previous section. The geometry fabrication constraints are adjusted for electron beam (e-beam) lithography and thus include a minimum pixel dimension of 100 nm. A minimum total FSS thickness of 0.5 µm is also used in the GA so that the final sample is strong enough to be released from the wafer and mounted on a slide for characterization as a freestanding device. Each design is evaluated against an ideal filter response with specified passband and stopband frequencies. The metallodielectric FSS response is predicted using a full-wave periodic method of moments (PMM) code [20,52]. Dispersive material parameters including the measured dielectric constant for polyimide and a published metallic loss model for Ag at optical and IR wavelengths [52] are incorporated into the PMM model. The dielectric constant for polyimide films cured under our experimental conditions was measured using infrared variable angle spectroscopic ellipsometry (IR-VASE) from 2 µm to 20 µm in wavelength and incorporated into the GA fitness function. The measured permittivity data for polyimide is shown in the Appendix. The minimizing fitness function used in the GA is given by

\[
Fitness = \frac{1}{N_{pass} N_{pass}} \sum (\text{MIN}(|\tau|, 0.95) - 0.95)^2 + \frac{1.5}{N_{stop} N_{stop}} \sum (\text{MAX}(|\tau|, 0.1) - 0.1)^2 \tag{3.2}
\]
where $N_{pass}$ and $N_{stop}$ are the number of pass band and stop band frequencies, respectively, and $T$ is the transmission coefficient calculated by the PMM model.

Figure 3.11: (a) Unit cell geometry of a metallodielectric FSS filter optimized by a GA to exhibit dual stop bands at 3.3 and 4.1 µm. The period $d$ of the unit cell is 1.87 µm. The thickness $h$ of the polyimide dielectric layers is 1.07 µm on each side of the silver metal elements. The binary chromosome is shown over one triangular fold of the unit cell. (b) SEM image of a fabricated filter without the top polyimide dielectric layer. The inset shows an enlarged image of one unit cell. The bright areas are the silver elements and the dark areas are the dielectric.
Because polyimide has strong absorption bands in the mid-IR for frequencies lower than 55 THz, the frequency band chosen for optimization was 50 THz to 150 THz (2 µm to 6 µm in wavelength). Two target stop band locations were chosen at 75 THz and 90 THz, each specified to the GA by three closely spaced frequency points. Pass bands were specified elsewhere from 50 THz to 150 THz at 29 frequency points. The GA optimized a population of 75 members over 500 generations to arrive at the design shown in Figure 3.11(a) with a unit cell size of 1.87 µm on a side and with matching polyimide substrate and superstrate thicknesses of 1.07 µm. The predicted response in Figure 3.12 shows strong dual stopbands at the design frequencies of 75 THz and 90 THz.

Figure 3.12: Transmission spectra of the dual-band fabricated FSS measured using FTIR spectroscopy as well as the PMM simulation including metallic and dielectric losses.
and passbands elsewhere from 50 THz to 150 THz aside from some polyimide absorption bands at lower frequencies.

This design was fabricated using e-beam lithography to print a 75 nm thick Ag FSS screen on a 1.07 µm polyimide substrate. A second 1.07 µm polyimide superstrate was then spun and cured over the FSS screen before removing the entire structure from the silicon wafer and mounting it on an aluminum slide for characterization. A scanning electron microscope (SEM) image of the fabricated structure is shown in Figure 3.11(b). The Fourier transform infrared (FTIR) spectrometer measurements of the fabricated structure shown in Figure 3.12 reveal shifted stopbands centered at 80 THz and 100 THz. The small blue shift and increase in bandwidth are due, at least in part, to rounding at the corners of the silver pixels during electron-beam patterning. In addition, the metallodielectric FSS filter was characterized with a focused beam in the FTIR rather than a plane wave as used in the model. This may also account for the lower attenuation and broadening of the transmission stop-bands relative to the model. These results demonstrate that this design optimization process can be applied to design mid-infrared metallodielectric photonic devices that meet user-input-defined performance criteria using only a single layer of metallic elements.

3.2 All-Dielectric Frequency Selective Surfaces

The optical properties of two-dimensional dielectric gratings, known as photonic crystal (PC) slabs or all-dielectric frequency selective surfaces (DFSS), have received significant attention over the past several years because of their application as
narrowband filters [95,96,97]. In Section 3.1.2 metallodielectric FSS were exploited to achieve dual stop bands in the mid-IR for use in filtering applications [7]. However, the bandwidths of metallodielectric FSS filters are somewhat large in comparison with those reported for all-dielectric FSS slabs due primarily to the intrinsic loss of metals at IR/optical wavelengths [24,70]. In order to realize a narrow bandwidth IR filter with low absorption loss, DFSS containing low-loss dielectrics can be considered. In Section 3.2.1 a DFSS filter with dual, sharp resonances for the mid-IR is considered. However, the stop bands for this design are strongly dependent on the incidence angle of the characterization beam, which is very typical of DFS structures [95,97]. The focus of Section 3.2.2 is to increase the angular tolerance of a mid-IR resonant DFSS through the use of GA optimization.

3.2.1 Dual-band Filter Design, Fabrication and Characterization

Although there has been extensive work in the analysis and design of DFSS, most of this work is limited to the structures that are based on waveguide gratings. In the case of DFSS with 2D periodic inhomogeneous dielectric layers, simple structures such as rectangular blocks are expected to give rise to one or more stopband frequencies, depending on the properties of the dielectric materials and dimensions of the structure. For the purpose of this study, a simple square block geometry was considered for a 2D inhomogeneous dielectric layer as shown in Figure 3.13, which will produce the same filter response for both polarizations at normal incidence. The blocks are composed of amorphous silicon (a-Si) surrounded by air and have a relative permittivity of 11.6 in the
mid-IR. A homogeneous polyimide substrate is chosen for a support layer because it is robust, flexible, and highly transmissive in the mid-IR over the wavelength range from 2 \( \mu \text{m} \) to 5 \( \mu \text{m} \).

Figure 3.13: All-dielectric FSS designed to have dual stop-bands at about 80 THz and 91 THz in the mid-IR. (a) Cross-section view of the unit cell with dimensions; (b) 3-D drawing of the DFSS showing square a-Si blocks on a polyimide substrate; (c) SEM image of the fabricated DFSS, scale bar 1 \( \mu \text{m} \).
A full-wave periodic finite element-boundary integral (PFEBI) technique was employed in this work to perform the electromagnetic simulations of the DFSS structures because it is a powerful and efficient full-wave numerical method for handling inhomogeneous problems [81]. Measured material properties were incorporated into the PFEBI code for polyimide. The filter response of the DFSS was calculated across a range of geometry dimensions, including the polyimide substrate thickness, the a-Si block thickness, the square block width, and the unit cell periodicity. The design was limited by a minimum polyimide substrate thickness of 0.5 µm, a minimum feature size of 100

Figure 3.14: Simulated and measured transmission response for the DFSS shown in Figure 3.13. The excellent agreement with experiment validates the PFEBI code used to simulate DFSS structures in this work.
µm for electron beam (e-beam) lithography, and a maximum aspect ratio for the a-Si block height to width of 1:1. Optimizing the design parameters by hand for dual stopbands in the mid-IR around 3.5 µm in wavelength resulted in the design shown in Figure 3.13(a) and Figure 3.13(b). The polyimide and a-Si block thicknesses are 0.895 µm and 0.54 µm, respectively. The block length and width are 1.491 µm, and the cell dimension is 1.909 µm on a side. The PFEBI predicted transmission response for this structure is shown in Figure 3.14. Two strong stopbands can be seen at around 80 THz and 91 THz with greater than 10 dB attenuation. Passbands occur elsewhere from 65 THz to 105 THz.

Fabrication of the DFSS shown in Figure 3.13 starts with spin-coating and curing a thin layer of polyimide film on an oxidized Si wafer. The polyimide precursor used in this experiment is *HD Microsystems PI2556* diluted by 85% using *HD Microsystems T9039* polyimide thinner. The curing process is carried out in a nitrogen-purged oven by first heating at 150°C for 30 min, then at 250°C for two hours. On top of the polyimide film, an a-Si layer is deposited in a Trion ICP-PECVD system by introducing silane (SiH₄) gas into the reaction chamber. During the deposition process, the substrate temperature is kept low at 300°C to prevent the polyimide film from glass transition. The thicknesses of the polyimide and a-Si layers are measured to be approximately 1000 nm and 500 nm, respectively, using a J. A. Woollam BASE-160 spectroscopic ellipsometer.

E-beam lithography is used for patterning the a-Si blocks. First a layer of positive e-beam resist (ZEP 7000A) is spun onto the wafer and covered with 10 nm thick gold coating to avoid charging during e-beam exposure. The resist is then exposed in a Leica EBPG-5HR system to define the 2D square block array into the resist. The dose of the
electron beam current is adjusted to minimize blooming of features due to proximity effects. Following exposure, the resist is developed in ZED 500 for deposition of 100 nm thick chrome and lift-off. With the chromium square patches as a mask, the a-Si layer is etched through in a Trion ICP-RIE system to form square blocks. After the chromium mask layer is dissolved with chromium etchant, the DFSS structure is peeled off from the handling Si wafer with diluted buffered oxide etchant and mounted onto a testing frame for characterization. The overall sample size of the DFSS structure is about 5 mm in square (i.e. 2500 by 2500 unit cells). The SEM image in Figure 3.13(c) shows a SEM image of the fabricated DFSS sample.

The sample was characterized using Fourier transform infrared (FTIR) spectroscopy to measure the non-polarized transmission at normal incidence. The transmission plot in Figure 3.14 shows that the fabricated DFSS filter has two strong stop-bands in the mid-IR centered at 79.6 THz and 91.4 THz. We also note that the excellent agreement between our simulation and measurement provides validation for the accuracy of the full-wave PFEBI analysis tool. The transmission loss observed in the passbands is due primarily to reflection, as the absorption predicted by simulation is less than about 10 dB over the entire plotted region.

### 3.2.2 Genetic Algorithm Optimized Filter Design for Angular Tolerance

In Section 3.2.1 a DFSS filter with dual, sharp resonances for the mid-IR was presented. However, the stop bands were strongly dependent on the incidence angle of the characterization beam, which is very typical of PC slab or DFSS structures [95,97].
The focus of the current study is to increase the angular tolerance of a mid-IR resonant DFSS through the use of GA optimization. In this section, the experimental realization of a DFSS having a narrow, single stop band around 3 µm in wavelength with attenuation greater than -25 dB in the mid-IR and high angular stability up to 10° off normal incidence for both polarizations is presented. The angular and polarization stability performance requirements for this filter were met by incorporating fabrication constraints and accurate material properties into a robust GA [21] synthesis method for optimizing the DFSS geometry. As described in the previous section, strong agreement is found between the predicted and experimental scattering coefficients by incorporating measured dispersive material properties into a full-wave electromagnetic simulation of the DFSS structure. This agreement indicates that all-dielectric filters with user-defined characteristics can be optimized for direct fabrication.

The DFSS filter considered here consists of an inhomogeneous layer of dielectric nanostructures with air holes supported by a uniform dielectric substrate. The inhomogeneous top layer is periodic in two dimensions, with a unit cell divided into a 7x7 grid of pixels representing blocks of air (“0”) or dielectric (“1”). The unit cell is constrained to have eight-fold symmetry, so that the filter response will be identical for both TE and TM polarizations at normal incidence. A GA optimizes the unit cell geometry as well as the unit cell dimension and layer thicknesses. The scattering parameters for each geometry are calculated by the PFEBI code and then evaluated against an ideal filter response to determine its cost. The minimizing fitness function used in the GA is given by
where \( N_{\text{pass}} \) and \( N_{\text{stop}} \) are the number of pass and stop band frequencies, while \( T_{\text{TE}} \) and \( T_{\text{TM}} \) are the TE and TM polarized transmission coefficients. The ideal filter response, then, would be a transmittance greater than \(-0.45 \text{ dB}\) in the pass bands and less than \(-26 \text{ dB}\) in the stop band for both polarizations. Fabrication constraints are incorporated in the fitness function by limiting the pixel size and layer thicknesses to ranges compatible with our nanofabrication scheme. Diagonal connections between pixels are also not allowed as they are difficult to fabricate.

