Multi-Layer Aperiodic Dielectric Stack Structures for High Performance Electromagnetic Spectral Shaping from mm-Wave to mid-IR Frequencies

by

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Abstract

Multi-layered stacked dielectric devices provide the mechanism of using resonance cavities, based on Fabry-Perot interferometer theory, for spectral shaping for filtering or beam emission purposes. This thesis describes the completion of two projects to demonstrate the capabilities of such structures. The first focused on the design and fabrication of a stacked dielectric structure to achieve a broadband filtering response at millimeter-wave (mm-wave) frequencies. The measured structure consists of a periodic arrangement of different dielectric materials (aperiodic designs demonstrated in simulation) to exhibit a bandpass (BP) response. These structures are designed using a transmission line (t-line) model and confirmed with full-wave simulations. Compared to standard printed circuit board (PCB) fabrication, stacked dielectric structures are expected to exhibit better loss performance, due to absence of metallic patterns, and are easier to fabricate at mm-waves because of the absence of constraints from PCB line-width/gap dimension tolerances. An example structure was designed, fabricated, and measured with a center frequency 57 GHz consisting of three dielectric slabs and two air gaps. ANSYS FEM-HFSS simulations of this structure show well-matched BP performance, insertion loss of less than 1 dB, and a 3-dB bandwidth of 4.5 GHz. Measurement of the fabricated structure shows excellent performance and correlation with simulation. The second project focused on the design, fabrication, and direct thermal testing of a multi-layer aperiodic all-dielectric thermal emitter, with its high quality factor (Q-factor) and emissivity properties being experimentally demonstrated for carbon dioxide gas sensing applications. Using a 7-layer dielectric stack consisting of alternating layers of silicon and silicon dioxide, backed by a metallic ground plane, an emittance of 0.7 and Q-factor of 113 is achieved at 70°C. This is the first time a direct thermal testing of such a structure is reported, thereby showing narrowband emission properties of such structures when heated above room temperatures. An all-dielectric stack is thus found to be a simple, deposition-based, structure that does not require any lateral mask preparation as the frequency selectivity is achieved using an aperiodic arrangement of alternating dielectrics with contrasting permittivities. For both projects, superior performance of the aperiodic stacked dielectric structures over their periodically stacked counterparts is demonstrated using numerical examples.

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List of Acronyms

ALD	atomic layer deposition
BP	bandpass
EM	electromagnetic
FEM	finite element moment
FSS	frequency selective structure
FTIR	Fourier transform infrared spectroscopy
GA	genetic algorithm
HFSS	high frequency structure simulator
HP	high-pass
IL	insertion loss
IR	infrared
LP	low-pass
MC	Monte-Carlo
MTIR	multiple total internal reflection
PCB	printed circuit board
PEC	perfect electric conductor
PECVD	plasma enhanced chemical vapor deposition
PMC	perfect magnetic conductor
SCCM	standard cubic centimeters per minute
SEM	scanning electron microscope
VNA	vector network analyzer

Nomenclature

c	speed of light in air or vacuum, 3×10^8 m/s
ω	angular frequency, rad/s
f	frequency, Hz
λ	wavelength, m
β	phase constant, rad/m
k	wave number, rad/m
ϵ	electric permittivity, F/m
ϵ_0	electric permittivity in free space, 8.854×10^{-12} m/s
ϵ_r	relative electric permittivity
μ_r	relative magnetic permeability
γ	complex propagation constant
α	attenuation constant, Np/m
Γ	reflection coefficient
η	wave impedance, Ω
η_0	wave impedance of air or vacuum, $120\pi \Omega$
$\tan \delta$	loss tangent

Chapter 1

Introduction

1.1 Motivation and Contribution

1.1.1 Motivation

Many types of surfaces have been explored for the manipulation of electromagnetic (EM) waves for various applications. Metasurfaces, in particular, have been designed and used for the control of the phase and polarization of EM waves [1], while frequency selective surfaces are used as spatial filters [2]. Thin film-based metasurfaces can be used as thermal emitters for important applications such as the detection of toxic gasses [3], antibody detection for human health [4], and measuring atmospheric composition changes [5] to name a few. The importance of these applications become evident with the observance of deaths from exposure to toxic gases, the lack of ability to detect dangerous biological markers, and poor air quality due to pollution. Novel solutions can be developed with proper detection using sensors such as what has been described in [3, 4, 5].

Hence, narrowband emission devices based on periodic, or aperiodic, cell-based microstructures using metamaterial concepts have recently emerged as topics of important research. A device emitting a narrow, high quality factor (high-Q), peak in frequency is the goal to use in the applications of the previous paragraph. The majority of emittance device research consists of large number of sub-wavelength resonators (in the planar dimension) tuned to produce an emission at the desired wavelength [6, 7, 8, 9]. There is lot of flexibility in engineering the thermal emission through the unit cell design by using either a periodic or an aperiodic arrangement of these resonators, which can subsequently be used for steered or tailored emission in space for instance. While the measured fabricated devices show that high-Q designs can be obtained using these microstructures, they are complex and typically difficult to implement at mm-wave frequencies due to requirements on implementing small fea-

ture sizes, and are limited by tolerances as seen through variations in deposition rates and a difficulty in implementing minimum-size dimensions. Multi-layer all-dielectric stacked structures show promise in producing the required performance with several advantages over microstructure-based designs to be discussed throughout this thesis [10].

An alternative technique is using a vertical stack of alternating uniform dielectrics of different permittivities. By engineering the permittivity contrast and the thickness of the layers, narrowband thermal emission at the desired frequency can be achieved. Compared to the periodic surface microstructure devices, this technique eliminates several steps in fabrication and has no limitations due to feature dimension tolerances as the various layers are uniform with no micro-patterns. This benefit becomes particularly advantageous at smaller wavelengths, where the microstructure dimensions becomes smaller, more challenging to implement, with tolerances having a greater effect on the resulting performance, for instance a reduced quality factor (Q-factor) [11]. These structures comes at an expense of optimal performance solely along a fixed direction normal to the surface, which is nevertheless useful in several typical applications including gas sensing [12, 13], for instance. The stack can either be longitudinally periodic or aperiodic. Periodic stacked structures are formed by a periodic arrangement of dielectric layers with contrasting permittivities, while aperiodic stacked structures are formed by an aperiodic arrangement, each layer potentially having a different permittivity, loss tangent, and thickness.

In this thesis, an algorithm based on the transmission line (t-line) model method was designed and used to implement a mid infrared (mid-IR) thermal emitter design, which was then thermally tested and validated as being a high-Q candidate for thermal emission devices. To verify the algorithm and design process before proceeding to the thermal emitter, a periodic millimeter wave (mm-wave) frequency selective structure (FSS) was designed, fabricated and tested, thus validating the process to pursue the mid-IR thermal emitter project. Aperiodic structures are shown for both frequency ranges to have superior performance over their periodic counterparts. Further contributions are described in the following section.

1.1.2 Contributions

With the advent of 5G telecommunications, structures are required to provide spatial filtering for the purpose of suppressing unwanted signals to reduce interference with the loss-prone 60 GHz 5G signals. Multi-layer aperiodic all-dielectric BP FSS have been explored in this thesis, which led to the fabrication of a periodic structure, which was measured showing promising performance for use as a spatial filter. Simulation results of an aperiodic structure shows improved performance, where unwanted adjacent passband were suppressed due to the aperiodic nature of the structure. An example real-world application of these structures is the mass-production of ‘smart’

window blinds which can enable rooms that only allow 5G signals to propagate within when the blinds are blocking the windows. Potential enhancements of 5G performance within that room may result. Other applications include using the structure as large radomes for antennas and anti-jamming purposes (such as suppressing multi-path signals).

The work done on the mm-wave BP FSS project demonstrates the capabilities of using numerical methods for the design of this Fabry-Perot resonator-based structure. Expanding this to mid-IR thermal emitter devices was the next step, where a 7-layer multi-layer aperiodic structure was designed, fabricated and thermally tested; the first thermal testing of an aperiodic stack of this nature in literature. These devices enable high-Q narrowband emission beams to be used within a sensing system. A beam is emitted from this stacked dielectric device towards a receiver. A receiver measures the incoming beam. As an example, gas may be contained within a chamber, where the ratio of the power absorbed by the gas is proportional to the amount of gas present within that chamber. A narrower beam means the measurement can be more precise to detect only the element of interest, ignoring all others that are contained within the chamber. Thus high-Q emission characteristic is shown to be important, and this thesis demonstrates a device achieving that characteristic in thermal measurements.

In particular, the work presented in this thesis has led to two contributions to literature [14], [15], one for each of the projects; the mm-wave BP FSS leading to the mid-IR thermal emitter:

1. “Millimeter-wave Bandpass Frequency Selective Structure Using Stacked Dielectric Slabs” has been accepted to the 14th European Conference on Antennas and Propagation (EuCAP) to take place in March 2020.
2. “Direct Thermal Emission Testing of Aperiodic Dielectric Stack for Narrowband Thermal Emission at mid-IR” has been submitted to the Journal of Applied Physics (JAP), which was reviewed with minor revisions necessary for acceptance.

