ALL-DIELECTRIC METASURFACE THERMAL EMITTERS FOR MID-IR SPECTROSCOPY

by

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A thesis submitted to the Faculty of Graduate and Postdoctoral
Affairs in partial fulfillment of the requirements
for the degree of

Doctor of Philosophy

in

Department of Electronics

Carleton University
Ottawa, Ontario

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DOCTOR OF PHILOSOPHY (PH.D.)
(DEPARTMENT OF ELECTRONICS)
AUG 2019

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Presented by: ALI Muhammad O.

To obtain the degree of : Doctor of Philosophy (Ph.D.)

ABSTRACT

A thermal emitter using a metasurface to tailor the emission spectrum in the mid-infrared for gas-sensing applications is demonstrated. The design consists of an array of high index dielectric elliptical pucks above a metal back-reflector. Using full-wave simulations in HFSS (Ver. 19.0.0), it has been shown that the achievable Q-factor ($Q \approx 150$) in this structure is an order of magnitude larger than in plasmonic arrays ($Q \approx 16$), attributed to the low-loss in the dielectric materials. Furthermore, the thermal emission properties of the structure can be engineered by manipulating the geometry of the unit cell, and these unit cells can provide polarized thermal emission simultaneously in two separate frequency bands determined by the ellipticity parameter of the puck. Design of the thermal emitter requires accurate knowledge of frequency dependent optical constants of specific deposited materials in the mid-infrared region. Optical parameters for thin film Silicon and Silicon Dioxide deposited by Plasma Enhanced Chemical Vapor Deposition (PECVD) are not readily available in the literature. These parameters were measured and used in simulation of the thermal emitter with a resonant frequency corresponding to the absorption spectra of a known industrial gas Sulphur Dioxide (SO_2). The narrow-band thermal emitter was fabricated in the Carleton University Micro Fabrication Facility and tested for thermal emissivity. Measured emissivity was found to match simulation when variations in the resonator structure due to process variation were taken into account.

Acknowledgements

Accomplishment of my thesis would not have been possible without the support of a few special people.

I would like to acknowledge and thank my thesis supervisors Dr. Niall Tait and Dr. Shulabh Gupta from the bottom of my heart for providing consistent support and encouragement to complete this task. Specially going through and fixing the multiple drafts of my thesis and help with the journal papers.

This project involved a lot of nanofabrication which is time consuming and requires a lot of expertise in terms of equipment usage and experience. I would like to extend my sincere thanks to Robert Vandusen, Angela M. Williams and Rodney Aiton for their continuous support during fabrication failures and encouragement and appreciation on my successes.

I would like to specially thank Nagui Mikhail for helping me specially when it came to simulation and technical support related to my project. Thanks to the Department of Electronics Engineering, particularly Nagui Mikhail, Blazenka Power, Anna Lee and Valerie Daley for their help.

I would like to extend gratitude to my close friend Muhammad Asif for being my continuous support during this project. His words of encouragement and advises throughout my stay in Ottawa helped me navigate the highs and lows of my academic journey. I would also like to thank my dear friend Raheel Ahmed for his help and support towards the completion of my project. I would specifically like to acknowledge his mastery on graphical designing software that helped me in translating my fabricated devices into figures.

My deepest thanks goes to my family for being my continuous support in this journey. My Wife, Naureen Aqueel was always there to help me specially raising our two sons Muhammad Abdurrahman Ali and Muhammad Yasir Ali while I was working late hours at Carleton University working on my projects and writing my thesis. She was my constant support and encouragement and believed in me for successful completion of my project.

I have no words to thank my parents Dr. Muhammad Abid Ali and Shaheen Abid Ali from the bottom of my heart for supporting me throughout my academic journey and for praying for me and for all the sacrifices they gave to enable me to be where I am right now. I would also like to thank my late father in law who passed away during the course of this research and my mother in law Tasnim Aqueel for her continuous prayers for me and my family.

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Chapter 1 Motivation

1.1 Mid-Infrared Spectroscopy

Mid-infrared (mid-IR) spectroscopy has become a widely used sampling and characterization technique [11, 12, 13]. It corresponds to light in the region of 12 THz to 120 THz ($25\ \mu\text{m}$ to $2.5\ \mu\text{m}$). It can provide qualitative analysis to identify materials by measuring the reflection, absorption, and transmission of light influenced by the presence of specific chemical bonds.