The constituent dielectric materials are chosen to have low loss, a large refractive index contrast over the wavelength range of interest, and good adhesion between the two materials. a-Si and polyimide were chosen as the grating and substrate materials, respectively. The a-Si provides a large refractive index contrast to air and polyimide, whereas the polyimide film offers good mechanical stability and flexibility. The use of a polyimide film substrate has the added benefit of eliminating a wet etch required to remove the silicon wafer under the sample [98,99].

The user-defined filter properties of polarization insensitivity, a narrow single stop band at 3 µm with several pass band frequencies specified over 2.5 to 3.75 µm, and a moderate angular tolerance up to 10° were fed into the GA with the measured refractive index values of polyimide and a-Si to evaluate the frequency response of each candidate filter design using a FEBI code. The square unit cell size was constrained in the GA to vary around half of the target wavelength, eliminating the possibility of exciting higher order propagating waves. The pixel size was also limited to be greater than

\[
Fitness = \frac{1}{N_{\text{pass}}} \sum_{i=1}^{N_{\text{pass}}} \left( \min \left( T_{\text{TE,TM}} \left| 0.95 \right| - 0.95 \right) \right)^2 + \frac{2}{N_{\text{stop}}} \sum_{i=1}^{N_{\text{stop}}} \left( \max \left( T_{\text{TE,TM}} \left| 0.05 \right| - 0.05 \right) \right)^2
\]  

(3.3)
100 nm for ease of fabrication. The thickness of the polyimide substrate was allowed to vary between 0.5 and 1 μm, and the a-Si varied in the range from 0.2 to 0.5 μm. The GA evolved a population of 16 over 33 generations to produce the DFSS filter design shown in Figure 3.15. Figure 3.15(a) shows the unit cell of the converged single stop band DFSS filter design with 246 nm pixels and a unit cell dimension of 1.72 μm on a side. The optimized thicknesses of the a-Si and polyimide layers are 338 and 762 nm, respectively. It is feasible to fabricate isolated a-Si blocks due to the presence of the supporting polyimide layer.

Figure 3.15: (a) Schematic of the DFSS filter unit cell optimized by a GA to exhibit a single stop band at 3 μm with polarization insensitivity and angular stability. (b) Scanning electron micrograph of the GA optimized DFSS displaying a vertical side wall profile.
Simulated transmission spectra of the GA optimized design are plotted for both TE and TM polarizations in Figure 3.16 for incidence angles of 0º and 10º and with the azimuth angle fixed to 0º. The angular tolerant resonance point was initially optimized at

Figure 3.16: Calculated and experimental TE and TM polarized transmission spectra for the DFSS filter shown in Figure 3.15. “Original” simulation represents the dimensions shown in Figure 3.15(a), whereas the “adjusted” simulation possesses a polyimide undercut and slightly thicker polyimide substrate to better match the experiment. Data is shown for comparison at normal (black solid line) and 10º oblique (red short dot) incidence.

Simulated transmission spectra of the GA optimized design are plotted for both TE and TM polarizations in Figure 3.16 for incidence angles of 0º and 10º and with the azimuth angle fixed to 0º. The angular tolerant resonance point was initially optimized at
3 µm, as exhibited by the “original” design simulation curves in Figure 3.16. This resonance point then shifted a little bit after fabrication errors, including a small polyimide undercut and slight increases in the polyimide and a-Si layer thicknesses were considered in the spectra calculation to match the fabricated sample more closely. In the resulting “adjusted” simulation, a Fano-shaped resonance at 2.95 µm maintains its position and depth almost identically up to 10° for both polarizations with transmission suppressed by 25 dB. Even though the resonance position is slightly red shifted by 0.68% at 10° for the TE case, the stop band profile is maintained. For oblique incidence angles, two more resonances appear for each polarization at the smaller wavelength edge of the primary stop band. However, these weak resonances do not affect the main resonance profile at 2.95 µm. These modes cannot be excited by an externally incident field at normal incidence due to the fact that the field profile of these modes share the full symmetry of the lattice. Meanwhile, the resonances at 2.61 µm and 2.95 µm are doubly degenerate states with field profiles that have the same parity as the incident wave and therefore can be coupled by a normally incident wave. In Figure 3.17(a) and Figure 3.17(b), the electric field distributions of the mode at 3.0 µm for the original geometry are shown to be a guided resonant mode, which has strong field confinement to the a-Si blocks without sharing the square lattice symmetry.

The optimized DFSS design was fabricated to experimentally verify the user-defined requirements. In Figure 3.15(b), a scanning electron micrograph of the fabricated single stop band DFSS filter is shown. Crisp features with highly anisotropic profiles were attained, and the fabricated film is shown to be mechanically stable and flexible.
The fabricated DFSS sample was characterized by measuring its transmittance at the operating frequencies using FTIR spectroscopy. The “measured” TE and TM transmission spectra in Figure 3.16 are shown to be in excellent agreement with the

Figure 3.17: Electric field distribution within the DFSS structure at the resonance wavelength of 3.0 µm. (a) The horizontal cross-section through the center of the a-Si layer reveals an asymmetric field pattern, indicative of a guided resonance. (b) The vertical cut through the a-Si blocks shows that the field is concentrated in the a-Si blocks.

The fabricated DFSS sample was characterized by measuring its transmittance at the operating frequencies using FTIR spectroscopy. The “measured” TE and TM transmission spectra in Figure 3.16 are shown to be in excellent agreement with the
simulated TE and TM results for two different angles of incidence. The position and attenuation of the main stop band at 2.93 µm for both TE and TM polarizations are well maintained up to 10° as predicted in the theoretical calculations performed by a full-wave FEBI simulation. The measured fractional 3 dB bandwidth of this optimized stop band is 13.5%, which is a bit broader than those of dielectric gratings, but still much narrower than those of reported metallo-dielectric FSS structures in this wavelength range of interest [7]. The optimized stop band positioned at 2.93 µm in the measured spectrum at normal incidence is shifted by less than 1.67% from the “adjusted” simulated value. This minor shift can be explained by the sensitivity of the stop-band location to the polyimide and a-Si layer thicknesses, undercutting into the polyimide layer during etching, and feature dimensions for the a-Si block pattern. The transmission attenuation of the stop band at 2.61 µm is reduced to -17.5 dB in the measurement, while the measured attenuation of the optimized stop band at 2.93 µm is close to the calculated value. This is caused by a finite cone angle in the measuring IR beam, which averages the transmission spectra over a range of angles as mentioned above. It is known that broader bandwidths give greater angular tolerance in a guided resonance [100]. Thus, there is no noticeable degradation in filter response for normal incidence at the optimized stop band, despite the angular spread in the measurement.

3.3 Liquid Crystal Tuned Metallo-dielectric Frequency Selective Surface Filters

There is currently interest in developing tunable filters and switches for IR and optical applications. Research discussed in the previous sections demonstrated the
synthesis of FSS for use as band-reject and band-pass filters with applications in various IR signal-processing devices. The frequency responses of these metallodielectric and all-dielectric FSS can be altered by incorporating a tunable dielectric, such as liquid crystal (LC), into the FSS structure [101]. Section 3.3.1 considers different methods for tuning the response of FSS filters and discusses in detail the application of LC to tunable IR FSS filters. Section 3.3.2 presents and compares several design examples for LC-tunable FSS filters.

### 3.3.1 Background on Liquid Crystals and FSS Tuning Methods

Current research and development in nonlinear and electro-optical materials for photonic applications are largely centered on nano-structured materials that exhibit unique physical and optical properties [41,42,101,102,103,104,105,106]. For advanced applications, it is highly desirable that the properties and functions of the resulting devices can be reconfigured or tuned. This can be accomplished by adjusting the effective permittivity and permeability of the medium supporting the device. Among existing materials, nematic liquid crystals (LCs) stand out as the preferred choice for the supporting medium as they possess extraordinarily large electro-optical and nonlinear optical responses, allowing both electrical and/or all-optical tuning. Furthermore, they are also compatible with almost all widely used optoelectronic materials and possess very broadband (near UV to infrared) transparency and large optical birefringence $\Delta n$ [101]. Recent studies indicate that LC can also be used for microwave tuning applications [105,106]. Their fluid nature allows easy incorporation into various geometries and
nanometer scale pore sizes [101]. Recent studies [42,104] of liquid crystal infiltrated 3-D inverse opal structures, for example, have demonstrated their exceptionally large spectral transmission tunability. The focus of this paper is directed towards the use of these various LC properties in the construction of tunable filters for terahertz applications based on micro- and nano-structured frequency selective surfaces (FSSs) and metamaterials that can exhibit tunable indices of refraction in the infrared (IR).

Band-reject and band-pass filters that exhibit single- or multi-band filter responses in the IR can be formed from a single layer metallodielectric FSS and have been designed using fractal and genetic algorithm (GA) techniques [6,24,94], where fabrication constraints were developed and incorporated within a GA synthesis procedure to achieve designs that could be accurately manufactured [24]. For applications at optical wavelengths, however, the metallic losses start to affect the performance of metallodielectric FSS filters. Thus, for optical applications, all-dielectric frequency selective surfaces (DFSSs) are preferable and can be synthesized as planar, polarization insensitive filters. In Section 3.3.2 metallodielectric FSS filters are designed to be widely tunable by incorporating a nematic LC into the FSS structure.

The filter response of a metallodielectric FSS is determined by both the 2D periodic geometry and by the electromagnetic properties of dielectric substrates or superstrates surrounding the screen [20,52]. The metallic screen resonates at certain frequencies dependent on the unit cell geometry and the periodicity between unit cells. At resonance, incident electromagnetic waves induce currents on the FSS screen, which reradiate in reflected waves. Because this stop-band resonance is determined by the electrical dimensions of the screen, the location of the stop-band will shift down in
frequency if the permeability or permittivity of a substrate or superstrate is increased. The resonant frequency is also dependent upon the thickness of the dielectric slabs surrounding the FSS screen as described in [52]. Thus, the substrate or superstrate thickness could be changed in order to tune the resonance frequency. Another method for tuning the frequency response of the FSS is to alter or reconfigure the unit cell geometry of the metallic screen. A novel reconfigurable frequency selective surface (RFSS) concept is described in [107].

Several demonstrations of FSSs with tunable substrates that operate in the microwave regime can be found in the literature. The most common method uses a ferrite for the substrate material [107,108,109,110,111]. As a dc bias is applied across the ferrite substrate, the electrical properties of the material change, making the electromagnetic waves in the material longer or shorter and tuning the stop-bands of the FSS lower or higher in frequency. While ferrite substrates offer tuning at microwave frequencies, there are some serious disadvantages associated with the concept. Ferrites have high mass, and large currents are required to maintain the dc bias across the substrate. Furthermore, ferromagnetic materials cannot be found for terahertz frequencies. Another novel tuning technique introduced in [15] uses a liquid dielectric as the substrate. A substrate cavity below the metallic screen is filled with a liquid dielectric or drained leaving air to tune the frequency response of the FSS. This novel technique has been demonstrated to tune the FSS frequency response, but it requires a complex design to properly handle the liquid substrate. Finally, a very recent paper reports passband tuning in the mm wave regime by using a LC sandwiched between two FSS screens [112].
The FSS tuning method we propose uses LC as a dielectric superstrate as shown conceptually in Figure 3.18. At IR and optical frequencies, LCs are excellent tunable dielectric materials due to their transparency and wide tuning range. While LCs have absorption bands due to mechanical resonances scattered throughout the IR, many LCs

Figure 3.18: (a) Conceptual illustration of a metallodielectric FSS with cross-dipole elements and a tunable nematic LC superstrate. (b) Side-view illustration showing how an actual LC cell could be encapsulated by a glass slide on top and the FSS (or DFSS) on the bottom.
exhibit high transmission from 95% to 100% from optical to IR wavelengths [101]. In
the literature, new LCs and LC mixtures are being reported with birefringences as high as
$\Delta n = 0.8$ [113]. For the tuning examples in this paper, we assume a lossless LC with a
birefringence of $\Delta n = 0.6$ and a permittivity ranging from 2 to 4 in our model. The
previous metallodielectric FSSs we have demonstrated in the IR were fabricated by
lithographically patterning Al and Ag metallic features on a thin polyimide substrate
[6,24,94]. In this case of a tunable IR metallodielectric FSS, a nematic LC cell is
incorporated directly on the metallic screen. The cell is made by sandwiching LC
between the FSS and a slide with a polymer rubbing layer that maintains the orientation
of the LC molecules in the relaxed state as illustrated in Figure 3.18(b). While rubbing
layers are typically incorporated on both sides of the LC cell, the molecule alignment can
be maintained with a single rubbing layer for thin cells and will exhibit only minor
degradation in LC molecule orientation on the opposite side of the cell. The LC is then
tuned by applying a static or alternating electric or magnetic field or by illumination with
polarized laser light in order to change the orientation of the LC molecules. While a
thick quartz or glass slide would be used to encapsulate the LC and hold it against the
FSS in actual implementation, the effects of the slide are not considered in this work.