1.2 Theory of Stacked Dielectric Structures

The basic operation of EM waves travelling through a dielectric slab is explained through wave impedance mismatch, transmission and reflection. In particular, a concept known as ‘stepped impedance filters’ from [16] can be applied to implement not only low-pass (LP) filters, as per Pozar’s example, but also BP filters, by combining LP structures with high-pass (HP) equivalents. T-line models of these filters are used to implement stepped-impedance filters, which can be realized using a series of stacked dielectrics. Simulation tools for dielectric stack structures are available, but

Figure 1.1: First-order (a) LP and (b) HP filter schematic diagrams based on LC-resonance.

Figure 1.2: BP filter schematic diagram, combining the circuits from Fig. 1.1.

were not used in this thesis. Examples of these tools include FreeSnell and Lumerical, and are alternatives to what will be discussed here.

The concept of using stepped-impedance filters involves alternating between very high and very low characteristic impedance lines [16]. An LC-resonance based LP filter is modelled according to Fig. 1.1(a), where the cutoff frequency, f_{cLP} , is given by Eq. 1.1. Similarly, LC-resonance based HP filters can be modelled according to Fig. 1.1(b), with the cutoff frequency also given by Eq. 1.1

$$f_{cLP} = f_{cHP} = \frac{1}{2\pi\sqrt{LC}} \quad (1.1)$$

Combining the unit filters from Fig. 1.1 in series, with each filter providing a unique cutoff frequency, a BP response results with roll-off slopes for the lower and upper ends, and a bandwidth determined by the respective cutoff frequencies. Fig. 1.2 shows the circuit of an LC-resonator BP filter, comprised of one LP and one HP filter combined in series, with the 3-dB bandwidth given by Eq. 1.2, and the center frequency given by Eq. 1.3.

$$BW_{3\text{-dB}} = |f_{cHP} - f_{cLP}|, \quad f_{cHP} < f_{cLP} \quad (1.2)$$

Figure 1.3: Stepped-impedance t-line implementation of Fig. 1.2.

$$f_{\text{center}} = \frac{f_{c_{\text{LP}}} + f_{c_{\text{HP}}}}{2} \quad (1.3)$$

Ignoring resistive and conductive components of the distributed t-line model, the BP filter can be modelled as a series of t-lines of varying impedances, Z_n , for $n \in [1, N]$ with N being the number of filters. Each filter is represented by two t-lines of characteristic impedances Z_l and Z_h and each t-line representing a dielectric slab. This is shown in Fig. 1.3. Putting more of these t-lines in series allows for further control of the filter response, due to the addition of more poles, as described in [16], whereby the stepped-impedance BP filter can be designed approximately using the ‘ABCD’ parameters of the t-line based circuit.

A dielectric slab with thickness, l , and wave impedance, η , replaces each t-line from Fig. 1.2. Using numerical methods to allow for added complexity of the structure, the design of a series of dielectric slabs stacked aperiodically, in the sense of varying thickness and wave impedances, can theoretically perform the function of a BP filter, a LP filter, a HP filter, or any spectral response required for a given application. For this thesis, multi-layer aperiodic all-dielectric stacked structures provide the mechanism allowing a BP response to fulfil the two applications as will be discussed in the following Chapters 2 and 3.

The basic principle of operation, discussed earlier in this section, is that interfaces exist at the surfaces of the dielectric slabs, between the dielectrics (or air) surrounding them. These interfaces mean impedance mismatch exists between the wave impedances of the surrounding media which causes some of the wave to be reflected at the interface, some absorbed in the media, as a function of the loss tangent, and the rest transmitted through the interface.

As finite planar structures, these can be described by rectangular resonant cavities [16]. However, to simplify the problem, the structures are assumed to be infinite in the planar dimensions, thus reducing the structure to a series of Fabry-Perot resonators [16]. Standing plane waves can exist within the various cavities that make up the stacked dielectric structure, with the electric field (E-field) given by Eq. 1.4, when constructive interference occurs between the incident wave and the wave reflected from the second interface.

$$E_x = E_0 \sin(k_0 z) \quad (1.4)$$

With E_0 being the amplitude (arbitrary), and k_0 being the wave numbers which satisfy the standing wave conditions that $E_x = 0$ at $z = 0$ and $z = d$, the location, in z , of two interfaces of the resonator. In reality, the electric field at these points will not be zero, because the surfaces of dielectric slabs are not conductive. Thus, the device will behave as a series of Fabry-Perot interferometers [17], with the equations modelling transmission and reflection through each dielectric slab given in [17].

The multiple internal reflections, that may cause standing waves, results in the spectral response illustrated in Fig. 2.2 in Section 2.2 as characterized in [17]. Depending on the frequency of the wave, or thickness of the dielectric slab, constructive or destructive interference between the incident wave and the wave reflected from the second interface results in spectral shaping of the incident wave. The superposition of many dielectric slabs of various wave impedances and thickness allows for the design of a particular spectral response, as will be discussed in the following Chapters 2 and 3.

1.3 Thesis Organization

This thesis has the following structure.

- **Chapter 1** introduces the twin-project approach of this thesis, with the motivation and contributions discussed in depth, along with a general overview of the theory which makes stacked dielectric slab devices an attractive area of research.
- **Chapter 2** describes, in depth, the first project undertaken for the completion of this thesis, dealing with the optimization algorithm, the design and simulation of an aperiodically stacked structure, and the design, fabrication, and measurement of a periodically stacked dielectric slab structure, both for use as FSSs for 5G telecommunications. A background and literature review introduce the chapter, followed by discussion of the algorithm, then the discussion of the mm-wave FSS project, with emphasis on the measurement portion being the validation of the whole design process, allowing progression to the second project. A spatial BP filter operating at the center frequency of around 57 GHz, with a 4.5 GHz 3-dB bandwidth, was fabricated and measured, showing correlation to the corresponding simulation results.
- **Chapter 3** describes, in depth, the second project undertaken for the completion of this thesis, dealing with the algorithm-based design, fabrication, and thermal measurement of a multi-layer aperiodic dielectric stacked structure as a mid-IR thermal emitter. Again, a background and literature review introduce

the chapter, followed by a discussion of the proposed structure, then the details of the fabrication and measurement of the devices. Samples of a 7-layer aperiodic stacked dielectric structure were fabricated, based on IC fabrication methods for deposition of layers, then thermally tested showing a high-Q thermal emission peak at 71.2 THz.

- **Chapter 4** concludes the thesis with remarks summarizing the results of both projects, as well as outlining directions for future work to be undertaken in the highly interesting topic of stacked dielectric devices.

Chapter 2

All-Dielectric Structures

2.1 Overview of Frequency Selective Structures

Frequency selective surfaces are typically based on sub-wavelength resonators which are tuned at the design frequencies to provide either full transmission or reflection. While literature is available on narrowband FSS designs, and FSS at low frequencies, limited work has been done in broadband FSS, with spectral shaping in transmission, at mm-waves. With the upcoming 5G applications, and a greater focus on mm-wave systems, the development of novel high frequency, broadband, surfaces is an attractive direction of research.

To demonstrate a proof-of-concept for stacked dielectric devices, and the eventual design and fabrication of a multi-layer aperiodic device for mid-IR applications, a multi-layer stacked dielectric frequency selective structure (FSS) is presented and its BP response is shown with promising performance for use at mm-wave frequencies. Theoretically, loss performance is improved since the structure does not require metallization. Naturally, it also offers polarization-independent operation. Using t-line theory to model the impedances of the layers, an algorithm was created to obtain the BP design as required, using the genetic algorithm (GA) optimization routine.

2.2 Algorithm for Design of Stacked Dielectric Structures

The transmission and reflection through one dielectric slab, with air on either side as shown in Fig. 2.1, is shown in Fig. 2.2. The response of such a slab is inherently periodic with frequency (i.e. commensurate) due to the theory discussed in Section 1.2, where the thickness of the slab primarily controls its frequencies of maximum trans-

mission and the properties of its corresponding pass-bands. A periodic arrangement of these slab will also retain its commensurate behavior. Such a structure can be used as a spatial BP filter where the number of dielectric layers will control the roll-off behavior of the pass-bands. Moreover, if this periodicity is broken, and a cascade of non-uniformly thick or spaced dielectrics slabs; an aperiodic structure, is formed realizing a non-commensurate structure, great flexibility in tailoring the passband can be achieved. The theory was discussed in more detail in Section 1.2.

Figure 2.1: T-Line model of a single dielectric stack, using η as the EM impedance for the characteristic impedance of the dielectric slab, with η_0 as the impedance of free space on either side of the slab.

Figure 2.2: Spectral response of the t-line model shown in Fig. 2.1.

To minimize computational time for quick design, accelerating the computation of the transmission and reflection response for plane-wave excitation, a model was created based on t-line theory modelling wave propagation through dielectric slabs, as explored in [18, 19]. A similar approach using a transfer matrix (t-matrix) was used in [20]. For multiple stacked dielectric slabs, a load-to-source recursive approach

of calculating the response is taken, and the GA is used to obtain the design needed for a BP response. Fig. 2.3 shows the implementation of the theory for N stacked dielectric slabs. Appendix A shows samples of the algorithm code for reference.

Figure 2.3: An illustration of the t-matrix method by applying the t-line model from Fig 2.1 on N dielectric slabs.