Optical gas sensing is a widely used application of mid-IR spectroscopy. This includes detection of toxic gases in industries [14] and mines, medical applications [15], monitoring of air quality in enclosed spaces [16], leak detection [17], and breath analyzers [18] among other applications. These sensors are also in high demand in the fields of atmospheric science to measure different gas species, including greenhouse gases [19, 20]. Gas sensing applications have varying requirements for sensitivity or response time, and may operate under different conditions of gas concentration and composition.

This project focuses on design, fabrication, and testing of an all-dielectric metasurface thermal emitter that can be used for mid-IR spectroscopic applications with specific emphasis on optical gas sensing applications.

1.2 Optical Gas Sensing

Gas sensors based on optical measurements exhibit unique characteristics for several applications. These systems can be sensitive, selective, stable, repeatable and exhibit long lifetime, and also show consistent performance after multiple uses. They can also provide fast response time, which makes them ideal for real-time gas sensing needs [21].

Optical gas detection is based on the spectral variation in the absorptivity of gases. Gases exhibit strong absorption at specific frequencies in the electromagnetic spectrum due to their molecular structure. Optical sensors can selectively identify gases by their unique absorption spectra. Some common gases identified using this technique include CO, CO₂, SO₂, NO₂, CH₄ [22, 23, 24].

Infrared light sources are a vital component in the sensing assembly. Many optical sensors make use of an inexpensive but relatively broadband IR source where emission is produced by resistive heating of the emitter. Thin film IR filters are used to pass the desired frequency that interacts with the sample gas and is measured at a detector [25, 26]. However, filtering results in wasted energy outside of the filter passband. In this type of application it is desirable to have a narrow-band

source, emitting light only at a frequency specific to the target gas. The following section describes the working principle and some typical topologies for optical gas sensors. It also describes some common mid-IR optical sources and detectors with their pros and cons.

1.2.1 Working Principle

Fundamental molecular vibrations at discrete energy levels for some common gases lie in the mid-IR region [27]. In this region, which is also referred to as the finger print region, gases can be identified by their unique absorption spectra as shown in Figure 1.1. An optical gas sensing assembly consists of three major components, an optical source, a gas sample chamber and a detector [28]. An optical source emits a mid-IR radiation that passes through the gas and an attenuated signal is received at the detector depending on the concentration of the target gas.

The absorption of the radiation through the sample can be quantified using the Beer-Lambert Law [29] $I(\lambda) = I_o(\lambda)e^{-\alpha(\lambda).c.\ell}$, where I_o [W/m^2] is the spectral intensity of light incident upon the gas sample (light intensity emitted by the source), α [L/gm] is the absorption coefficient of the target gas, c [g/L] is the concentration of the target gas, ℓ [m] is the path length along which the gas reacts with the emitted radiation and I [W/m^2] is the attenuated intensity of the signal after it passes through the target gas (signal received at the detector). The absorption is measured in “absorbance units” (AU), which is the ratio of the change in intensity and the original emitted intensity. According to the Beer-Lambert law, a long optical path length increases attenuation of the target frequency at the detector and increases the resolution of the gas concentration. A reference channel is used to correct for effects such as fluctuation in emission from the optical source. As most sources do not produce collimated output and are often anisotropic, optical systems are used to direct the beam through the target gas. The power passing through the target gas is lower than the total power emitted from the source.

Sensitivity of an optical gas sensor can be described as the magnitude change in the detector signal per unit change in gas concentration [30]. The detection limit is the minimum amount of target gas concentration required to obtain a precise repeatable signal. Conventionally, the detection limit is measured in parts per million (ppm). Precision refers to the repeatability of a reading and accuracy refers to true and consistent reading of the optical gas sensor. The sensitivity as well as the detection limit are directly related to the intensity of the emitter, optical path length, the type of detector, and the signal to noise ratio [31].

Figure 1.1 mid-IR absorption spectrum of some common gases

1.2.2 Optical Gas Sensing Topologies

Various optical gas sensing topologies have been reported and demonstrated to detect gases. These topologies vary depending on the type of source and detector used, the concentration of target gas in ppm, the available volume in terms of optical path and the application in terms of mobility. In some systems the emitter is aligned with the detector in such a way that they are facing each other separated by the gas cell, while in other configurations, the emitter and detector are either on the same plane or not facing each other and carefully designed multiple reflections enable emitted radiation to fall on the detector. A commonly used configuration is to have a broadband mid-IR source with a filter that passes radiation corresponding to the absorption spectrum of the target gas and passes it through a gas cell containing the sample. Another topology is to have a broadband source pass through the sample in the gas cell, and have an optical filter in front of the detector to detect the radiation at the target frequency. An optical source such as a laser produces narrowband and coherent radiation which would avoid use of any filter at the source although the detector may still require filtering of background light.