3.3.2 Liquid Crystal Tuned IR FSS Filter Design Examples

In order to design a tunable metallodielectric FSS filter for the mid-IR, the screen
gamestry and substrate parameters must be optimized to give an isolated, narrow stop-
band. In keeping with our previous experimental efforts in the mid-IR, the substrate is
chosen to be a 1 µm thick polyimide layer, while the FSS screen consists of a 70 nm thick Ag film, patterned using electron beam lithography. Polyimide has very low loss and a permittivity of about 2.6 from 2 µm to 5 µm. Within this wavelength range the maximum measured polyimide loss tangent is \( \tan \delta = 0.0084 \). The superstrate is a 1 µm thick layer of liquid crystal with a permittivity varying from 2 to 4 and no loss.

A full-wave PMM analysis technique was employed to perform the electromagnetic simulations of the metallodielectric FSS with LC superstrate. At IR frequencies the loss in the metallic screen begins to affect the performance of FSS filters and should be incorporated into the simulation of the FSS [67]. Measured optical and infrared properties of the Ag fit to a Lorentz-Drude fitting model [82] were incorporated into the PMM code as a wave impedance calculated according to the expression given by Eq. 2.10.

![FSS screen geometries optimized to exhibit a single tunable stopband around 100 THz when used in conjunction with a LC superstrate. (a) Jerusalem cross element; (b) Minkowski fractal element.](image)

Figure 3.19: FSS screen geometries optimized to exhibit a single tunable stopband around 100 THz when used in conjunction with a LC superstrate. (a) Jerusalem cross element; (b) Minkowski fractal element.
Figure 3.20: Simulated transmission responses for the tunable FSS elements shown in Figure 3.19 with a 1µm LC superstrate.
Two well-known elements, the Jerusalem cross [20] and the Minkowski fractal loop [114], are considered for the screen geometry because they are known to produce narrow stop-band resonances. The geometry dimensions for these two elements, shown in Figure 3.19(a) and Figure 3.19(b), were optimized by hand to achieve strong attenuation at 100 THz, a narrow bandwidth, high pass-band transmission, and a large separation in frequency from neighboring resonances. The optimizations were performed for the case where the liquid crystal permittivity was set equal to 3. Next, the designs were simulated for $\varepsilon_{LC} = 2$ and 4 as shown in Figure 3.20(a) and Figure 3.20(b) to verify that the stop-band could be tuned in frequency by adjusting the superstrate permittivity. Table 3.1 compares the performance of these two designs, revealing that there is a trade-off between a strong stop-band, demonstrated by the Jerusalem cross, and a narrow bandwidth, demonstrated by the Minkowski fractal loop.

Table 3.1: Performance comparison between the FSS tunable filters presented in this section and a DFSS tunable filter [1].

<table>
<thead>
<tr>
<th></th>
<th>Jerusalem Cross</th>
<th>Minkowski Fractal</th>
<th>GA FSS</th>
<th>DFSS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Tuning Range</strong></td>
<td>18.3 THz</td>
<td>18.3 THz</td>
<td>18.1 THz</td>
<td>9.1 THz</td>
</tr>
<tr>
<td><strong>Avg. 3 dB Bandwidth</strong></td>
<td>17.6 THz</td>
<td>12.2 THz</td>
<td>12.6 THz</td>
<td>0.31 THz</td>
</tr>
<tr>
<td><strong>Avg. Stop-band Attenuation</strong></td>
<td>20.5 dB</td>
<td>11.8 dB</td>
<td>18.0 dB</td>
<td>23.4 dB</td>
</tr>
<tr>
<td><strong>Min. Insertion Loss</strong></td>
<td>0.5 dB</td>
<td>0.9 dB</td>
<td>0.6 dB</td>
<td>0.001 dB</td>
</tr>
<tr>
<td><strong>Max. Insertion Loss</strong></td>
<td>4.4 dB</td>
<td>2.2 dB</td>
<td>2.6 dB</td>
<td>1.2 dB</td>
</tr>
</tbody>
</table>

A third design was optimized using a genetic algorithm (GA) synthesis technique with fabrication constraints [24] in order to find a better balance between stop-band
attenuation and narrow bandwidth. For this FSS design, the parameters represented in the chromosome were a 16x16 pixel grid describing the metallic screen geometry, the unit cell size and the substrate thickness. Eight-fold symmetry was applied to the unit cell to achieve polarization independence, and diagonal connections between metallic patches that are difficult to fabricate were suppressed. The fitness of each candidate FSS design is measured against a desired filter response. The minimizing fitness function used for the optimizations in this work is given in Eq. 3.4, where $R$ is the reflectance at each specified pass-band frequency and $T$ is the transmittance at each specified stop-band frequency.

$$Fitness = \sum_{\text{pass}} R^2 + \frac{3}{2} \sum_{\text{stop}} T^2$$  \hspace{1cm} (3.4)

A weighting coefficient of 3/2 is used to achieve greater attenuation at the specified stop-band frequencies.

Figure 3.21: Pixelized FSS screen geometry optimized using a GA to exhibit a single tunable stopband around 100 THz when used in conjunction with a LC superstrate.
For a LC-tunable metallodielectric FSS filter design, we specified a single stop-band frequency at 100 THz (3 µm wavelength) and 32 pass-band frequencies spaced at 1 THz intervals from 80 THz to 95 THz and from 105 THz to 120 THz. The superstrate was constrained to be a 1 µm thick LC and was assigned a permittivity of 3, while the polyimide substrate was allowed to vary in thickness from 0.5 to 1.5 µm. The unit cell size was limited to 0.8 to 1.4 µm on a side, where the minimum pixel size could be fabricated by electron beam lithography. Measured loss models for both the polyimide substrate and the Ag metallic screen were incorporated into the PMM modeling code used in the evaluation of the GA fitness function. After optimizing a population of 75

Figure 3.22: Simulated transmission responses for the tunable FSS element shown in Figure 3.21 with a 1µm LC superstrate.
over 500 generations, the GA converged on the screen geometry shown in Figure 3.21. The unit cell measures 1.32 µm on a side, and the optimized polyimide substrate thickness is 1.05 µm. The response of this LC-tunable metallodielectric FSS shown in Figure 3.22 illustrates how the single narrow stop-band is tuned from 92.7 THz to 110.8 THz as the permittivity of the LC superstrate changes from 2 to 4. Table 3.1 reveals that the GA-designed tunable filter has a 3 dB bandwidth comparable with the Minkowski fractal loop design and an average stop-band attenuation of 18.0 dB, indicating that the GA allowed us to find a good balance between narrow bandwidth and stop-band performance.

Looking toward optical frequencies, all-dielectric FSSs offer better narrow-band filter performance because metallic losses are much more significant, whereas dielectric materials with low loss are readily available. For tunable filters that can operate in the IR or optical regimes, DFSSs with a LC superstrate have been considered in [1], where a similar shifting in stop-band resonances is observed as the superstrate permittivity changes. The LC-tunable DFSS example considered in [1] has been included in the performance comparison in Table 1, revealing that the DFSS has both stronger stop-band attenuation and narrower bandwidth than the metallodielectric FSS filters. With such an extremely narrow stop-band, this LC-tunable DFSS filter offers high selectivity in frequency over the entire tunable range from 83 THz to 92 THz [1].
A second GA optimized example was considered for which the substrate was not fixed to be polyimide. This FSS filter was optimized to provide a strong stop-band in the mid-IR that tunes in frequency from 71 THz to 92 THz (3.1 µm to 4.3 µm). The substrate parameters and screen geometry were optimized by the GA to have a single stopband within the frequency range from 60 THz to 100 THz. The optimized screen geometry is illustrated in Figure 3.23. The dimensions of the FSS unit cell are 2.17 µm x 2.17 µm, and the optimized substrate thickness is 0.94 µm with a dielectric constant of $\varepsilon_r$. 

Figure 3.23: Frequency Selective Surface screen geometry optimized by a Genetic Algorithm to exhibit a single tunable stopband over the range from 60 THz to 100 THz. (a) Unit cell geometry; (b) 3D depiction of the optimized structure.
The response of this LC-tunable FSS is shown in Figure 3.24. As the permittivity of the LC superstrate changes from 2 to 4, the stop-band location tunes from 93 THz to 71 THz. By allowing the GA to select the substrate permittivity, the GA could find a narrower band solution than when the FSS substrate was limited to polyimide.

Figure 3.24: Simulated transmission response for tunable FSS shown in Figure 3.23 with a 1 µm liquid crystal superstrate. Metallic losses for Ag are included in the PMM model.
Chapter 4

Single-Layer Metallodielectric Metamaterials

In this chapter, the design and characterization of planar zero index metamaterials (ZIMs) using frequency selective surfaces (FSS) is discussed. In order to design FSS metamaterials, a genetic algorithm (GA) is employed to evolve the metallic FSS screen geometry and dielectric layer properties in order to achieve the desired refractive index and impedance values. In Section 4.1 the design approach is described in depth along with several optimized FSS ZIM designs for the far-IR and mid-IR regimes. The synthesis, fabrication, and characterization of an optimized low loss ZIM that exhibits a low/zero index of refraction at far-IR wavelengths around 20 μm is presented in Section 4.2.

4.1 Zero-Index Metamaterial Design Approach

Figure 4.1: Cross-section of the single FSS screen metamaterial structure optimized in this chapter for ZIM properties.
The planar ZIM proposed here consists of an FSS screen supported backed by a dielectric substrate and superstrate as shown in Figure 4.1. Polyimide is chosen for the dielectric layers because it is robust and flexible and has very low loss in the far-IR for wavelengths larger than 15 µm and in the mid-IR from 2 µm to 6 µm in wavelength. The FSS screen is a 75 nm thick Ag metal film patterned by electron beam (e-beam) lithography. A GA is used to optimize the metamaterial structure for low loss and a low/zero effective refractive index. The metamaterial design parameters, including the FSS screen geometry, unit cell dimension, and dielectric layer thicknesses are all determined by the GA. The FSS screen geometry is pixellized into a 16 by 16 unit cell with eight fold symmetry enforced to achieve polarization insensitivity at normal incidence. A minimum pixel dimension is specified corresponding to the limitations of e-beam lithography.