The t-lines have characteristic impedance, Z_0 , being the intrinsic impedance η of the materials: air (η_0) and the dielectric slabs (η_n), where n is the slab number from the air ‘load’. The input impedance is calculated by applying Eq. 2.1, with γ_n being the lossy propagation constant, calculated using Eq. 2.5, t_n being the dielectric thickness, and Z_{L_n} being the load, calculated using Eq. 2.2, of the n th dielectric slab. Z_{L_0} is η_0 , for air, with t_0 being ∞ .

$$Z_{IN_n}(t_n) = Z_0 \frac{Z_{L_n} + Z_0 \tanh(\gamma_n t_n)}{Z_0 + Z_{L_n} \tanh(\gamma_n t_n)} \quad (2.1)$$

$$Z_{L_n} = Z_{IN_{n-1}}(t_{n-1}), \quad n \geq 1 \quad (2.2)$$

The final load impedance for N slabs, Z_{IN_N} , is used to calculate reflection and transmission coefficients, calculated by applying Eqs. 2.3 and 2.4, respectively. The complex (lossy) propagation constant is found by applying Eq. 2.5. Auxiliary equations are explained below.

$$\Gamma = \frac{Z_{IN_N} - \eta_0}{Z_{IN_N} + \eta_0} \quad (2.3)$$

$$T = \frac{2Z_{IN_N}}{Z_{IN_N} + \eta_0} \quad (2.4)$$

The propagation constant is found as follows, with the complex permittivity being

calculated based on the dielectric slab parameters, including loss tangent, using Eq. 2.6. These equations are for the n th dielectric slab.

$$\gamma_n = i\omega\sqrt{\epsilon_n\mu_0} \quad (2.5)$$

$$\epsilon_n = \epsilon_{r_n}\epsilon_0(1 - i\tan\delta_n) \quad (2.6)$$

As all of these parameters depend on frequency, being $\omega(f) = 2\pi f$, these equations are applied for all frequencies in the range $f \in [f_L, f_H]$, with f_L and f_H being the lower and upper frequency limits of the solution range, respectively.

2.2.1 Genetic Algorithm Solution

For a fast design process, a similar method to that in [20] is used in the design and development of the stacked dielectric structures. The GA is used to minimize a residue function by choosing a set of N dielectrics for the stack. These are either chosen from a database of commercially available dielectrics (mm-wave FSS project) or optimized for thicknesses of a particular set of chosen dielectrics (mid-IR thermal emitter project) to obtain a design with a performance resembling a goal scattering response function, such as the BP response, $G(f)$, defined as in Eq. 2.7.

$$G(f) = \begin{cases} 1, & f \in \mathbb{R} \\ 0, & \text{otherwise} \end{cases} \quad (2.7)$$

With $\mathbb{R}$ being the frequency range where transmission is required. All other frequencies, within the solution range $f \in [f_L, f_H]$, will have suppressed transmission. The frequencies, f_L and f_H , are chosen such that they are near $\mathbb{R}$ to emphasize $G(f)$ in the optimization. The residue function, R , is shown in Eq. 2.8 being the sum of the square absolute differences (over frequency) between a goal transmission function, and the transmission of the current iteration, $T(f)$, based on the equations above.

$$R = \sum_f |G(f) - T(f)|^2 \quad (2.8)$$

Here, the optimization variables are the ϵ_r , $\tan\delta$, and thickness t of the various, commercially available, dielectric slabs. The number of layers, N , is constrained prior to optimization. Air gaps are included in the database, which can be implemented in fabrication using nylon washers or rigid foam.

2.3 mm-Wave Frequency Selective Structure at 60 GHz

2.3.1 Background

Many applications exist for mm-wave FSS such as for use as radomes to block signals that may cause interference within the receiver, surfaces for anti-jamming purposes, or smart window blinds that render spaces blocked from certain EM signals. For these applications, large conformal surfaces are needed, with low-loss performance necessary to minimize the signal attenuation, a sensitive parameter for 5G telecommunications, while keeping maximal signal strength in transmission. Using multi-layer stacked dielectric slabs is a solution to be discussed in this section.

The conventional methods of fabricating FSS is using printed circuit boards (PCB) [21, 22, 23, 2, 24, 25, 26] and IC technology [27]. These processes rely on several steps and masks. At higher frequencies, typically beyond 20 GHz, adverse dimension variation due to fabrication tolerances have an effect on electrical (loss) performance of FSS and standard PCB fabrication becomes challenging. All-dielectric structures are alternatives to PCB-based fabrication and, while they have been proposed in literature [19], little work was done to verify and fabricate these structures. Similar work has been done in the infrared (IR) spectrum with multi-layered dielectric thin films [20] to be explored in Chapter 3.

2.3.2 Literature Review

This literature review will highlight various key articles in literature demonstrating the need for novel techniques to improve BP performance for spatial filters, of which stacked dielectric structures is one.

PCB-based BP FSS have been shown at various frequency ranges in literature. Some from low frequency ranges will be discussed, followed by a review of the PCB structures designed for mm-wave frequencies, for which the proposed structure is designed. In [21] metallic patterns, shown in Fig. 2.4(a), based on the Jerusalem cross shape were used to design a BP FSS at 11.75 GHz, with a 3-dB bandwidth of around 2 GHz, similar to the response shown in [25]. The measured insertion loss (IL) ranged from 1.5 dB to 2.7 dB, and the response was stable for oblique angles of wave incidence up to 40°. The work done in [22] shows a BP FSS designed using GA optimized metallic structures to fit a required response. The BP response was centered at 10 GHz, with a 3-dB bandwidth of around 2 GHz, with minimal variation for oblique angles of incidence up to 15° shown in simulation. Another multi-layer metallic topology was used in [23] to design a BP FSS centered at around 3.8 GHz.

Moving to a higher frequency, dual dipole-slot resonators were used to design a BP FSS with high selectivity, meaning no transmission in the bandstop regions, for the Ku-Band at around 18 GHz in [24]. This shows promise when moving to higher frequencies, although feature sizes begin to become challenging for fabrication with the thickness of the substrate used being 0.508 mm. Moving up, a 28 GHz BP FSS with a 3-dB bandwidth of 6 GHz was designed, fabricated and measured in [2], using a 3-layer metallic resonator approach, based on the structure shown in Fig. 2.4(b), as per the lower frequency examples. Angular independence is still maintained, i.e. the response remains stable, for oblique incidence angles up to 40° as shown. A 7-layer approach was taken to design a 62 GHz BP FSS with a 3-dB bandwidth of 4 GHz in [26], which is comparable to the design proposed in this chapter. This one in particular was tested within a rectangular waveguide, and was not tested as a spatial filter.

With higher frequency requirements, feature sizes of the resonators become smaller, and more difficult to implement using standard PCB technology. Photolithographic IC technology becomes an alternative, which allows the implementation of smaller feature sizes. A BP FSS was designed in an IC process for operation at 320 GHz with a wide bandwidth of around 15 GHz in [27], with the structure, illustrated in Fig. 2.4(c), demonstrating polarization-independent operation. Another IC-based structure is proposed using Maltese cross shaped resonators for BP operation at around 550 GHz in [28]. However, IC-based fabrication is not ideal for 5G applications as the feature sizes become large in retrospect, introducing a variety of new problems. In [19] multi-layer stacked dielectric structures are proposed, supported by simulations, showing how narrowband 10 GHz BP FSS can be produced by stacking uniform non-patterned dielectric slabs. Polarization independence, low-loss performance, and realizability are some of the possible advantages for these structures designed at mm-wave frequencies.

(a)

(b)

(c)

Figure 2.4: Example structure designs from the literature review showing (a) the Jerusalem cross structure from [21] (J. H. Choi et al. ©2013 IEEE), (b) the PCB-based structure from [2] (D. Li et al. ©2017 IEEE), and (c) the IC-based Maltese cross structure from [28] (T. Manabe et al. ©2017 IEEE).

Table 2.1: mm-Wave BP FSS project dielectric slab parameters. The material properties were obtained from the data sheets, being observed the frequency f .

Brand	Name	f (GHz)	ϵ_r	$\tan \delta$
Rogers	TMM 10	10	9.2	0.0022
	TMM 10i	10	9.8	0.0020
	TMM 13i	10	12.85	0.0019

2.3.3 Proposed Structure and Simulation

2.3.3.1 Aperiodic Proposition

The algorithm discussed in Section 2.2.1 was used to design a multi-layer aperiodic BP FSS centered at 60 GHz with a 3-dB bandwidth of 2.5 GHz. The stack consisted of four dielectric slabs, and three air gaps, for a total of 7 layers, as shown in Fig. 2.5. The dielectric slab parameters are shown in Table 2.1.

Figure 2.5: 7-layer aperiodic FSS design for center frequency f_c of 60 GHz.

The ANSYS FEM-HFSS model, with simulation setup, is shown in Fig. 2.6. It was used to validate the optimization procedure to ensure it produced a correct result. An exact match with the t-line model result is expected. Fig. 2.7 shows the simulated scattering responses, S_{11} and S_{21} , indicating a well-matched filter response and a near-zero flat transmission response. The phase response and group delay are shown in Fig. 2.8.

Figure 2.6: Full-wave simulation setup in ANSYS FEM-HFSS of the aperiodic FSS design showing the simulation model of the FSS, with boundary conditions shown.

Figure 2.7: Simulated scattering parameters of Fig. 2.6 showing the S_{11} results of the simulation (S_{11H}) and the t-line model (S_{11T}) overlapping.