Considerable work has also been done to improve the interaction of radiation with the target gas. One commonly used method is to have a long gas cell to maximize the interaction length for the radiation. While this method can provide high sensitivity, the size of the cell can be impractical for on-chip gas sensing applications. An integrating sphere has been demonstrated to increase the optical path length [32], due to multiple reflections of the light before reaching the detector. For

on-chip applications several designs have been reported that attempt to increase the interaction of the light with the gas while maintaining a compact cell size. For example, enhancement layers such as photonic crystals have been introduced that enable slow light [33].

1.2.3 Filters for Optical Gas Sensors

Optical filtering techniques have been demonstrated to convert a broadband source into a narrow-band source. However there are several drawbacks associated with using filters for optical gas detection. One issue is the attenuation of the signal as it passes through the filter requiring a higher power source, while another issue is the alignment of the filter with the surface, specifically for system on chip applications, where it is desirable to have the source, filter as well as the detector on the same substrate. While optical filters can effectively pass the desired frequency, this sometimes results in wasted energy for frequencies in the stop band.

Linear variable optical filters (LVOF) have been demonstrated as a CMOS integrable filter to spatially separate emission frequencies from a broadband source [34]. The filter is made up of a tapered resonator layer between a flat and tilted mirror, the resonator thickness at each point determines the filtered frequency. They have achieved a transmission of about 50% with these filters. Pyroelectric detectors with uncooled arrays of linear variable filters in mid-IR are also commercially available. These filters have a working range from $2.5\mu\text{m}$ to $11\mu\text{m}$. Integrated electrostatically tunable micro-machined Fabry-Perot filters have also been demonstrated [35]. A bulk micro-machined Fabry-Perot interferometer has been fabricated on top of a pyroelectric detector and has been shown to work in the wavelength range $3\mu\text{m}$ to $5\mu\text{m}$.

1.2.4 Optical Sources and Detectors

The type of optical source used in optical gas sensing is dependent on various parameters such as cost, application, fabrication complexity, absorption spectrum of target gas as well as available gas sensor topology. In certain cases an optical fiber is needed to deliver light to a sample in a remote location, or a hollow core fiber might be used to form a thin long gas cell. For these configurations a laser is the preferred source as it is relatively easy to couple it with the fiber. For other low cost and low powered applications a broadband source such as a microbulb is commonly used. These sources are simple and inexpensive, and can be used with passive optical filters to achieve frequency dependent emission [36]. CMOS compatible MEMS thermal sources have been demonstrated for integrated on-chip gas sensing applications [37] [38]. MEMS thermal sources have a low thermal mass and good thermal isolation which makes it possible to modulate the temperature rapidly and efficiently, creating a useful low-power IR source.

Various optical detectors have been used for optical gas sensing applications. Detectors are often chose based on the source used in the sensor assembly. For sensor assemblies with QCL sources, mercury cadmium telluride (MCT) is often used for the detector. For sensor assemblies using MEMS heated sources, thermopile, bolometer and pyroelectric detectors have been used. A thermopile is a combination of series connected thermocouples. A bolometer uses high temperature coefficient of resistance thin metal films to create a resistive device that is very sensitive to absorbed infrared radiation. Pyroelectric sensors are based on classes of materials that exhibit strong polarization in response to temperature change. Table 1.1 shows some reported optical gas sensor assembly systems, with their common features.

A number of configurations for optical gas sensing assemblies have been proposed as well as demonstrated. While a high intensity narrowband coherent source such as a laser can create an accurate and sensitive optical gas sensor, it is a relatively expensive source and can require high power input. While various optical filtering techniques have been demonstrated with broadband sources, they generally result in a loss of power at the stop band as well as an attenuation of the the pass band frequency depending on the type of filtering technique. Moreover it is also challenging to integrate these filters for system on chip applications. Creation of a CMOS integrable MEMS based narrowband optical source with emission only in a desired frequency range will can result in a simple and low power infrared source.