Each step in the evolutionary process the GA evaluates the candidate design to determine how well it meets three criteria after imposing the fabrication design rule constraints. These criteria are: achieving the user-specified refractive index ($\Re[n_{\text{eff}}] = n_{\text{target}}$), minimizing power loss in the effective material (minimize $\Im[n_{\text{eff}}]$), and maximizing power transmission through the effective material (maximize $|T|^2$). Meeting these criteria also leads to an impedance match between the metamaterial and free space ($Z_{\text{eff}} \sim 1$). The minimizing fitness function used to evaluate each design is given by

$$
\text{Fitness} = \min_{\text{freqs}} \left[ \Re(n_{\text{eff}})^2 + \Im(n_{\text{eff}})^2 + (1-|T|^2)^2 \right]
$$

(4.1)

where $T$ is the predicted transmission coefficient, \text{freqs} are the frequency points over which the GA will search, and $n_{\text{target}} = 0$. 

To evaluate the cost function, $n_{\text{eff}}$ is determined by inverting the transmission $T$ and reflection $\Gamma$ scattering coefficients predicted by PMM analysis using the Nicolson-Ross-Weir algorithm [22,39,83]. In our previous studies on multi-band far and mid-infrared planar metallodielectric filters described in Chapter 3, the measured and modelled scattering parameters agreed well with experimentally measured values when the frequency-dependent dispersion properties of the metal screen and dielectric substrate were included in the simulations [6,7,24,94]. However, the solution for $n_{\text{eff}}$ is multivalued, and additional measures must be taken to ensure that the proper root is chosen during the inversion procedure. To eliminate ambiguity for $n_{\text{eff}}$ and choose the proper inversion root, a refractive index continuity test is performed. During the optimization, scattering data is calculated over a sweep from low frequency up to the band of interest. In the low frequency limit, the inverted permeability $\mu_{\text{eff}}$ is expected to approach $1-0j$. This is because there are no magnetic component materials ($\mu_{\text{Ag}} = \mu_{\text{polyimide}} = 1-0j$) and any magnetic resonances in the metamaterial would possess a limited frequency band dependent on the geometry of the metamaterial inclusions. The correct root for $\Re [n_{\text{eff}}]$, selected at a low frequency, is traced up to the band of interest enforcing $\Re [n_{\text{eff}}]$ to be continuous across frequency. Screen geometries having inverted constitutive parameters that are magnetic in the low frequency limit check are eliminated from the GA optimization process by assigning them a poor fitness.
The first design example was optimized for a range of target frequencies from 15 THz to 20 THz in the far-IR. As described in Section 4.2, it was found that in order to more closely match the experiment for far-IR wavelengths a loss factor $\alpha_{\text{Ag}}$ can be added to the bulk metallic model [44]. The adjusted model for silver is given by

$$\epsilon_{\text{Ag, adjusted}} = \Re[\epsilon_{\text{Ag}}] + \alpha_{\text{Ag}} \cdot \Im[\epsilon_{\text{Ag}}] j$$

(4.2)

where $\epsilon_{\text{Ag}}$ is the measured model for bulk Ag [82]. In this design example a loss factor of $\alpha_{\text{Ag}} = 4$ was included in the GA optimization and PMM simulations, and the surface impedance for the metallic FSS screen was calculated according to Eq. 2.15. The unit cell size was allowed to vary from 1 $\mu$m to 5 $\mu$m, and the polyimide substrate and superstrate were restricted to have the same thickness, which could vary from 250 nm to 500 nm. Optimizing a population of 75 over 1000 generations, the GA converged to the screen.

Figure 4.2: Unit cell geometry for a ZIM optimized for the far-IR with an optimum frequency of 17 THz. The unit cell measures 4.41 $\mu$m on a side.
geometry shown in Figure 4.2. The period in the x and y dimensions is 4.41 µm, and the polyimide substrate and superstrate layers are both 0.96 µm thick for a total thickness of 1.91 µm. The inverted refractive index and normalized impedance for this design are shown in Figure 4.3. The optimum frequency for this design was chosen by the GA to be 17 THz (17.6 µm wavelength), where the effective refractive index is \( n_{\text{eff}} = 0.331 - 0.333j \) and the normalized impedance is \( Z_{\text{eff}} = 1.69 + 1.72j \). The inverted permittivity and permeability are shown in Figure 4.4. The permittivity exhibits Drude behaviour, which is expected from the interconnected metallic mesh contained in the unit cell geometry shown in Figure 4.2. The permeability does not exhibit much dispersion and is close to 1, indicating that there is no magnetic resonance in the metamaterial structure. Thus, the ZIM behaviour of this metamaterial is due primarily to the permittivity approaching 0 at its plasma frequency, and the impedance is expected to become large. However, because the transmission was also optimized to be high, the effective impedance is maintained on the order of the impedance of free space. The scattering parameters calculated by the PMM code for a TE wave at 15° oblique incidence are shown in Figure 4.5. The transmission magnitude is -1.16 dB at the optimum wavelength.
Figure 4.3: Inverted (a) $n_{\text{eff}}$ and (b) $Z_{\text{eff}}$ for the ZIM design shown in Figure 4.2.
Figure 4.4: Inverted (a) $\varepsilon_{\text{eff}}$ and (b) $\mu_{\text{eff}}$ for the ZIM design shown in Figure 4.2.
Figure 4.5: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 4.2 for a TE polarized wave at 15° oblique incidence calculated using a PMM code.
The second design example was optimized for a band around 10 µm where polyimide has low loss (see the Appendix). The GA searched from 28 THz to 31.5 THz for an optimum ZIM band. Because this band is still at the edge of the far-IR, an alpha factor $\alpha_{Ag} = 4$ was used in the metal model as with the previous example. The surface impedance for the metallic FSS screen was calculated according to Eq. 2.15. The unit cell size was allowed to vary from 1 µm to 3 µm, and the polyimide substrate and superstrate were given matched thicknesses, which could vary from 250 nm to 1 µm. Optimizing a population of 75 over 1000 generations, the GA converged to the screen geometry shown in Figure 4.6. The unit cell dimension for this design is 2.98 µm, and the total thickness of the structure is 1.63 µm. The inverted refractive index and normalized impedance for this design are shown in Figure 4.7. The optimum frequency for this design is 28.5 THz (10.5 µm wavelength), where the effective refractive index is $n_{eff} = 0.366 - 0.425j$ and the normalized impedance is $Z_{eff} = 1.48 + 1.79j$. The inverted permittivity and permeability are shown in Figure 4.8. Once again, the permittivity has a characteristic Drude...
behaviour due to the interconnected metallic geometry in the unit cell, and the permeability varies only slightly near 1. The index and permittivity both also exhibit additional resonances above and below the optimal ZIM band, which are due to absorption bands in the polyimide dielectric (see the Appendix). The scattering parameters calculated by the PMM code for a TE wave at 10º oblique incidence are shown in Figure 4.9. The transmission magnitude at 28.5 THz is -2.5 dB.

Figure 4.7: Inverted (a) $n_{eff}$ and (b) $Z_{eff}$ for the ZIM design shown in Figure 4.6.
Figure 4.8: Inverted (a) $\varepsilon_{\text{eff}}$ and (b) $\mu_{\text{eff}}$ for the ZIM design shown in Figure 4.6.
Figure 4.9: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 4.6 for a TE polarized wave at 10° oblique incidence calculated using a PMM code.
The final design example was optimized for the mid-IR 4 \( \mu \text{m} \) in wavelength. Polyimide has low loss characteristics in the mid-IR from 2 \( \mu \text{m} \) to 5.5 \( \mu \text{m} \) (see the Appendix). The GA targeted the frequency range from 60 THz to 75 THz for an optimum ZIM band. Because the mid-IR FSS filter measurements presented in Section 3.1.2 did not require additional metal loss included in the model, an alpha factor \( \alpha_{\text{Ag}} = 1 \) was used for the GA optimization and simulations for this mid-IR ZIM example. The surface impedance for the metallic FSS screen was calculated according to Eq. 2.15. The unit cell size was allowed to vary from 1 \( \mu \text{m} \) to 1.6 \( \mu \text{m} \), and the polyimide substrate and superstrate were given matched thicknesses, which could vary from 250 nm to 1 \( \mu \text{m} \). A population of 75 was optimized for 1000 generations to arrive at the screen geometry.

Figure 4.10: Unit cell geometry for a ZIM optimized for the mid-IR around 4 \( \mu \text{m} \) in wavelength. The unit cell measures 1.60 \( \mu \text{m} \) on a side.
shown in Figure 4.10. The unit cell dimension for this design is 1.60 µm, and the total thickness of the structure is 0.50 µm. The inverted refractive index and normalized impedance for this design are shown in Figure 4.11. The optimum frequency chosen by the GA for this design is 75 THz (4 µm wavelength), where the effective refractive index is $n_{\text{eff}} = 0.159 - 0.230j$ and the normalized impedance is $Z_{\text{eff}} = 2.36 + 3.44j$. The refractive index for this design is significantly lower than those of the far-IR ZIM designs, but the impedance match is worse. The inverted permittivity and permeability are shown in Figure 4.12. The permittivity shows the expected Drude characteristic behaviour from the metallic mesh geometry. At the lower frequency of 52 THz, an absorption band can be found arising from a polyimide resonance. The permeability is flat and close to 1 indicating no magnetic resonances are present in the metamaterial. The scattering parameters calculated by the PMM code for normal incidence are shown in Figure 4.13. The transmission magnitude at the best frequency of 75 THz is high with an attenuation of -1.11 dB.
Figure 4.11: Inverted (a) $n_{\text{eff}}$ and (b) $Z_{\text{eff}}$ for the ZIM design shown in Figure 4.10
Figure 4.12: Inverted (a) $\varepsilon_{\text{eff}}$ and (b) $\mu_{\text{eff}}$ for the ZIM design shown in Figure 4.10.
Figure 4.13: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 4.10 for normal incidence calculated using a PMM code.
4.2 Far-Infrared ZIM Design, Fabrication and Characterization

For experimental fabrication and characterization of a ZIM, the far-IR wavelength range of 15 to 20 µm was chosen for the design optimization. During GA optimization, the polyimide superstrate and substrate layers were constrained to have equal thicknesses between 0.25 and 6 µm. The square pixel of the silver metallic screen were also restricted to between 62 nm and 312 nm, corresponding to a unit cell range of 1 to 5 µm. These constraints guaranteed that the optimized structure could be reproduced using conventional nanofabrication techniques and would behave as an effective medium (e.g., thickness < ½ λ and unit cell < ½ λ) [115]. The targeted refractive index used to evaluate ZIM performance was $n_{\text{target}} = 0-0j$ within the 15 THz to 20 THz band. Beginning with a population of 75 randomly generated chromosomes, the GA converged on an optimized screen geometry shown in Figure 4.14. The final ZIM design is comprised of a planar

Figure 4.14: Unit cell geometry for a ZIM optimized for the far-IR over the wavelength range from 15 µm to 20 µm. The unit cell measures 2.8 µm on a side.
array of $2.8 \times 2.8 \ \mu m^2$ unit cells sandwiched between a substrate and superstrate that are each $1.08 \ \mu m$ thick. The inverted refractive index and impedance are shown in Figure 4.15. At the optimum frequency of 18.2 THz (16.5 \mu m wavelength), $n_{\text{eff}} = 0.43 - 0.21j$ and $Z_{\text{eff}} = 2.2 + 1.1j$. In Figure 4.15(a) $\Re [n_{\text{eff}}]$ shows a near zero region from low frequencies up to the optimization band. However, $\Im [n_{\text{eff}}]$ is large for lower frequencies, indicating that any energy entering the metamaterial will be quickly attenuated. Further, $\Re [Z_{\text{eff}}]$ is small below the optimization band, which results in a poor impedance match to free space and high reflection. At 18.2 THz, $Z_{\text{eff}}$ does not provide an exact match to the impedance of free space, but it represents a trade-off between minimizing the effective index and maximizing transmission through the metamaterial. Figure 4.16 shows the inverted effective permittivity and permeability of the ZIM design. The inverted permittivity $\varepsilon_{\text{eff}}$ shows a Drude type curve due to the metallic mesh screen geometry [116] with an effective plasma frequency $\omega_p \approx 17.8$ THz, where $\Re [\varepsilon_{\text{eff}}]$ transitions from negative to positive (Figure 4.16(a)). A spike in $\Im [\varepsilon_{\text{eff}}]$ can be observed around 21.5 THz and corresponds to a strong absorption band in the polyimide layers. The effective permeability $\mu_{\text{eff}}$ varies slowly around 1+0j and does not show any strong magnetic resonance.
Figure 4.15: Inverted (a) $n_{\text{eff}}$ and (b) $Z_{\text{eff}}$ for the far-IR ZIM design shown in Figure 4.14.
Figure 4.16: Inverted (a) $\varepsilon_{\text{eff}}$ and (b) $\mu_{\text{eff}}$ for the far-IR ZIM design shown in Figure 4.14.
The ZIM was fabricated by first spin-casting a 1.08 \( \mu m \) thick layer of polyimide onto a sacrificial silicon wafer. A 5 \( \times \) 5 mm\(^2\) array of metallic screen elements was then defined by lift-off of a 75 nm thick silver film patterned by electron-beam lithography.