Figure 2.8: Phase of S_{21} , and group delay, τ_g of the aperiodic structure simulated in Fig. 2.11.

This assortment of dielectric slabs was difficult to obtain from the manufacturer as samples. To accelerate the process of measurement and validate the design propose to progress to the mid-IR thermal emitter project, an alternative approach of using a *periodic* structure was used to design, fabricate and measure the BP FSS performance of multi-layer stacked dielectric structures. A comparison of periodic multi-layer BP FSS, aperiodic multi-layer BP FSS, and a PCB-based BP FSS operating at around 60 GHz center frequency is made in Section 2.3.6.

2.3.3.2 Periodic Proposition

To demonstrate the method, an example design was obtained using 5 layers: three dielectric slabs, and two air gaps. A periodic solution was found as one solution for the prescribed passband centered at around 60 GHz, with a 3-dB bandwidth of 4.5 GHz. As shown previously, the algorithm can produce aperiodic structures as well and multiple solutions for the stacked configuration may exist for a given goal response. Fig. 2.9 illustrates the final design for the periodic structure, with the thickness of each layer shown.

Air
TMM 10i — $t = 3.175$ mm
Air Gap — $t = 1.524$ mm
TMM 10i — $t = 3.175$ mm
Air Gap — $t = 1.524$ mm
TMM 10i — $t = 3.175$ mm
Air

Figure 2.9: 5-layer example FSS design for center frequency f_c of 60 GHz.

Where the dielectric slab parameters are shown in Table 2.1. Fig. 2.10 shows the ANSYS FEM-HFSS (simulation) model that was used to verify the result from the optimization code. Fig. 2.11 shows the simulated scattering responses, S_{11} and S_{21} , indicating a well-matched filter response within the design bandwidth with a near-zero flat transmission response, thereby validating the usage of stacked dielectrics to achieve a spatial BP filtering response with low loss performance. The phase response and group delay are shown in Fig. 2.12.

Figure 2.10: Full-wave simulation setup in ANSYS FEM-HFSS of the *periodic* FSS design showing the simulation model of the FSS, with boundary conditions shown.

Figure 2.11: Simulated scattering parameters of Fig. 2.10 showing the S_{11} results of the simulation (S_{11_H}) and the t-line model (S_{11_T}) overlapping.

Figure 2.12: Phase of S_{21} , and group delay, τ_g of the periodic structure simulated in Fig. 2.11.

Due to the periodic nature of this device, the response is also expected to be periodic. Expanding the spectral sweep to $f \in [40, 80]$ GHz, this periodicity is

demonstrated in Fig. 2.19(a) as opposed to the suppressed periodicity shown in the performance of the aperiodic structure in Fig. 2.19(b). Aperiodicity of the structure can eliminate this periodicity, and can also be thinner than periodic structures, as will be shown in this chapter, as well as in Chapter 3 for the mid-IR thermal emitter project.

2.3.4 Fabrication and Measurement

Square TMM 10i samples, with an area of 225 cm², were obtained for fabrication of the BP structure of Fig. 2.9. Small plastic spacers of 1.524 mm thickness were used on the corners of the slabs to create the air gaps. The FSS structure was assembled mechanically using a multi-purpose Elmer's 'Glue-All' adhesive. The measurement setup is shown in Fig. 2.13, with images of the actual configuration in Fig. 2.14, where a vector network analyzer (VNA) was used to measure transmission through the FSS between two WR-15 standard horn antennas. The response was measured for both normal and oblique angles of incidence by varying the angle of the FSS, as shown in Fig. 2.14. A measurement was taken with the absence of the FSS to de-embed path loss as per Eq. 2.9

$$S_{21_N} = S_{21_{FSS}} - S_{21_{PL}} \quad (2.9)$$

With S_{21_N} being the de-embedded transmission, $S_{21_{FSS}}$ the original FSS-inclusive transmission measurement, and $S_{21_{PL}}$ the transmission measurement without the FSS; the units for all being dB.

Figure 2.13: Diagram showing the mm-wave FSS measurement setup.

The dimensions of the fabricated FSS were measured to account for any errors due

Figure 2.14: Experimental setup for characterizing the stacked dielectric FSS. (a) No FSS, calibration measurement setup, (b) normal incidence setup and (c) oblique incidence setup (angle varies).

to mechanical assembly to re-simulate the structure then compare the measurement results to those simulations. The dielectric thickness was around 3.28 mm (designed 3.175 mm) and the air gap thickness around 1.6 mm (1.524 mm). This variation shifted the response down, in frequency, by around 3 GHz, from the designed 60 GHz to 57 GHz. The normal incidence transmission measurement is shown, compared to the simulation result, in Fig. 2.15. Oblique incidence transmission measurements from 0° to 45° are shown in Fig. 2.16.

At normal incidence, the BP response agrees well with simulations over a 4.5 GHz bandwidth. The BP response shifts in frequency, and the bandwidth becomes narrower as the incident angle increases. In all cases, the IL is less than 1 dB. This shows some degree of incidence angle independence. As an example, a signal with a frequency of 58 GHz will be unimpeded through the FSS at any incident angle in the range of $\theta \in [0^\circ, 45^\circ]$.

2.3.5 PCB-Based Example

While PCB based FSSs are well-known in realizing BP responses, they suffer from challenging fabrication tolerances when small line widths and gaps, such as the

Figure 2.15: Transmission measurement result (S_{21_M}) compared to its simulation (S_{21_H}) counterpart, with simulation reflection also shown.

Figure 2.16: Oblique incidence analysis, varying FSS angle from 0° to 45° .

0.2 mm from Fig. 2.17, are required, in addition to transmission losses associated with both small physical features and ohmic losses from metallization. The proposed all-dielectric structures offer a potential solution to mitigate these issues at mm-wave frequencies and above.

Figure 2.17: PCB-based BP FSS model based on [24] using RO3035 substrates with data sheet values being $\epsilon_r = 3.5$, $\tan \delta = 0.0017$, observed at 10 GHz, with a metal thickness of $30 \mu\text{m}$. An airbox was defined, with Floquet ports defined on the top and bottom layers, and master-slave boundaries on the sides. The dimensions are as follows: $p_x = p_y = 1 \text{ mm}$, $w_{\text{slot}} = 0.2 \text{ mm}$, $l_{\text{slot}} = 0.45 \text{ mm}$, $w_{\text{line}} = 0.2 \text{ mm}$, $l_{\text{line}} = 0.7 \text{ mm}$, $d_{\text{slot}} = 0.125 \text{ mm}$, $H = 0.1252 \text{ mm}$.

To compare loss performance to a PCB-based mm-wave FSS, the PCB dipole-slot coupling resonator structure from [24] was scaled from 18 GHz to around 60 GHz. Fig. 2.17 shows the ANSYS FEM-HFSS model and setup, with the dimensions noted in the caption. Fig. 2.18 shows the spectral response of this structure showing a BP response centered at 61.6 GHz with a 3-dB bandwidth of 4 GHz, and an IL of 0.81 dB at the center frequency. There are no unwanted bands in the stop-band.

At this frequency, implementing small feature sizes, such as the line widths and gaps shown in Fig. 2.17, become the main challenge with fabricating PCB-based designs, as they will be difficult to fabricate with strict tolerances due to process limitations, such as a minimum line width of 0.1 mm for instance. Further work, to be discussed in Chapter 4, will present the next steps to show whether loss-performance improves with the proposed all-dielectric structures.

2.3.6 Discussion and Conclusion

In this Chapter, a method of designing aperiodic multi-layer all-dielectric FSS for mm-wave applications has been demonstrated, verified by full-wave simulation. Us-

Figure 2.18: Spectral response of the PCB-based mm-wave BP FSS from Fig. 2.17 showing a matched response, and good transmission, at around 62 GHz.

ing dielectric stacks minimizes the effect of fabrication tolerances on electrical performance, improves loss performance, introduces polarization-independence, and allows some degree of incidence angle independence. It was shown that aperiodic stacked devices can outperform periodic structures by reducing unwanted bands in the stop-band regions and by having an overall lower thickness than their periodic counterparts. Figs. 2.19(a) and 2.19(b) demonstrate the reduction in unwanted bands for aperiodic structures. Table 2.2 compares the performance of the aperiodic multi-layer BP FSS, the periodic multi-layer BP FSS, and the PCB-based BP FSS example discussed previously.

For comparison, in simulation the proposed aperiodic structure has an IL of 0.5 dB at 60 GHz, the periodic structure has an IL of 0.56 dB at 60 GHz, and the aperiodic structure has an IL of 0.81 dB, presenting a difference to the PCB-based FSS value that seems insignificant in practice. However, analyzing Table 2.2 will further emphasize advantages for one structure over another. The PCB-based structure has 5 layers, 3 being metallization layers, and 2 being dielectric substrates.

Although the implementation of stacked dielectrics is immune to alignment tolerances, and is polarization-independent, the three main drawbacks to this method are (1) the overall thickness of the stack increases with complexity of the required response (e.g.: for multi-band filters), (2) the limited number of commercially available dielectrics, meaning some responses may be practically unrealizable, and (3) the requirement of mechanical assembly. However, these drawbacks become negligible

(a)

(b)

Figure 2.19: Wide spectral response of (a) Fig. 2.11 showing periodicity due to the periodic nature of this structure, and of (b) Fig. 2.11 showing suppressed unwanted adjacent transmission bands due to the aperiodicity of the structure.

where higher frequency applications are needed, such that the scale of the structures is reduced to allow for IC-based fabrication. Also, aperiodic structures were shown to have advantages over periodic ones.