Figure 4.17: Photograph of a fabricated ZIM sample removed from the silicon support wafer and glued to an aluminium slide for characterization.

Figure 4.18: SEM image of an array of the ZIM pattern. Scale bar, 3 \( \mu m \).
Finally, a second 1.08 µm thick layer of polyimide was cast on top of the screen elements to complete the device. The entire ZIM sample was removed from the sacrificial silicon wafer and mounted as a freestanding device onto a test frame for optical characterization (see Figure 4.17). High-magnification field emission scanning electron microscope (FE-SEM) images of one unit cell (Figure 4.18) show that the screen geometry was accurately reproduced during ZIM fabrication, underscoring the importance of incorporating fabrication constraints in the GA optimization procedure.

Figure 4.19: Transmission (red) and reflection (blue) intensity measured using FTIR spectroscopy and compared with simulation. Adding an additional loss parameter of $\alpha_{Ag} = 4$ into the silver permittivity model and adjusting the screen geometry slightly to match the SEM images of the fabricated sample brings the simulation into very close agreement with the measured intensities.
Figure 4.20: (a) Experimental and simulated transmission ellipsometry $\Delta$ ($p$-$s$ phase difference) at normal incidence as well as 30° and 50° oblique incidence. (b) Experimental and simulated transmission ellipsometry $\Psi$ (arc tangent of the ratio of $p$ and $s$ amplitudes). The simulated data includes the additional metallic loss with $\alpha_{Ag}=4$ and follows the ellipsometry data extremely well for normal incidence as well as 30° and 50° oblique incidence.
To verify the refractive index experimentally, the amplitude and relative phase of the scattering coefficients were measured using Fourier-transform (FTIR) spectroscopy and transmission ellipsometry and compared with simulation. The amplitude measurements (Figure 4.19) indicate where cutoff frequencies occur and quantify loss in the metallodielectric structure, whereas relative phase measurements taken by transmission ellipsometry (Figure 4.20) demonstrate that the simulated phase values, necessary for calculating $n_{\text{eff}}$ and $Z_{\text{eff}}$, are reasonable. The original full-wave electromagnetic modeling of the metamaterial follows the same trend as the transmission and reflection intensity measurements, but the measurement exhibited higher reflection and lower transmission than the simulation (see Figure 4.19). In order to more closely model the experiment, a 32 × 32 pixel screen geometry was refined to match the SEM image in Figure 4.18 (inset) and a loss factor $\alpha_{\text{Ag}}$ was added to the bulk metallic model. Simulating the ZIM design with the adjusted geometry and a loss factor $\alpha_{\text{Ag}} = 4$ results in excellent correspondence with the measured scattering amplitudes (Figure 4.19). Transmission ellipsometry was performed at normal incidence as well as at 30° and 50° oblique incidence angles. Figure 4.20(a) shows the difference in phase between the $p$ and $s$ polarizations $\Delta$, while Figure 4.20(b) shows the arctangent of the $p/s$ ratio $\Psi$. At normal incidence, there is little phase or amplitude difference between the two polarizations because the metamaterial geometry is symmetric. However, for oblique incidence there is a significant phase shift and amplitude variation between the $p$ and $s$ polarizations. Simulating the ellipsometry experiment with the adjusted geometry and $\alpha_{\text{Ag}} = 4$ shows that the model accurately predicts the relative phases and amplitudes between polarizations. The correlation between measured and modelled scattering data provides
verification of the full-wave simulation accuracy and, hence, the metamaterial properties $n_{\text{eff}}$ and $Z_{\text{eff}}$.

Finally, with strong agreement found between the simulated and experimental scattering data, it is also important to study the effect of the refined geometry and additional metal loss on the inverted metamaterial effective properties. Figure 4.21(a) shows the simulated refractive index for the original design compared with the adjusted design with $\alpha_{\text{Ag}} = 4$. The frequency of the low/zero index band is shifted by about 1 THz and absorption loss ($\Imag[n_{\text{eff}}]$) is 0.18 larger. At 19.2 THz, the adjusted $n_{\text{eff}}$ is approximately 0.41-0.39j, and the normalized effective impedance $Z_{\text{eff}}$ is 1.6+1.5j (Figure 4.21(b)). The increased loss in the adjusted constitutive parameters is due primarily to the additional loss factor introduced into the Ag material model. While the material losses cannot be avoided, optimizations including a metallic loss factor will be able to find an optimum trade-off between the target refractive index and losses due to impedance mismatching and absorption. Generalizing the approach to multilayer structures (i.e., two or more FSS screens) is also expected to provide more design flexibility for achieving a better impedance match to free space. Chapter 5 investigates the exploitation of magnetic resonances due to multiple metal FSS screens to achieve better impedance matches to free space and to achieve optimal designs for planar negative index metamaterials (NIMs) with simultaneously low absorption and reflection losses.
Figure 4.21: Inverted (a) refractive index and (b) effective impedance from simulation comparing the original design with an adjusted design matching the geometry and adding an $\alpha_{Ag}=4$ metallic loss parameter. The adjusted simulation shows an increase in absorption loss indicated by a larger $\Im[n_{eff}]$. The optimum point has also shifted higher in frequency.
Chapter 5

Multi-Layer Metallodielectric Metamaterials

In this chapter, the synthesis of zero index metamaterials (ZIMs) and negative index metamaterials (NIMs) using frequency selective surfaces (FSS) with multiple metallic screens is discussed. In order to design multi-layer FSS metamaterials, a genetic algorithm (GA) is employed to optimize the metallic FSS screen geometry and dielectric layers in order to achieve the desired refractive index and impedance values. Section 5.1 discusses the synthesis of ZIMs for the mid-IR using cascaded FSS with two or four metallic screens. The synthesis of multi-layer NIMs is presented in Section 5.2 along with a study on increasing the number of layers in an optimized metamaterial. Section 5.3 covers preliminary efforts on fabricating multi-layer metallodielectric metamaterials.

5.1 Multi-Layer Mid-Infrared Zero-Index Metamaterials

The ZIM structure considered in this section is a freestanding device consisting of cascaded metallic FSS screens sandwiching layers of dielectric. The thicknesses of the dielectric layers separating metallic screens can vary within the structure but are constrained to be symmetric about the center slab. It is expected that the metallic screens will load the metamaterial with a negative permittivity due to the characteristic Drude-type behavior of metals. Neighboring metallic screens will also form parallel plate magnetic resonators, resulting in Lorentz-type resonances in the effective permeability.
Compared with the ZIM synthesis approach presented in Chapter 4, the multi-layer FSS ZIMs considered here have additional control over the metamaterial permeability. Thus, the metamaterial structure can be optimized for all three cases considered in Table 2.1. Section 5.1.1 considers a ZIM example optimized for the first case, where $\varepsilon$ approaches zero. This results in a value for large effective impedance. Section 5.1.2 presents two ZIM optimizations for the second case in Table 2.1, where $\mu$ approaches zero faster than $\varepsilon$, resulting in a small $Z$. Section 5.1.3 considers the final case of a ZIM with matched impedance to free space. Several examples are presented, and a comparison is made with the single FSS screen ZIM approach discussed in Chapter 4.

5.1.1 ZIM Example with $\varepsilon$ Approaching Zero

The first ZIM impedance condition show in Table 2.1 is arrived at then the zero refractive index is achieved by the permittivity of the metamaterial approaching zero. In this case, the impedance, which is proportional to the inverse of the square root of the permittivity, becomes very large, approaching infinity under ideal conditions. Furthermore, the reflection coefficient from such a ZIM half-space would be $\Gamma = +1$, where the reflected wave is in phase with the incident wave. This type of boundary condition is consistent with a perfect magnetic conductor (PMC), or artificial magnetic conductor (AMC), and could be useful for applications such as a perfect mirror or low-profile antenna systems.

A FSS with two 75 nm Au screens separated by a glass ($\text{SiO}_2$) dielectric layer is chosen as the metamaterial structure for realizing a ZIM. The design flexibility afforded
by this structure is exploited by optimizing the screen geometry, unit cell size, and SiO$_2$ thickness parameters via a genetic algorithm (GA) [21]. Fabrication constraints, including a minimum pixel size and prohibiting diagonal connections in the geometry are enforced throughout the optimization. Single non-connected pixels are also eliminated from the geometry. Each metamaterial geometry is simulated in a full-wave periodic finite element boundary integral (PFEBI) code to calculate the scattering coefficients. Measured material properties for Au metal [82] and SiO$_2$ dielectric (see the Appendix) are incorporated into the model to ensure good correspondence with experimental data. The surface impedance model used to represent the metal is given by Eq. 2.20. The Nicolson, Ross, and Weir (NRW) inversion algorithm [22,83] is applied to the scattering coefficients in order to obtain the effective parameters $n$ and $Z$ or $\varepsilon$ and $\mu$ of the metamaterial. The ambiguity for the real part of $n$ is resolved by sweeping from a low frequency, where we expect the inverted permeability $\mu$ to approach 1-0j. The fitness function used to evaluate the performance of each member is given by

$$Fitness = \text{MIN}_{freqs} \left[ |n - n_{\text{target}}|^2 + |\varepsilon - \varepsilon_{\text{target}}|^2 \right]$$  \hspace{1cm} (5.1)$$

where $n_{\text{target}} = 0+0j$ and $\varepsilon_{\text{target}} = 0+0j$ are the desired refractive index and permittivity and $freqs$ is a range of target frequencies over which the GA will search for the best performance.

A design example was optimized for a range of target frequencies from 86 THz to 100 THz, around 3 $\mu$m in wavelength in the mid-IR. The unit cell size was allowed to vary from 0.8 $\mu$m to 1.8 $\mu$m, providing a minimum pixel size of 73 nm. The SiO$_2$ dielectric layer varied from 300 to 600 nm in the optimization. Optimizing a population of 32 over 500 generations, the GA converged to the screen geometry shown in
Figure 5.1. The optimized unit cell dimension is 1.8 µm, and the thickness of the device is 452 nm. The inverted refractive index and normalized impedance for this design are shown in Figure 5.2. The optimum frequency for this design was chosen by the GA to be 99.5 THz (3.02 µm wavelength), where the effective refractive index is \( n = 0.13 - 0.12j \) and the effective impedance is \( Z = 3.29 + 3.17j \). We find that the real and imaginary parts of \( n \) are approaching zero, whereas the impedance is several times the impedance of free space, as one would expect when the ZIM condition is achieved by \( \varepsilon \) approaching zero. The inverted permittivity and permeability are shown in Figure 5.3. The permittivity exhibits Drude behavior with a plasma frequency at the optimum wavelength, and the permeability does not show any magnetic resonances near the optimized band. The scattering parameters calculated by the PFEBI code for a normally incident wave are shown in Figure 5.4. The transmission magnitude for this design is still quite high at -0.77 dB because the metamaterial thickness is thin with respect to the wavelength.