Table 2.2: Comparison between aperiodic multi-layer, periodic multi-layer, and PCB-based FSS structures as demonstrated in this chapter. All frequencies are in GHz, with IL in dB.

Type	# Layers	t (mm)	$IL(f_{\text{center}})$	f_{center}	$BW_{3\text{-dB}}$
Aper.	7	8.54	0.50	59.8	2.5
Per.	5	12.6	0.56	59.7	4.5
PCB	5	0.34	0.81	61.6	4.0

In conclusion, a 57 GHz center frequency periodic stacked dielectric structure was fabricated, based on a 60 GHz design, and measured, with the measurements correlating well with ANSYS FEM-HFSS simulation results. The FSS operated with a 3-dB bandwidth of 4.5 GHz and less than 1 dB IL within the passband. It was shown that the response shifts, in frequency, with a change in the angle of incidence, but a good BP response was shown to be present in the range of incident angles of 0° to 45° . The variation in the passband (wiggle) was determined to be interference from multipath signals and unwanted reflections due to taking the measurements in an open environment without EM-absorbing foam. Regardless, this work opens the path for fabricating multi-layer aperiodic stacked dielectric devices on a smaller scale for higher frequency applications as will be demonstrated in Chapter 3.

Chapter 3

Narrowband Mid-IR Thermal Emitter

3.1 Background

All objects emit IR radiation when heated. An increase in temperature means an increase in the radiation [17]. An ideal blackbody is an object that emits over all frequencies, according to Planck's law [11], but realistically objects emit over specific frequency ranges. Knowing this, devices can be designed to emit only at specific frequencies, which can be shown to emit at a specific intensity at those frequencies when superimposed over the blackbody radiation at a given temperature [29]. Discussions in literature of the future of mid-IR sources shows promise in this area of research [30].

For example, mid-IR optical devices have important applications, one of which is sensing of a wide variety of gases such as carbon dioxide (CO_2) and sulfur dioxide, (SO_2), with work demonstrating this application [31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43]. In this work, a direct thermal testing of an aperiodic all-dielectric stack is performed, with its high-Q characteristics being experimentally verified, where samples are heated to produce the mid-IR emission at around 71 THz, being near to the absorption peak of CO_2 .

The superiority of the aperiodic stack over similarly performing devices is further confirmed by comparison to the literature, and using numerical examples, where an optimal narrowband emittance, without spurious peaks over wide spectral bandwidth, is achieved using an aperiodic design. In contrast, a periodic stack design is found to suffer from a trade-off between emittance, number of dielectric layers and undesired emission peaks. The emitter can be stimulated by being heated by a microhotplate as shown in [44, 45], whereby emitting the desired peak.

3.2 Literature Review

Details will be provided in this literature review to highlight the contributions made by this work to existing research. Of great importance is the high performance characterization and detection of the *purity* of the mid-IR signal generated by the source emitter, whereby a narrowband emission is highly desirable. Having a high-Q emission peak maximizes the detection resolution, where individual elements, molecules, or gases can be detected in a medium with minimal error. Several emitters have been reported to produce these narrowband emissions [46, 47, 48, 49, 50, 51, 52, 7, 53, 6, 8, 54, 29], based on various methods that can be classified as follows.

In three dimensions, there are six distinct major classifications of cell-based all-dielectric stacked structures as mid-IR thermal emitters, with most of them discussed in a well-done review of optical nanostructures [6]. In particular, there are three sets of aperiodic and periodic structures, giving the six groups: **(1)** periodic cells on the surface [46, 11, 55, 47, 49, 50, 56, 52, 7, 53, 54, 57, 58, 59, 60, 61], **(2)** aperiodic cells on the surface [8], **(3)** periodic cells in the z-direction [62], **(4)** aperiodic cells in the z-direction [20, 63, 64, 65], **(5)** periodic cells in all dimensions [48, 50, 51, 66, 67], and **(6)** aperiodic cells in all dimensions. Groups three and four encompass the entirety of research for multi-layered stacked dielectric devices for thermal emission, with the work done in this Chapter being a subset of group four: a multi-layer *aperiodically* stacked structure of dielectrics with contrasting permittivity. In particular a periodic structure is where a sub-stack of dielectrics with two or more specific thicknesses forms a unit cell that is repeated along the vertical (longitudinal) direction [62], and an aperiodic structure is where the layer thickness can vary from one to the other [20, 63].

Most of the work in literature for narrow-band thermal emitters focuses on planar microstructure-based designs; group one. Using dielectric pucks, such as that shown in Fig. 3.1(a), it was shown that a high Q-factor of up to 650 can be achieved in [46], where finalization of that work in [11] showed a more realistic value of 150 being achievable, with a measured Q-factor of 38 being reported, with an $|\mathcal{E}|$ of 0.38 at around 42 THz. Another work done on resonant dielectric pucks shows a higher-Q peak than [11], in absorption instead of emission, but with many unwanted emission peaks surrounding at around a wavelength of $1\ \mu\text{m}$ [55]. In [61], a review of plasmonic structures is done, showing a cross pattern being the best performing structure, which is again confirmed in [11].

Less-common are the designs which fall under the group two category, where in [8] aperiodic structures are used to induce multiple emission peaks. This can enhance the accuracy of gas sensing for those gases with multiple absorption peaks, and reduce error further, however, the Q-factor was lower than the proposed single-peak periodic designs, and the author suggests energy-harvesting applications, which do not need high-Q emission peaks.

Groups 3 and 4 make up the set of stacked dielectric devices for thermal emitters and absorbers. In [20], the method used in this thesis for designing an algorithm to use the GA to obtain designs of aperiodically stacked dielectric slab devices was demonstrated in simulation with the promise of high-Q peaks. The demonstration shows the use of silicon (Si) and silicon dioxide (SiO₂) layers, as was done, and will be discussed within this chapter. The design is taken further by [63] with germanium used instead of Si, samples of these aperiodic structures being fabricated and measured using reflectance-based FTIR, emissivity being calculated via the equations in Section 3.3. Xingxing Liu et al. proposed a periodically stacked structure of Si and SiO₂, with a thermal emission measurement and full characterization of the emitters done.

It is well known in EM filter theory that aperiodic structures offer optimized filtering response with greater flexibility in a more compact size compared to their periodic counterparts [16]. Various structures reported in the literature and designed for narrowband thermal emission (acting as spectral filters) are aperiodic in nature. While aperiodic all-dielectric stack-based thermal emitters have been proposed in literature, discussed above, their thermal emission performance has not been tested. In particular, the usage of multi-layered dielectric stacks for IR emission shows promise in simulation [20] and in FTIR reflection measurement [63]. On the other hand, while detailed thermal testing of periodic dielectric stacks have been presented in [62], the structure being illustrated in Fig. 3.1(b), it requires large number of dielectric layers and thus forming a thick stack and suffers from spurious emission peaks due to the non-optimal periodic nature of the device.

Finally, work was done to combine elements of the previous 4 groups such that there are resonant structures in all three dimensions. These are also rarer than structures falling within the categories of groups 1, 3, and 4 due to the added complexity of fabricating such devices. In [48] coupled dipole resonators are placed in three dimensions periodically to produce narrow-band thermal emission at either 1.6 μm or around 11.6 μm wavelengths. Stacked Si and SiO₂ thin films are combined with surface planar Si resonators to produce emission peaks at a wavelength of 2.2 μm , with unwanted peaks also observed in the shown spectrum. Another combination is [51] which uses circular slots in a stacked dielectric structure to produce these peak, which was also thermally tested, with a similar structure proposed in [66]. Three-dimensional Si crystals, with a shape varying in the z-direction, were used in [67]. The structure from [50], shown in Fig. 3.1(c), shows a periodic arrangement of resonators over a periodic dielectric stack for tailored dual-emissions.

$$\mathcal{E}(\omega) = 1 - |T(\omega)|^2 - |R(\omega)|^2 \quad (3.1)$$

Where $T(\omega)$ and $R(\omega)$ are the spectral transmission and reflection across the structure, when excited with a plane-wave. Since the structure is to be backed by an opaque metallic base, $T(\omega) = 0$, so that the emissivity is reduced to Eq. 3.2.

$$\mathcal{E}(\omega) = 1 - |R(\omega)|^2 \quad (3.2)$$

By designing the thicknesses of these dielectric layers for a set of given materials, large emittance (or absorption) can be achieved at the desired frequencies.

Figure 3.2: ANSYS FEM-HFSS model and setup, using floquet ports and master-slave boundaries for full-wave simulation of an infinite surface of the proposed stacked device.

A further development of the algorithm described in Section 2.2.1 was used to design the structures discussed in this chapter. A load-to-source recursive approach of calculating the response of an incident plane wave through multi-layer dielectric slabs is taken, and the GA optimization routine is used to obtain the design needed for any goal scattering response. The load, in this case, is a copper (Cu) layer, which ensures no transmission and only either reflection or absorption of incident radiation. Fig. 3.2 shows the ANSYS FEM-HFSS model and setup for the verification simulations of this chapter. The superposition of dielectric slabs with alternating high and low dielectric constants, with different thicknesses creates resonant cavities within the structure which is opaque to some frequencies (due to complete absorption in our case) and purely reflective to others [20].