Figure 5.1: Optimized ZIM two metallic screens for high impedance. (left) Unit cell geometry and (right) cross-section view of structure.
Figure 5.2: Inverted (a) $n$ and (b) $Z$ for the ZIM design shown in Figure 5.1.
Figure 5.3: Inverted (a) $\varepsilon$ and (b) $\mu$ for the ZIM design shown in Figure 5.1.
Figure 5.4: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 5.1 for a TE polarized wave at normal incidence calculated using a PFEBI code.
5.1.2 ZIM Examples with $\mu$ Approaching Zero

The second ZIM impedance condition shown in Table 2.1 is achieved when the ZIM condition is due primarily to the permeability approaching zero. Because $\mu$ approaches zero faster than $\varepsilon$ in this case, the metamaterial impedance should become small. A wave impinging on an ideal ZIM half space with an impedance approaching zero will have a reflection coefficient equal to -1. Thus, this type of ZIM is useful for application in a perfect mirror.

The first design example consists of two Au FSS screens separated by SiO$_2$ dielectric as in the previous section. The fitness function used by the GA is modified from the previous case in order to optimize for a small $\mu$ at the ZIM band and is given by

$$Fitness = \min_{f \in \text{freqs}} \left[ |n - n_{\text{target}}|^2 + |\mu - \mu_{\text{target}}|^2 \right]$$ (5.2)

where $n_{\text{target}} = 0+0j$ and $\mu_{\text{target}} = 0+0j$ are the desired refractive index and permeability and $\text{freqs}$ is a range of target frequencies over which the GA will search for the best performance. A design was optimized for a range of target frequencies from 86 THz to 100 THz, around 3 $\mu$m in
wavelength in the mid-IR. The unit cell size was allowed to vary from 0.8 µm to 1.8 µm, providing a minimum pixel size of 73 nm. The SiO$_2$ dielectric layer varied from 300 to 600 nm in the optimization. Optimizing a population of 32 over 500 generations, the GA converged to the screen geometry shown in Figure 5.5. The optimized unit cell dimension is 1.8 µm, and the thickness of the device is 545 nm. The inverted refractive index and normalized impedance for this design are shown in Figure 5.6. The optimum frequency for this design was chosen by the GA to be 94 THz (3.19 µm wavelength), where the effective refractive index is $n = 0.029 - 0.18j$ and the effective impedance is $Z = 0.55 + 0.062j$. We find that the real and imaginary parts of $n$ are approaching zero at the optimum frequency. However, the real part of $Z$ is only half the value of free space.

Examining the effective permittivity and permeability shown in Figure 5.7 reveals that while the GA met the goal of minimizing $\mu$, the lack of constraint on $\varepsilon$ allowed the permittivity to also approach zero. The scattering parameters calculated by the PFEBI code for a normally incident wave are shown in Figure 5.8. The scattering coefficients reveal that the metamaterial has low reflection due to the permittivity also approaching zero at the ZIM band.
Figure 5.6: Inverted (a) $n$ and (b) $Z$ for the ZIM design shown in Figure 5.5.
Figure 5.7: Inverted (a) $\varepsilon$ and (b) $\mu$ for the ZIM design shown in Figure 5.5.
Figure 5.8: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 5.5 for a TE polarized wave at normal incidence calculated using a PFEBI code.
A second design example was synthesized in order to further constrain the permittivity. The fitness function for this optimization was modified to optimize $n$ and $Z$ directly and is given by

$$
Fitness = \min_{f_{\text{freqs}}} \left| n - n_{\text{target}} \right|^2 + \left| Z - Z_{\text{target}} \right|^2
$$

(5.3)

where $n_{\text{target}} = 0+0j$ and $Z_{\text{target}} = 0+0j$ are the desired refractive index and effective impedance and $f_{\text{freqs}}$ is a range of target frequencies over which the GA will search for the best performance. By minimizing $Z$, the permittivity is also constrained to not approach zero. The optimization parameters were the same as for the previous design, except the population size and number of generations were changed to 16 and 300, respectively. The optimized structure is shown in Figure 5.9 and possesses a unit cell dimension of 1.33 $\mu$m and a thickness of 600 nm. The inverted refractive index and normalized impedance for this design are shown in Figure 5.10. The optimum frequency for this design was chosen by the GA to be 100 THz (3 $\mu$m in wavelength), where the effective refractive index is $n = 0.11 - 0.75j$ and the effective impedance is $Z = 0.12 +
0.67j. For this design example, the real parts of $n$ and $Z$ are both approaching zero. However, the larger imaginary parts indicate higher absorption losses. Examining the effective permittivity and permeability shown in Figure 5.11 reveals that the permeability is significantly smaller than the permittivity for this design. The scattering parameters calculated by the PFEBI code for a normally incident wave are shown in Figure 5.12 with the $|R| = -3.6$ dB indicating a poorer impedance match to free space at the optimum frequency.

Figure 5.10: Inverted (a) $n$ and (b) $Z$ for the ZIM design shown in Figure 5.9.
Figure 5.11: Inverted (a) $\varepsilon$ and (b) $\mu$ for the ZIM design shown in Figure 5.9.
Figure 5.12: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 5.9 for a TE polarized wave at normal incidence calculated using a PFEBI code.
5.1.3 ZIM Examples with Matched Impedance

The final ZIM case described in Table 2.1 is a matched impedance condition, where $\varepsilon$ and $\mu$ approach zero together such that the $Z$ approaches the impedance of free space. A matched ZIM is an important component in transmissive applications such as electromagnetic cloaking [33,34] and a directive radiator [28,29]. In order to realize a matched ZIM, the fitness function given by Eq. 5.3 is used with $n_{\text{target}} = 0+0j$ and $Z_{\text{target}} = 1+0j$. The metamaterial structures optimized in this section consist of multiple Ag FSS screens separated by layers of polyimide. An additional constraint was added to the GA requiring all metallic patches to be interconnected across the screen. This requirement ensures that the resulting design can be a self-supporting free-standing device. Examples with two and four screens will be presented.

![Optimized matched ZIM with two metallic screens](image)

Figure 5.13: Optimized matched ZIM with two metallic screens. (left) Unit cell geometry and (right) cross-section view of structure.

The first example with two Ag screens was optimized for a target frequency range from 85 THz to 90 THz. The unit cell size was permitted to vary from 0.8 $\mu$m to 2.0 $\mu$m, and the thickness of the structure ranged from 150 nm to 500 nm. The Ag screen thickness was also included in the GA as an optimization parameter and could vary from 50 nm to 70 nm. The GA optimized a population of 32 for 600 generations and
converged on the design shown in Figure 5.13. The unit cell dimension for this design is 1.76 µm, and the thickness is 500 nm. The optimized thickness of the Ag screen is 70 nm. The best frequency chosen by the GA is 89.5 THz (3.35 µm), where $n = -0.068 - 0.13j$ and $Z = 0.96 - 0.036j$, indicating a very low index and good impedance match have been found. Plots of $n$ and $Z$ are shown in Figure 5.14. The inverted $\varepsilon$ and $\mu$ are shown in Figure 5.15. At 89.5 THz, $\varepsilon = -0.066 - 0.14j$ and $\mu = -0.070 - 0.12j$ are both matched and close to zero. As expected, the scattering coefficients shown in Figure 5.16 reveal a null in the reflection coefficient and a high transmission coefficient of -1.04 dB.

![Figure 5.14: Inverted (a) $n$ and (b) $Z$ for the ZIM design shown in Figure 5.13.](image)
Figure 5.15: Inverted (a) $\varepsilon$ and (b) $\mu$ for the ZIM design shown in Figure 5.13.
Figure 5.16: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 5.13 for a TE polarized wave at normal incidence calculated using a PFEBI code.
The second impedance matched ZIM example consists of four Ag screens separated by polyimide layers. The thicknesses of the polyimide layers were allowed to vary from 150 nm to 500 nm in the optimization, but the top and bottom layers were restricted to have the same dimension so that the entire structure would be symmetric in the vertical direction. The other optimization parameters were identical to those in the previous example. The optimized geometry is shown in Figure 5.17 with a unit cell dimension of 2.0 µm and a Ag screen thickness of 70 nm. The thicknesses of the center and outer polyimide layers were 0.24 µm and 0.46 µm, respectively, for a total thickness of 1.16 µm. The refractive index and impedance curves are shown in Figure 5.18. At the optimum frequency of 88.5 THz (3.39 µm), \( n = 0.040 - 0.066j \) and \( Z = 1.03 - 0.012j \), indicating a near-zero index and excellent impedance match. The inverted \( \varepsilon \) and \( \mu \) shown in Figure 5.19 also are near zero at the optimal frequency. The scattering coefficients shown in Figure 5.20 exhibit a null in the reflection coefficient, highlighting the excellent impedance match of this four layer ZIM design.
Figure 5.18: Inverted (a) $n$ and (b) $Z$ for the ZIM design shown in Figure 5.17.
Figure 5.19: Inverted (a) $\varepsilon$ and (b) $\mu$ for the ZIM design shown in Figure 5.17
In order to evaluate the performance of matched ZIMs, two figures of merit are introduced. The first figure of merit $FOM_n$ evaluates how near zero the real and imaginary parts of the index are and is given by

![Figure 5.20: Scattering (a) amplitudes and (b) phases for the ZIM design shown in Figure 5.17 for a TE polarized wave at normal incidence calculated using a PFEBI code.](image)
where $n$ is the effective impedance of the metamaterial. The second figure of merit $FOM_Z$ evaluates how close the impedance of the metamaterial is matched to free space and is given by

$$FOM_Z = \frac{1}{|Z - 1|}$$  \hspace{1cm} (5.5) 

where $Z$ is the effective impedance normalized to free space. The figures of merit are calculated for the single FSS design example shown in Figure 4.10 as well as the example with two and four FSS screens presented in this section and are tabulated in Table 5.1. While all three examples could achieve a near zero $n$, the multi-layer designs were able to achieve a superior impedance match to free space due to the added control over the permeability. It is interesting to note that the example with four FSS screens is twice as thick as the design with two FSS, but the transmission does not drop much because the entire metamaterial stack was optimized to minimize absorption and reflection loss.

Table 5.1: Performance comparison between mid-IR ZIMs with one, two, and four FSS screens described in Figure 4.10, Figure 5.13, and Figure 5.17.

| Number of Screens | $FOM_n$ | $FOM_Z$ | $|T|$  |
|-------------------|--------|--------|-------|
| 1 FSS             | 3.58   | 0.27   | -1.11 dB |
| 2 FSS             | 6.90   | 18.08  | -1.04 dB |
| 4 FSS             | 12.95  | 36.06  | -1.23 dB |
5.2 Multi-Layer Mid-Infrared Negative-Index Metamaterials

The NIM structures considered in this section are freestanding devices consisting of stacked metallic FSS screens separated by layers of dielectric. The dielectric layer thicknesses are permitted to vary within the structure but are constrained to be symmetric about the center slab. It is expected that the metal elements will produce Drude or Lorentz shaped resonances in the metamaterial effective permittivity due to the characteristic Drude-type behavior of metals, and the neighboring metallic screens produce Lorentz-shaped resonances in the effective permeability. The desired properties for the NIMs presented here are a refractive index of -1 and an impedance matched to free space. Section 5.2.1 presents several multi-screen FSS NIM designs optimized by a GA for low absorption and impedance mismatch losses. Section 5.2.2 examines the bulk properties (i.e., approaching those of an infinite stack) of the metamaterial by adding a FSS screen to the designs presented in Section 5.2.1. This analysis demonstrates that it is more effective to optimize a metamaterial stack with many layers in order to achieve a practical low-loss NIM. Optimizing a large stack also results in a metamaterial with properties approaching those of a bulk material. Finally, Section 5.2.3 considers a design optimized for fabrication and discusses experimental progress.

5.2.1 NIM Examples with Matched Impedance

The planar NIM proposed here consists of two cascaded FSS screens sandwiched between uniform layers of dielectric. Polyimide is chosen for the dielectric layers because it is robust and flexible and has very low loss in the mid-IR from 2 µm to 5 µm.
The FSS screens are 75 nm thick films of Ag metal patterned by electron beam (e-beam) lithography. A GA is used to optimize the metamaterial structure for low loss and a negative effective refractive index. The metamaterial design parameters, including the FSS screen geometry, unit cell dimension, and dielectric layer thicknesses are encoded into a binary string, or chromosome, and an initial population is generated with random chromosome values. The FSS screen geometry is pixellized into a 10 by 10 unit cell and divided into eight mirrored triangular folds, one of which is encoded into the chromosome. Fabrication constraints are also incorporated into the GA prohibiting diagonally connected metallic pixels. A minimum pixel dimension of 100 nm is set corresponding to the limitations of e-beam lithography.

The fitness of each design is evaluated against specified target metamaterial effective properties as specified in Eq. 5.3. This fitness function seeks to achieve both a negative refractive index and low loss as quantified by the two figures of merit for $n$ and $Z$. FOM$_n$ is given by

$$FOM_n = \left| \frac{n'}{n''} \right|$$

(5.6)

where $n$ is the effective refractive index of the metamaterial. FOM$_n$ is the ratio of the real part of the index to the imaginary part and provides a measure of the absorption loss in the metamaterial. FOM$_Z$, given in Eq. 5.5, describes the impedance match of the metamaterial to the free space and is often neglected in the NIM literature. By optimizing for large values of FOM$_n$ and FOM$_Z$, a NIM design can be achieved with the smallest possible absorption and reflection.
The scattering parameters of the cascaded FSS structure are predicted using a full-wave periodic finite element boundary integral (PFEBI) code [81]. Dispersive material parameters including the measured dielectric constant for polyimide and a published metallic loss model for Ag at optical and IR wavelengths [82] are incorporated into the PFEBI analysis code. For the first example the Ag screen surface impedance are calculated using Eq. 2.15, while Eq. 2.20 is used for the later two examples.

Figure 5.21: (left) FSS screen geometry optimized by a GA for low loss and a negative refractive index. (right) Cross-section view of a two-layer cascaded FSS NIM.

The design goals provided to the GA were a negative refractive index with minimum absorption ($n_{\text{target}} = -1+0j$) and an impedance match to free space ($Z_{\text{target}} = 1+0j$). A range of target frequencies from 90 THz to 110 THz around 3 µm was also specified to the GA. The GA optimized a population of 16 members over 100 generations to arrive at the design shown in Figure 5.21. The unit cell geometry in Figure 5.21 is shared by both FSS screens and measures 1.46 µm on a side. The polyimide layer between the FSS screens is 226 nm thick, and the polyimide superstrate and substrate are both 113 nm thick. As seen in Figure 5.21 the FSS screen geometry has
eight-fold symmetry, so that at normal incidence the two orthogonal polarizations will have the same scattering response.

![Graph showing refractive index and effective impedance](image)

Figure 5.22: Inverted (a) $n$ and (b) $Z$ for the NIM design shown in Figure 5.21.
Figure 5.23: Inverted (a) $\varepsilon$ and (b) $\mu$ for the NIM design shown in Figure 5.21.
Figure 5.24: Scattering (a) amplitudes and (b) phases for the NIM design shown in Figure 5.21 for a TE polarized wave at normal incidence calculated using a PFEBI code.
The inverted metamaterial \( n \) and \( Z \) are shown in Figure 5.22, revealing a negative index band around 3 \( \mu \)m. The optimum frequency chosen by the GA is 99 THz, where the predicted effective properties \( n = -0.97-0.28j \) and \( Z = 1.15+0.21j \) show a negative refractive index with low absorption loss and a good match to free space. The figures of merit at 99 THz for this design are calculated to be \( \text{FOM}_n = 3.5 \) and \( \text{FOM}_Z = 3.9 \). The effective constitutive parameters \( \varepsilon \) and \( \mu \) shown in Figure 5.23 reveal that at the negative index band around 3 \( \mu \)m the metamaterial also has a simultaneously negative permittivity and permeability. The scattering parameters for this design are shown in Figure 5.24. At the optimum frequency of 99 THz, there is a low return loss of -16.3 dB and a transmission loss of only -2.34 dB.

![Figure 5.25: NIM geometry consisting of two FSS screens separated by polyimide and perforated by air holes. (left) Top and side views of the unit cell, which is periodic in two dimensions. (right) 3D isometric view of the metamaterial.](image)

The metamaterial structure proposed for the second NIM example consists of stacked Ag metallic screens sandwiching layers of polyimide dielectric. The metal-dielectric stack is perforated by air holes in a periodic pattern defined by a unit cell such as the one shown in Figure 5.25. The design parameters that need to be optimized to
achieve a desired \(n\) and \(Z\) include the unit cell dimension, the thicknesses of the polyimide layers, and the pixilated geometry differentiating between Ag/polyimide pixels and air holes. In addition to the fabrication constraints used previously, the pixels representing Ag/polyimide were required to be fully connected across the screen. Any islands of pixels that were not connected to the rest of the screen were eliminated in the GA fitness function. This additional constraint ensures that the final design with air holes can be a free-standing device. The distance between Ag screens was permitted to vary between 150 nm and 300 nm, and the unit cell dimension ranged between 0.8 \(\mu\)m and 2.0 \(\mu\)m. The GA searched for an optimum NIM band from 2.85 \(\mu\)m to 3.15 \(\mu\)m in wavelength. A population of 32 members was evolved over 100 generations converging to the design shown in Figure 5.25. The inverted effective \(n\) and \(Z\) for the design are shown in Figure 5.26. The index approaches -1 at \(\lambda = 2.93\ \mu\)m wavelength, where \(n = -1.04 - 0.21j\) and \(Z = 1.01 + 0.03j\). The figures of merit at \(\lambda = 2.93\ \mu\)m for this design are calculated to be \(\text{FOM}_n = 5.0\) and \(\text{FOM}_Z = 31.6\). The effective permittivity and permeability shown in Figure 5.27 both approach -1 at the optimum wavelength. The scattering parameter magnitudes at \(\lambda = 2.93\ \mu\)m are transmission \(|T| = -1.1\ \text{dB}\), reflection \(|R| = -34.7\ \text{dB}\), and absorption \(|A| = -6.7\ \text{dB}\) as can be seen in Figure 5.28. The reflection null is indicative of an excellent impedance match to free space, and the absorption loss is minimized along with \(n''\). It is interesting to note that this metamaterial possesses a broad band with high transmission and matched impedance extending from the optimum NIM band to higher frequencies where \(n\) passes through zero and becomes positive. This behavior indicates that this design or similar structures could be exploited for low loss negative- zero- positive- index metamaterial (NIM-ZIM-PIM) applications.
Figure 5.26: Inverted (a) $n$ and (b) $Z$ for the NIM design shown in Figure 5.25.
Figure 5.27: Inverted (a) $\varepsilon$ and (b) $\mu$ for the NIM design shown in Figure 5.25.
Figure 5.28: Scattering (a) amplitudes and (b) phases for the NIM design shown in Figure 5.25 for a TE polarized wave at normal incidence calculated using a PFEBI code.
The third design example contains five Ag screens sandwiching four layers of polyimide. For this optimization, the distance between Ag layers could vary between 130 nm and 500 nm, and the unit cell dimension ranged between 0.8 µm and 2.0 µm. After 220 generations, the GA converged on the design shown in Figure 5.29. The effective $n$ and $Z$ are shown plotted in Figure 5.30. At $\lambda = 2.86$ µm the optimum effective parameters are $n = -0.99 - 0.13i$ and $Z = 1.01 + 0.08i$. At this wavelength FOM$_n$ = 7.6, which is higher than the figure of merit for the design containing only two Ag screens, meaning that this design will have lower absorption per unit thickness. On the other hand, FOM$_Z$ = 12.4 is lower than the first design, resulting in a higher reflection. The inverted $\varepsilon$ and $\mu$ plotted in Figure 5.31 are both very close to -1 at the optimum wavelength. The scattering parameter magnitudes at the optimum wavelength $\lambda = 2.86$ µm are transmission $|T| = -1.3$ dB, reflection $|R| = -23.6$ dB, and absorption $|A| = -5.9$ dB as can be seen in Figure 5.32. Despite the better FOM$_n$ for this design, the transmission is slightly lower because this
design has approximately double the thickness of the two-screen design, resulting in an increased absorption. Nevertheless, the transmission properties are still remarkably good. The excellent performance of this design indicates that for practical, thicker NIMs at optical wavelengths, the losses can be minimized by optimizing a metamaterial stack in its entirety. Table 5.2 summarizes the performance characteristics of the three NIM designs presented in this section.

![Image](image_url)

Figure 5.30: Inverted (a) \( n \) and (b) \( Z \) for the NIM design shown in Figure 5.29.
Figure 5.31: Inverted (a) $\varepsilon$ and (b) $\mu$ for the NIM design shown in Figure 5.29.
Figure 5.32: Scattering (a) amplitudes and (b) phases for the NIM design shown in Figure 5.29 for a TE polarized wave at normal incidence calculated using a PFEBI code.
Table 5.2: Performance comparison between mid-IR NIMs for designs with two FSS screens without air holes and two and four FSS screens with air holes described in Figure 5.21, Figure 5.25, and Figure 5.29.

|                | FOM$_{in}$ | FOM$_{Z}$ | $|T|$ |
|----------------|------------|-----------|------|
| 2 FSS without Air Holes | 3.5        | 3.9       | -2.34 dB |
| 2 FSS with Air Holes      | 5.0        | 31.6      | -1.1 dB  |
| 5 FSS with Air Holes      | 7.6        | 12.4      | -1.3 dB  |

5.2.2 Effect of Increasing Number of Layers on Metamaterial Properties

Figure 5.33: Metamaterial cross-section when adding a third metallic screen to the NIM design in Figure 5.21.

In order to evaluate how closely the effective parameters for the two designs match the desired bulk metamaterial properties, the effect of adding an Ag screen to each design will be analyzed. Figure 5.33 shows a cross-sectional view of the first design with two FSS screens and no air holes when adding a third metal screen. Overlay plots
showing the effect of adding another FSS screen on $n$ and $Z$ are presented in Figure 5.34. The loading effect from the third FSS screen causes the negative index band to disappear entirely and the impedance to lose its match to free space. At the optimized frequency of 99 THz, the effective properties are now $n = 0.13 - 1.44j$ and $Z = 0.34 + 1.82j$.