Using this theory, and the optimization algorithm, a design can be obtained to be perfectly absorptive at a single frequency with a high Q-factor meaning high spectral

selectivity, and opaque at all other frequencies. In particular, a frequency of 70.3 THz was chosen as the design frequency as it is near the absorption frequency of CO₂. Following Kirchoff's law of thermal emission, when heated this device will radiate at that single frequency, providing the high-Q IR emission peak for gas sensing. The GA is used to minimize a residue function by choosing the thicknesses for a set of N alternating layers of SiO₂ and Si for the stack. These are chosen to obtain a design that best matches the goal scattering response, as given as an input to the algorithm. The number of layers, N , is constrained prior to optimization.

Initially, the material parameters for all three materials, i.e. Cu, Si, and SiO₂, were kept frequency-independent and constant. The dielectric constant, ϵ_r , was constrained to 11.1 and 2.18, for Si and SiO₂ respectively, and the loss tangent, $\tan \delta$, was constrained to 10^{-6} (based on material measurements from Section 3.3.1) and 0.0024, for Si and SiO₂ respectively. Cu was taken as a perfect conductor for simplicity. Later on, for obtaining a realizable design, these parameters will be replaced with practical frequency-dependent measured values. Fig. 3.3 shows the results of a 7-layer example design using frequency-independent material parameters, as described above. Full-wave simulation using ANSYS FEM-HFSS was used to validate the results obtained using the t-matrix model and algorithm, with the FEM-HFSS model shown in Fig. 3.2. Master-slave boundaries were used to simulate the structure as an infinite surface. The reflectance was obtained and emissivity was calculated as above. As can be seen, a high-Q emittance, with a Q-factor of 175, was obtained at the desired frequency of 70.3 THz.

Figure 3.3: Emissivity of the dielectric stack from Fig. 3.2 showing exact correlation between full-wave simulation and the t-matrix model, as well as the calculation of Q-factor.

The dimensions of the ideal design are [1400, 354, 760, 344, 600, 360, 100] nm, starting at a 1000 nm Cu layer, followed by the first SiO₂ layer, then the first Si layer, to the last SiO₂ layer, with a total thickness of 3.92 μm . To show the advantages of aperiodic multi-layer dielectric stacks over their periodic counterparts, an analysis was done to obtain a periodic design exhibiting the same high-Q behavior as that of the aperiodic stack, which resulted in a 17-layer structure of alternating SiO₂ of Si with optimal thicknesses 1216 nm and 233 nm, respectively, whose response is shown in Fig. 3.4(a). Compared to the aperiodic stack, while the desired emission is successfully obtained, periodic stack features several spurious emission peaks. Decreasing the number of layers to 15 shows the adjacent peaks move further from the main emission peak, but also shows a reduction in the emissivity and Q-factor. Increasing to 19 layers shows an improvement in main peak performance, with the adjacent peaks becoming more prominent and closer in frequency to the main peak. Fig. 3.4(b) illustrates these findings while Table 3.1 provides a numerical summary. It is clear that the periodic stack not only requires more layers, than the aperiodic stack, to obtain a narrowband high emission response, but also suffers from the trade-off where the reduction of the extra peaks comes at an expense of compromised peak emittance. Overall, the aperiodic structure used in this work outperforms periodic structures, of the same materials, using only 7 layers thus being thinner than the periodic counterparts.

Table 3.1: Summary of periodic vs. aperiodic multi-layer all-dielectric stacks for mid-IR thermal emission showing advantages in using aperiodic designs, as proposed.

# Layers	t_{total} (μm)	f_{center}	$ \mathcal{E} $	Adj. f_{center}	Adj. $ \mathcal{E} $
7	3.92	70.3	0.97	95.5	0.15
15	11.37	70.6	0.93	74.8	0.56
17	12.81	70.3	0.98	73.7	0.65
19	14.26	70.1	0.99	72.9	0.74

Figs. 3.5(a) and 3.5(b) shows the angular dependence of the emission beam in both θ and ϕ directions in both polarizations, for the fixed frequency of 70.3 THz, demonstrating a 3-dB beamwidth of 5°. Unpolarized emission is also demonstrated, seeing the angular emission response nearly identical between horizontal and vertical polarizations.

3.3.1 Material Parameters for Precise Design

Obtaining a design suitable for fabrication involved making use of the frequency-dependent optical properties for the three materials used. Models are available to provide this information for Si, SiO₂ [69], and Cu [70], but actual measured data was used instead shown in Fig. 3.6, from work done previously to measure the optical properties of Si and SiO₂ using ellipsometry [11]. These material parameters correspond to Si and SiO₂ deposited using the process in the Carleton University Micro-fabrication Facility. As an example SiO₂ was shown to have a permittivity

(a)

(b)

Figure 3.4: Typical emission response of an aperiodic dielectric stack structure compared to its periodic counterpart. (a) Spectral responses of a 17-layer periodic structure, similar to that proposed and thermally characterized in literature [62], versus the proposed aperiodic structure, and (b) variation of periodic structure response with increase and decrease in the number of layers.

(a)

(b)

Figure 3.5: Angular-dependence of the ideal IR emitter showing the total emissivity from the IR emitter vs. θ and ϕ angles in (a) horizontal and (b) vertical polarizations for the center frequency of 70.3 THz.

of around 2.2, compared to the value of around 2.1 from literature [69]. Also, the measured parameters are strongly dependent on frequency and exhibit several material absorption regions. Fortunately, the materials have well-defined low-loss region around the frequency of interest around 70 THz. This allows for the most accurate simulations possible to ensure maximal measurement-simulation correlation.

(a)

(b)

(c)

Figure 3.6: Measured frequency-dependent material parameters for (a) Cu, (b) Si, and (c) SiO₂.

A 7-layered structure was obtained, using the methodology from Section 2.2 and using frequency-dependent parameters from Section 3.3.1. The dimensions of the the 7 layers, including the Cu layer, are as shown in Table 3.2. The results from the model used in the design process matched the results from full-wave simulations, using ANSYS FEM-HFSS, validating the use of the model once more.

3.3.2 Structure Design and Simulation

Fig. 3.7 presents the simulation results for the design which makes use of the measured material parameters from Section 3.3.1. Table 3.2, in the proceeding section, shows the design parameters for each layer starting with SiO₂ deposited over the Cu-layered wafer, followed by alternating Si and again SiO₂.

Figure 3.7: Emissivity of the simulated designed structure using the material parameters from Section 3.3.1.

3.4 Fabrication and Measurement

3.4.1 Fabrication of the Proposed Structure

The IR emitter was fabricated at the Carleton Micro-fabrication Laboratory using plasma-enhanced chemical vapor deposition (PECVD) via a Trion Minilock-Orion PECVD system. Firstly, a micron-thick layer of elemental Cu was deposited onto a

Si wafer of diameter 3.81 cm, using sputtering electron-beam evaporation in a Balzers evaporation system [11]. To ensure the Cu layer does not peel from the substrate, a 50 nm layer of titanium was used for Cu to the silicon wafer substrate for crystal adhesion, following the findings of previous work [11, 71]. Following Cu deposition, the wafer, being on a hot plate shown in Fig. 3.8, was placed into the vacuum chamber of the Trion, shown open after fabrication in Fig. 3.9. The wafer was transferred into the Trion quickly to avoid oxidation of the Cu. Using the pre-determined deposition rates of Si and SiO₂, 3.466 nm/s and 0.812 nm/s, respectively, the deposition times were calculated. The 7 layers were subsequently deposited, layer after layer, without removing the wafer from the vacuum chamber, and the fabrication was then complete. A nitrogen cleanse of the chamber was done between each deposition to reduce the risk of contamination of the proceeding layer during its deposition. Table 3.2 shows the deposition times for each layer. Table 3.3 shows the PECVD configuration on the Trion for deposition of both Si and SiO₂.

Figure 3.8: Carbon plate where the Cu-layered Si wafer is placed (at the center holder) for deposition in the Trion machine.

The titanium layer between the Cu base-layer and the substrate prevented the bubbling shown in the sample wafer in Fig. 3.10, which was fabricated without the titanium. Titanium is used due to its adhesion properties to metal and silicon. Also, following layer deposition, layer peeling, de-lamination, or separation due to thermal stress was a risk due to the different thermal expansion coefficients of Cu, Si, and SiO₂ [72] and the rapid cooling from 350°C to room temperature post-fabrication, but this phenomena was not observed in this experiment.

Tolerances of measured thickness were ± 20 nm taken as a one-pixel error due to measurement by counting pixels in the SEM image. An analysis is done in Section 3.4.3 to show how the dimension variation affects performance.

Figure 3.9: Trion PECVD machine used for fabrication of IR emitter samples.

Figure 3.10: Fabricated sample without the titanium layer between the substrate and the Cu layer, showing bubbling defects as a result.

Following fabrication, the wafer was cleaved into three square samples of 1.5 cm by 1.5 cm with the prime sample being the center most, labelled 'A', with two other samples taken from the left and right of the center, labelled 'B' and 'C' respectively, as shown in Fig. 3.11.