Figure 5.34: Overlay plots showing the (a) refractive index and (b) impedance when adding a third metallic screen to the design in Figure 5.21.
Figure 5.35 shows a cross-sectional view of the second design optimized with 2 FSS screens and air holes when adding a third metal screen. Overlay plots showing the effect of the third screen on $n$ and $Z$ are shown in Figure 5.36. While the NIM band for the modified metamaterial is still present, the location of the band has shifted and the loss characteristics have changed significantly. The optimum wavelength where $n' = -1$ has shifted to $\lambda = 2.88 \, \mu m$, where $n = -1.00 + 0.34i$ and $Z = 3.23 - 0.08i$. The scattering magnitudes at this wavelength are $|T| = -7.1 \, dB$, $|R| = -3.6 \, dB$, and $|A| = -4.2 \, dB$. The reduced $FOM_n = 2.94$ as well as the increased metamaterial thickness has contributed to a higher absorption, and the poor impedance match has resulted in a small $FOM_Z = 0.45$ and much higher reflection.
Figure 5.36: Overlay plots showing the (a) refractive index and (b) impedance when adding a third metallic screen to the design in Figure 5.25.
The cross-section view when adding a metal screen to the NIM design with 5 FSS screens and air holes is shown in Figure 5.37. Overlay plots showing the effect of the sixth screen on $n$ and $Z$ can be found in Figure 5.38. As can be seen in the overlay showing the index for the five screen design and the modified design, the NIM band has not changed (moved) significantly and retains its loss characteristics at the optimum wavelength. At $\lambda = 2.85$ the optimum effective parameters for the modified structure are $n = 0.99 - 0.14j$ and $Z = 1.35 + 0.14j$, and the scattering magnitudes at this wavelength are $|T| = -2.0$ dB, $|R| = -11.7$ dB, and $|A| = -5.1$ dB. The slightly lower NIM FOM$_n = 7.07$ and the increased metamaterial size contribute to an increased absorption, and the impedance match is not as good as the original design, resulting in a higher reflection and lower FOM$_Z = 2.7$. However, this design still performs very well with the added Ag screen, indicating that by optimizing for a larger metamaterial stack, the resulting design yields effective properties approaching those of a bulk material.
Figure 5.38: Overlay plots showing the (a) refractive index and (b) impedance when adding a sixth metallic screen to the design in Figure 5.29.
5.2.3 NIM Design for Fabrication

Fabrication and characterization methods are currently being developed to test the low-loss NIM designs presented here. The intended fabrication scheme for the metamaterial stacks begins by depositing alternating layers of Au and polyimide on a sacrificial wafer. A chrome etch mask containing the periodic geometry is then patterned on top of the stack using electron-beam lithography and lift-off. Reactive ion etching will be used to anisotropically etch air holes in the Ag-polyimide stack prior to removing the sample from the wafer and mounting it on a test frame as a free-standing device for characterization. Figure 5.39 shows side and top views of metal-dielectric stacks that are

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Figure 5.39: Scanning electron micrographs of preliminary fabricated metallo-dielectric stacks. (left) Side view showing alternating layers of polyimide and Au with vertically etched sidewalls, scale bar 100 nm. (right) Top view showing a stack with two metal screens and air holes, scale bar 2 µm.
perforated by anisotropically etched air holes. These preliminary samples look promising, but further efforts are required to refine the fabrication processes.

Following the design procedure detailed in Section 5.2.1, a new design with two FSS screens was optimized targeting Au as the screen metal and is shown in Figure 5.40. The optimum frequency for this design is 90.3 THz, where $n = -1.05 - 0.27j$ and $Z = 1.00 + 0.11j$ as shown in Figure 5.41. Because Au has more loss than Ag in the mid-IR, the figures of merit for this design are lower than the 2 FSS screen NIM with air holes presented in Figure 5.25. The optimum values for this design are $FOM_n = 3.89$ and $FOM_Z = 9.10$. The permittivity and permeability shown in Figure 5.42 both possess values near -1 at the optimum wavelength. The scattering parameters in Figure 5.43 reveal lower transmission magnitude of -2.5 dB when compared to the Ag design. The SEM image in Figure 5.44 shows an etched dose array for this design with an accurate reproduction of the synthesized geometry. A large sample for characterization is currently being fabricated.

Figure 5.40: NIM design optimized for fabrication consisting of a Au/polyimide stack with air holes.
Figure 5.41: Inverted (a) $n$ and (b) $Z$ for the NIM design shown in Figure 5.40.
Figure 5.42: Inverted (a) $\varepsilon$ and (b) $\mu$ for the NIM design shown in Figure 5.40.
Figure 5.43: Scattering (a) amplitudes and (b) phases for the NIM design shown in Figure 5.40 for a TE polarized wave at normal incidence calculated using a PFEBI code.
Figure 5.44: SEM image of a fabricated dose array for the NIM design shown in Figure 5.40.
Chapter 6
Conclusions and Ideas for Future Work

6.1 Conclusions

Often when a technology matures researchers can continue to make refinements to improve the state of the art or even reach beyond the original application and adapt the technology to solve new problems. This is also the case with frequency selective surfaces (FSS), which were originally developed as spatial filters for RF electromagnetic waves and often applied as radomes for antennas. Yet, in recent years FSS have also been adapted to a myriad of metamaterial applications, including artificial magnetic conducting (AMC) ground planes, electromagnetic bandgap (EBG) structures, metaferrites, and in this study, negative and zero index metamaterials (NIMs/ZIMs). A concurrent research effort has been to scale down the device dimensions, pushing the target frequency range from the RF to the millimeter wave, infrared (IR), and even optical regimes. This research has taken advantage of micro- and nano-scale fabrication techniques in order to synthesize and fabricate FSS-based devices for the far-IR and mid-IR, defined as 10 µm to 100 µm and 2 µm to 10 µm wavelength ranges, respectively.

Perhaps the simplest application of FSS with micron and nanometer scale features is an IR filter, following the original RF application. This research coupled a genetic algorithm (GA) with a periodic moment method (PMM) code to synthesize multi-band filters comprised of a freestanding FSS with a single metal screen and polyimide
supporting layers for the far-IR and mid-IR. Novel fabrication constraints that adjust the geometry for fabrication during the GA optimization were developed to ensure that accurate fabrication would be possible using contact lithography or electron beam (e-beam) lithography. Furthermore, accurate loss models for component metals and dielectrics in each design are vital to achieving excellent correspondence between synthesis, theory, and experiment. This research included studying various metal loss models for incorporation into the GA and full-wave simulation techniques. Several design examples were presented for the far-IR and one dual stop band example was synthesized, fabricated, and characterized for the mid-IR. In addition to metallodielectric FSS structures, all-dielectric FSS (DFSS) were also studied in this work for narrowband mid-IR filters. The advantage of DFSS is the high Q resonances made possible by low intrinsic losses in available dielectrics in this wavelength range. However, a drawback is the challenge of achieving polarization sensitivity over a broad angular range. A simple intuitive structure comprised of square amorphous silicon (a-Si) blocks on polyimide was studied as a dual band filter for normal incidence. In addition, a design was optimized by GA to have a polarization insensitive stop band for angles up to 10° oblique incidence. Another desirable feature for filters in the RF or IR regimes is reconfigurability or tunability. In the IR, liquid crystals (LC) offer an ideal tuning method because of their low losses and large birefringence. LC was exploited in this research as a FSS superstrate layer in order to realize mid-IR filters with a narrow stop band that can be tuned over several frequency channels. Both fractal and GA synthesis techniques were employed to find metallodielectric FSS designs with a sufficiently narrowband response.
ZIMs are an important building block for several applications that are currently receiving a very high level of popular and research interest including electromagnetic cloaking devices, directive radiators or emitters, perfect mirrors, and a variety of other transformation optics devices. This research investigated the realization of ZIMs for the far-IR and mid-IR by using FSS with a single metal screen or several cascaded metal screens. ZIM designs with a single FSS screen achieved a zero index by driving the effective permittivity to zero. The results presented represented a compromise between achieving a transmissive metamaterial and minimizing the real and imaginary parts of the refractive index through GA optimization. ZIM designs with two or more metal FSS screens were also able to exploit magnetic resonances in the structure to achieve an impedance match to free space. Figures of merit were introduced to evaluate the performance of ZIM designs. The multi-screen FSS ZIMs presented exhibited an increased figure of merit for the refractive index and impedance match (FOM$_n$ and FOM$_Z$).

NIMs have also been a highly pursued research topic in recent years, especially at optical wavelengths, because of their application as a perfect flat lens. This research studied metamaterials composed of multiple, stacked FSS screens in order to realize NIMs in the mid-IR. A negative refractive index arises from a simultaneously negative permittivity and permeability. The negative permittivity in FSS stacks comes from the Drude behavior of metals, while the negative permeability arises from magnetic resonators formed between neighboring metal screens. The flexibility afforded by the stacked FSS structure was exploited by a GA to achieve both a negative index of -1 and a matched impedance to free space. Several NIM examples were presented with optimized
large figures of merit representing low absorption loss and low impedance mismatch losses at the optimum wavelength. It was found that incorporating air holes in the dielectric layers produced higher values of $FOM_n$ and $FOM_Z$. Furthermore, a study in increasing the number of layers in an optimized NIM revealed that when a structure with many layers is optimized, the metamaterial properties will approach those of a bulk material (i.e., the addition of a layer will not change the metamaterial properties significantly). A fabrication process for stacked FSS metamaterials has been in development, and a FSS NIM design containing two Au metal screens sandwiching a polyimide layer was optimized targeting the proposed fabrication scheme.

6.2 Suggestions for Future Work

Work in the immediate future involves completing efforts to fabricate and characterize FSS metamaterials with multiple metallic screens for the mid-infrared. This achievement will enable the refinement of simulation models and fabrication constraints for synthesizing FSS stacks in the infrared with a variety of desired metamaterial properties. Succeeding with two layers will also provide a gateway toward fabricating metallo-dielectric stacks with many layers, such as those proposed in Chapter 5.

Also looking to the future, the concepts discussed in this dissertation can be applied to a variety of metamaterial applications from the RF through the IR/optical regimes by scaling the FSS dimensions and incorporating appropriate fabrication constraints and material properties into the optimization procedure. The synthesis techniques for FSS metamaterial stacks can be exploited in the RF regime to improve the
state of the art in minimizing absorption and impedance losses, where metallic losses are much lower than in the infrared.

The number of screens in FSS metamaterials must be further increased to realize practical devices with volumes on the order of several wavelengths. Also, synthesizing metamaterials with graded refractive index and effective impedance profiles are necessary in many practical device applications.

Finally, the FSS structures considered in this work are actually anisotropic and should be considered as such in the inversion procedure. Work needs to be done to develop anisotropic effective parameter extraction methods to better model FSS-based metamaterials.
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Appendix

Material Models

In this appendix, we introduce dispersive permittivity data for the dielectric films used throughout the course of this research. While some information on the dielectric constant of these materials can be found in the literature or from the vendor, the properties may shift depending on the processing conditions or tools used during fabrication. Thus, we have employed a J. A. Woollam Infrared Variable-Angle Spectroscopic Ellipsometer (IR-VASE) in order to measure the dispersive permittivity of dielectric films deposited using our fabrication techniques. The first polyimide sample was fabricated by spin-coating and curing two layers of HD Microsystem PI2556 resin with respective thicknesses of 0.49 µm and 0.51 µm on an oxidized silicon wafer. The polyimide film was released from the wafer and mounted onto an aluminum frame for IR-VASE characterization. Figure F.1 shows the measured permittivity from 2 µm to 30 µm in wavelength. Similarly, amorphous silicon (a-Si) and glass (SiO₂) films were deposited and characterized using IR-VASE as shown in Figure F.2 and Figure F.3.
Figure F.1: Dispersive permittivity for polyimide measured using IR-VASE.
Figure F.2: Dispersive permittivity for a-Si measured using IR-VASE.
The metal loss models used for Al, Ag, and Au in this work are Lorentz-Drude curves fit to experimental data [82]. The Lorentz-Drude models provide permittivity values at optical and infrared wavelengths, which are used to calculate the surface impedance $Z_s$ of a metal screen in the full-wave periodic moment method (PMM) and periodic finite element-boundary integral (PFEBI) codes employed throughout the dissertation. Figure F.4 compares the permittivity for Al, Ag, and Au from 1 µm to 60 µm in wavelength. Three methods for calculating the surface impedance are described in Section 2.3.3 based on an assumption that the metal slab is much thicker than the skin depth, using the volume equivalence theorem, and derived when calculating the
scattering from a slab. These surface impedance relations are given in Eq. 2.10, Eq. 2.15, and Eq. 2.20, respectively. Curves comparing the calculated surface impedances from a 50 nm metal sheet are plotted for Al, Ag, and Au in Figure F.5, Figure F.6, and Figure F.7, respectively. While these plots show some variation in the calculated surface impedance, the differences become more pronounced as the slab thickness approaches the skin depth of the metal.

Figure F.4: Permittivity for Al, Ag, and Au at mid-IR and far-IR wavelengths calculated from published Lorentz-Drude models.
Figure F.5: Surface impedance curves for a 50 nm Al slab calculated using the three models presented in Section 2.3.3.
Figure F.6: Surface impedance curves for a 50 nm Ag slab calculated using the three models presented in Section 2.3.3.
Figure F.7: Surface impedance curves for a 50 nm Au slab calculated using the three models presented in Section 2.3.3.
VITA

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