Table 3.2: Designed layer dimensions, estimated dimensions extracted from the SEM image, and computed deposition times for fabrication.

Layer #	Material	t_{design} (nm)	t_{SEM} (nm)	Dep. Time (s)
0	Cu	1000	1000	-
1	SiO ₂	1376	1356	397
2	Si	1012	1006	1246
3	SiO ₂	860	792	248
4	Si	212	266	260
5	SiO ₂	1168	1090	337
6	Si	999	959	1275
7	SiO ₂	170	168	49

Table 3.3: PECVD Trion deposition configurations for Si and SiO₂. Temperature was set to 350°C for all deposition steps.

Material	Type	Power (W)	P (mTorr)	Gas Flow (SCCM)
Si	RF	81	1000	SiH ₄ (25) Ar (50)
SiO ₂	ICP Triode	39	900	SiH ₄ (21) N ₂ O (355) N ₂ (110)

Figure 3.11: Fabrication results of the multi-layer all-dielectric IR emitter showing the Cu deposited wafer before and after deposition of the 7 layers, along with the cleaved samples.

A scanning electron microscope (SEM) image of the center sample, cleaved at the center and imaged post-measurement, is shown in Fig. 3.12, showing clear delineation between the 7 layers, with extracted dimensions shown in Table 3.2.

Figure 3.12: An SEM image of the middle of sample ‘A’; the layer dimensions being extracted and shown in Table 3.2.

3.4.2 Thermal Measurement

The samples were sent to Stony Brook University for thermal emission testing using the apparatus shown in Fig. 3.13. Each sample was placed in a system where it was heated to 70°C, and its emission was measured over a spectrum using Fourier transform infrared (FTIR) spectroscopy. An alternative method of measurement is to use multiple total internal reflection (MTIR) spectroscopy which measures absorption rather than emission [73]. The FTIR measurement apparatus is described in depth in Ali’s work [11]. The measured FTIR spectrum is compared with a blackbody reference at two temperatures, 70°C and 100°C, shown in Fig. 3.14(a), which provides the measurements necessary to obtain the sample emission only according to the methodology described by Ruff [74, 11]. The measured thermal emissivities of all three sample devices shown in Fig. 3.16.

Figure 3.13: Diagram showing the IR Emitter measurement setup from Stony Brook University, adopted from [11] (M. O. Ali, ©2019 Carleton University, CURVE).

Sample ‘A’ has the highest emittance of 0.7, with a Q-factor of 113, while samples ‘B’ and ‘C’ have lower emittance and a lower Q-factor. This is due to the radial unevenness of deposition onto the wafer. The center receives mainly uniform deposition, and the deposition rate decreases moving outwards toward the edges of the wafer. Table 3.4 outlines the measurement results of all samples, where the Q-factor was calculated as per Fig. 3.3. While the device was designed for near unity emittance, measured emittance was only 0.7. A frequency shift was also observed around 1.5 THz. The overall behavior of the device is otherwise similar to expectations. This could be attributed to the variation in the layer thicknesses during fabrication and variations in the materials parameters, such as an increase in loss tangent, at temperatures above room conditions.

To explore this possibility, SEM images of the dielectric stack were taken as shown in Fig. 3.12 and layer thicknesses were estimated, outlined in Table 3.2. To account for lower emittance, and variation in the the loss tangents, they were scaled by a constant factor throughout the stack. Fig. 3.16 compares the emissivity results of the design based on the SEM image’s extracted dimensions, and the loss tangents for all materials increased by a factor of 5. A good match is obtained, both in terms of the frequency shift and the emissivity between the two. This indicates that with a more controlled layer fabrication process, and with improved material characterization, the original high-Q response can be achieved.

(a)

(b)

Figure 3.14: FTIR Thermal Emission measurements showing (a) the background data for two temperatures, and (b) the raw data collected for the three samples, including the background measurement at 70°C.

(a)

(b)

Figure 3.15: Extracted thermal emissions of the samples using the methods described in [74] showing (a) the data over the whole measured spectrum, and (b) the measurements in the spectrum of interest.

(a)

(b)

Figure 3.16: (a) Thermal emission measurements of all samples, and (b) of Sample ‘A’ compared to original design simulated emissivity, and modified design emissivity based on matching the dimensions from the SEM image in simulation.

Table 3.4: Thermal emission measurement results for all samples.

Sample	f_{center} (THz)	$ \varepsilon(f_{\text{center}}) $	Q
A	71.2	0.70	113
B	71.7	0.41	49
C	71.6	0.49	62

3.4.3 Discussion and Conclusion

A direct thermal testing of aperiodic all-dielectric structures has been presented and an emittance of 0.7 and Q-factor of 113 has been experimentally achieved using a 7-layer dielectric stack for CO₂ gas sensing applications. This has been the first time a direct thermal testing of an aperiodic all-dielectric stack has been presented, thereby showing narrowband emission properties of such structures when heated above room temperatures. An all-dielectric stack is thus found to be a simple structure that does not require any lateral mask preparation as the frequency selectivity is achieved using an aperiodic arrangement of alternating dielectrics with contrasting permittivity. It has been further shown that the aperiodic structures leads to a significant reduction of the device thickness compared to its periodic counterpart without exhibiting any undesired spurious emission peaks. This simplicity comes with the limitation that thermal emission is uniform across the structure as opposed to metamaterials based devices, where phase gradients can be engineered for more diverse control over their emissivities.

A 1000-iteration Monte-Carlo (MC) simulation was performed to analyze the effects of thickness variation due to variable material deposition. The following layer variation constraint simulations were performed, with the worst case and best case results shown, with respect to lowest emittance and highest emittance peaks: ± 10 nm, ± 25 nm, and ± 50 nm, all shown in Fig. 3.17. The main impact of layer thickness variation was the shifting of the emission peak in frequency.

The MC simulations show that up to 25 nm of random variation in the layers shows that high emittance is maintained. If the layer variation is not random but uniform, being the same for all layers, then the behavior shown in Fig. 3.18 is expected.

As temperature increases, the material parameters of the material changes. As shown in [11], variation in the loss tangent reduces emissivity. This was not accounted for in the design process and, a five-times increase in the loss tangent for all three materials shows measurement agreement with simulation in terms of relative emissivity, shown in Fig. 3.16. A reduction in the loss tangent may also contribute to a lower emission, as shown in Fig. 3.19.

Using a multiplication factor of 5 for the loss tangents in the algorithm, a new design was obtained, as illustrated in Fig. 3.20, showing that the higher emittance

Figure 3.17: MC simulation results showing best and worst case emission peaks varied from the original design discussed in Section 3.3.2, for ± 10 nm, ± 25 nm, and ± 50 nm variations.

Figure 3.18: Uniform layer variation emission simulations compared to the original design. The simulations were done for ± 10 nm, ± 20 nm, and ± 30 nm variations in that order relative to the design simulation emission peak.

can be obtained, while maintaining high-Q performance (Q-factor remains over 100), by accounting for the temperature-variability of $\tan \delta$ in the future. This comes at the expense of a potential emittance shoulder, which cannot be verified as real until temperature-compensated material parameters are used in the design simulation.

Figure 3.19: Peak emittance of the design structure varying with a loss tangent scaling factor.

Figure 3.20: Re-design with an increase in $\tan \delta$ by a factor of 5, showing high-emissivity results possible at 70°C.

Chapter 4

Conclusions and Future Work

4.1 Conclusions

In this thesis, two projects presented the applications of using multi-layer aperiodic all-dielectric stacked devices for spectral shaping to serve as mm-wave BP FSS and mid-IR thermal emitters. The main focus became the mid-IR thermal emitter project from Chapter 3, as the mm-wave BP FSS results showed more promise for use at higher frequencies, which was proven in that chapter. An algorithm, based on the GA optimization routine, was designed and demonstrated by creating designs for the two projects. The algorithm was shown to match full-wave simulation results from ANSYS FEM-HFSS which validated its use as a high-speed and efficient method of obtaining designs through optimization and numerical techniques.

A 60 GHz aperiodic dielectric stack FSS was demonstrated in simulation as having fewer adjacent transmission peaks than corresponding periodic structures. With aperiodic structures, a multi-resonance flat BP response is more difficult to obtain with fewer layers, thus becomes impractical for fabrication as the thickness is increased. A 7-layer aperiodic design was simulated showing a good narrowband BP response at 60 GHz, with a 3-dB bandwidth of 2.5 GHz. As the scale is reduced at mid-IR frequencies, the thickness of these structures was taken as an advantage to move to higher frequencies toward the mid-IR thermal emitter project. To prove the design process, and function of these dielectric stack structures a 57 GHz center frequency periodic stacked dielectric structure was fabricated, based on a 60 GHz design, and measured, with the measurements correlating well with ANSYS FEM-HFSS simulation results. The FSS operated with a 3-dB bandwidth of 4.5 GHz and less than 1 dB IL within the passband. It was shown that the response shift, in frequency, with a change in the angle of incidence, but a good BP response was shown to be present in the range of incident angles of 0° to 45° . Although the incidence angle varied to 45° , the frequency shift is small because of the high permittivity of the slab

material resulting in a smaller transmitted angle according to Snell's law. Although loss performance did not improve significantly from PCB-based BP FSS, as shown through simulations, this work demonstrated the technique to enable fabrication of multi-layer aperiodic stacked dielectric devices, using IC fabrication technology, for higher frequency applications as was demonstrated in Chapter 3.

A direct thermal testing of aperiodic all-dielectric structures has been presented and an emittance of 0.7 and Q-factor of 113 has been experimentally achieved using a 7-layer dielectric stack for CO₂ gas sensing applications. This has been the first time a direct thermal testing of an aperiodic all-dielectric stack has been presented, thereby showing narrowband emission properties of such structures when heated above room temperatures. An all-dielectric stack is thus found to be a simple structure that does not require any lateral mask preparation as the frequency selectivity is achieved using an aperiodic arrangement of alternating dielectrics with contrasting permittivity. It has been further shown that the aperiodic structures leads to a significant reduction of the device thickness compared to its periodic counterpart without exhibiting any undesired spurious emission peaks. This simplicity comes with the limitation that thermal emission is uniform across the structure as opposed to metamaterials based devices, where phase gradients can be engineered for more diverse control over their emissivities.

It was also shown, for both projects, that aperiodic structures can outperform their periodic counterparts in terms of aperiodic structures being thinner, and having suppressed unwanted adjacent passbands or emission peaks. In addition, for the mid-IR thermal emitter, it was shown that fewer layers was required to get the single high-Q emission peak at the desired frequency in comparison with the periodic counterpart.

4.2 Future Work

There are several avenues of expansion that can be taken to further develop the work presented in this thesis, and the conclusions from that work from Section 4.1. Three main directions involve: (1) the improvement of the algorithm for better design of the structures, (2) comparison between fabricated aperiodic mm-wave FSS of both methods; all-dielectric and PCB-based, and (3) combination of the proposed mid-IR thermal emitters with a planar metasurface for beam-steering and other applications useful in the design of gas sensors, for instance. How this can be done is discussed in the following paragraphs.

As described in Chapter 2, the algorithm made use of the GA optimization routine to find a solution structure to fulfil a goal response. It was found that many solutions exist for any given goal function, and many iterations of the algorithm were required to create a database of solutions from which the optimal solutions are identified and chosen based on a the criteria of number of adjacent bands to the passband, the 3-dB

bandwidth of the passband, and the matching of the main passband. Modification of this algorithm to find the absolute best, i.e. the absolute minimum of the optimization function Eq. 2.8. In [20] the GA was used to minimize a different fitness function that is based on the integral of the emittance over angle of emittance from 0° to 90° . The function is constrained to ensure an emittance of over 0.95 for normal emission. In [63] Bayesian optimization was used, which begins by initializing 200 randomly selected candidate structures and uses an optimization routine to find the absolute minimum to the figure of merit function that they define in their work. This is a prolonged process, but the result is one ideal structure which eliminates the need to select from a set of many ‘solutions’ as was done for this thesis. Implementing and further developing on the work by these authors will improve the design process of these structures.

Further analysis must be done to verify loss performance of the mm-wave BP FSS for both the multi-layer periodic all-dielectric structure and the PCB-based structure. If it can be shown that at 60 GHz, PCB-based structures become impractical due to the higher loss performance, lower BP performance, and difficulty of implementing the small feature sizes, then all-dielectric structures are validated as an alternative method for producing these BP FSS. In that case, aperiodic structures, as demonstrated in Chapter 2, can be designed and fabricated. With tighter constraints on total thickness, and a more robust algorithm, a solution may be found that may mitigate the inherent bulkiness problems with regards to aperiodic multi-layer all-dielectric structures. If this does not solve the thickness issues, an alternative would be to introduce materials with very high dielectric constants into the algorithm pool, which would allow for thinner designs. For this thesis, only Rogers-based dielectrics were included in the pool which limited the peak dielectric constant to around 12.

The main project from this research was the mid-IR thermal emitter from Chapter 3. As much work was already done in the exploration of both periodic and aperiodic structures, in all three dimensions as described in the Section 2.3.2, there is little known further development that can be done on this structures, except for the development of fully three-dimensional aperiodic structure if they can be made practical. However, future work can be expanded to include using these aperiodic structures, explored in this thesis, in combination with planar devices on the top surface to add another level of control to the emitted beam, for example steering the beam in particular directions, modifying the polarization, or increasing the Q-factor further to improve sensing resolution. In this area there are many interesting directions that the research topic of stacked dielectric devices could take. Regarding fabrication, the following steps can be taken to improve prototyping of aperiodic stacked devices: (1) a more precise process control such as using atomic layer deposition (ALD) for layer deposition, and (2) material parameters measured at the thermal measurement temperature should be used in the design for the most accurate simulation.

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Appendix A

Optimization Algorithm Code

A.1 Core Optimization Function

The following is a sample of the core algorithm function, serving as a mechanism for obtaining designs for the mid-IR emitter project. Variations of this core function was used for other aspects of the thesis, including the mm-wave FSS project, and the multi-layer periodic stacked dielectric device analysis.

```
function x= main()
    %% core top level main function
    clc, clear, close all

    % Reading measured physical data for the materials.
    silicaData=csvread('silica.csv', 1,0);
    siliconData=csvread('silicon.csv',1,0);

    % Defining the bounds of the required bandpass response.
    fl = 70e12;
    fh = 71e12;

    % Initializing frequency range.
    freq0 = silicaData(:,1);

    % Defining new frequency range within measured material
    %  $\rightarrow$  property
    % limitations. Adjusting data to correspond accordingly.
    center=round(length(freq0)/2);
    freq=freq0(center+76:center+99);
    silicaDataN=silicaData(center+76:center+99,:);
    siliconDataN=siliconData(center+76:center+99,:);
```

```

% Defining optimization parameters.
N = 7;
FitFcn = @(x)solution(freq,fl,fh, N, x, silicaDataN,
    ↪ siliconDataN);
[LB, UB] = defineBounds(N,0.1e-6,1.4e-6); % Thickness bounds
options = optimoptions(@ga,'Display','iter');
options.PlotFcns = @gaplotbestf;
options.UseParallel = true;
options.UseVectorized = false;

% Running the GA optimization routine to find a solution.
[x, fval] = ga(FitFcn, nvars, [],[],[],[],LB, UB,[], options);
delete(gcp)

% Using the t-matrix approach to calculate response of
    ↪ solution.
[T,R] = solutionT(freq,fl,fh,N,x, silicaDataN, siliconDataN);
end

```

A.2 Response Calculation Function

A sample of the response calculation function is shown, which returns the residue for optimization purposes. A variation of this function is used to compute the response of the structure of the current GA iteration, where a residue value is passed back to the optimization routine to continue finding a better solution, if possible.

```

function residue = solution(freq, fl, fh, N, x, silicaData,
    ↪ siliconData)
    % Residue calculation function, based on current design
    % Setting the thicknesses of all layers from the variable 'x'
    for k=1:N
        d(k)=x(k);
    end

    % Extracting information from material property matrices.
    erSi=siliconData(:,5);
    tandSi=siliconData(:,7);

    erSiO2=silicaData(:,5);
    tandSiO2=silicaData(:,7);

    % Cu plate at back, short circuit, initial condition.

```

```

Zin0 = zeros(1,length(freq));

    % Recursively calculating the input impedance.
for j=1:N
    for i = 1:length(freq)
        % Odd is silicon, even is silica
        if (mod(j,2)==1)
            er=erSi02(i);
            tand=tandSi02(i);
        else
            er=erSi(i);
            tand=tandSi(i);
        end
        % Calculates the new input impedance, based on t-line
        % → theory.
        Zin(i)= one_slab(freq(i), Zin0(i), d(j), er, tand);
        i=i+1;
    end
    Zin0=Zin;
end

% Calculating the spectral response based on the t-line theory.
[~, R] = calcTrans(Zin);

    % Defining goal response in dB.
response = bp(fl, fh, freq);

% Calculating the delta between goal and actual responses.
diff = delta(mag2db(abs(R)), response);

% Defining the residue to be sent to the optimizer to adjust 'x'.
residue = totalDelta(diff);
end

```

A.2.1 One Slab Response Calculation

```

function Zin = one_slab(freq, ZL,d,er,tand)
mu0=(4e-7)*pi;
e0=8.854e-12;
omega=2*pi*freq;

%e=er*e0*(1+(1i*tand));
e = er.*(1 - 1i.*tand).*e0;

```

```

Z0=sqrt(mu0./e);

%Cbeta = 2*pi*freq*sqrt(er)/c;
gamma = 1i.*omega.*sqrt(e.*mu0);

%Zin = n*(ZL + 1i*n*tan(Cbeta*d))./(n + 1i*ZL*tan(Cbeta*d));
Zin = Z0.*(ZL+(Z0.*tanh(gamma.*d))./(Z0+(ZL.*tanh(gamma.*d))));

end

```

A.2.2 Defining the Goal Response

```

function bandpass = bp(fl, fh, freq)
    for i = 1:length(freq)
        if (freq(i) < fl) || (freq(i) > fh)
            bandpass(i) = 0;
        elseif (freq(i) > fl) && (freq(i) < fh)
            bandpass(i) = -20;
        end
    end
end

```

A.2.3 Residue Calculation

```

function diff = delta(slabs, goal)
    diff = abs(slabs-goal).^2;
end

function tot = totalDelta(delta)
    tot = sum(delta);
end

```