Ref	Source	Detector	Path Length	Wavelength(μm) /Freq(THz)	Gas	Power (mW)	Detection Limit(ppm)
[38]	MEMS Thermal	Thermopile	7.5 cm	4.26 / 70.8	CO ₂	80	
[39]	MEMS Thermal	Bolometer	8 cm	4.26 / 70.8	CO ₂	45	30
[40]	MEMS Thermal	Pyroelectric	30 cm	8.4 / 35.6	C ₂ H ₄ O ₂	-	165
[41]	QCL	MCT	1cm	4.23 / 70.8	CO ₂	-	5000
[42]	HeNe Laser	PbSe	0.15 cm	3.4 / 88	CH ₄	-	-

Table 1.1 Reported optical gas sensing systems with features.

1.3 Thermal Emitters as Sources for Mid-IR Optical Gas Sensing

An ideal optical source for Mid-IR gas sensing applications would produce a high-Q emission peak for a specific spectral line in the mid-infrared region of the spectrum. An interesting approach to realize this source is to take advantage of silicon micromachining to create a thermal source,

combined with a frequency selective metasurface structure fabricated on the emitter surface to narrow the emission bandwidth.

This has been an active area of research in recent years, combining microfabrication, materials, and optics. A number of thermal emitters have been demonstrated with engineered spectral response controlled through integration of photonic crystal, plasmonic, or metasurface structures.

Important features for optical sources in this application will include:

1. Efficient emission of mid-IR light in a narrow bandwidth around a wavelength of interest. Efficient emission corresponds to a low power sensor.
2. Ability to select the emission wavelength based on the geometry of the metasurface, ideally through layout alone. This allows the selection of different wavelengths for different gases or design of devices with multiple emission wavelengths.
3. A simple process using common materials. CMOS materials are ideal for low cost, integration potential, and volume scaling.

1.4 Thesis Objectives

Several thermal emitter designs have been proposed using plasmonic structures [43][44], owing to their property of strong wavelength compression leading to sub-wavelength designs. Even though metal-based emitters produce an emissivity close to that of a black body, they feature small Q-factors, primarily due to relatively high losses for metals in the mid-IR frequency range. Moreover, most metals are unstable at the high temperatures [9] required to achieve acceptable emission intensity. An alternative approach is to design and fabricate a dielectric based thermal emitter which would result in a high Q-factor as dielectrics have lower losses than metals in this frequency range. Moreover, common dielectrics such as silicon and silicon dioxide have proven to be stable at high temperatures.

Several dielectric designs have been reported to achieve narrowband thermal emission with higher Q-factors than the plasmonic based emitters. However little work has been done in the mid-IR region, which is of great interest for gas sensing applications. The few dielectric based designs that have been reported in the mid-IR are based on multi-layered Multiple Quantum Well (MQW) structures, featuring very high Q-factors at the expenses of complex fabrication requiring large number of dielectric layers [7].

This thesis proposes and demonstrates a simple dielectric metasurface thermal emitter with only two dielectric layers, that offers a Q-factor higher than conventional plasmonic-based structures,

and thus narrowband spectral response ideal for optical gas sensing applications. To illustrate the possibilities for this approach, thermal emitter structures for two specific resonant frequencies have been designed and simulated, corresponding to absorption spectra of Carbon Dioxide (CO_2) and Sulphur Dioxide (SO_2), taking them as examples.

1.5 Contributions

The specific contributions in this thesis are outlined as follows:

1. **Design of an All-dielectric Metasurface Thermal Emitter Structure for Mid-IR:** An all-dielectric metasurface thermal emitter operating in the mid-IR range has been proposed and demonstrated using numerical simulations. This structure is based on silicon resonators on top of a conductor-backed low index host dielectric. The thermal emitter has a simple structure and can be fabricated by standard CMOS processing. It has been found that Q-factors for dielectric metasurface based thermal emitters are theoretically greater than for plasmonic array based structures. In addition, a theoretical comparison between the thermal emission properties of the proposed structure has been done with state-of-the-art plasmonic thermal emitters. A paper in the Journal of Optical Society of America (JOSA-B) has been published describing this work [10].
2. **Optical Characterization of silicon and silicon dioxide in the mid-IR region:** Detailed characterization and investigation of frequency dependent optical constants of both Silicon and silicon dioxide deposited by PECVD has been performed in the mid-IR range. No reliable experimental data was available for silicon in this frequency range, and it was important to obtain accurate data for the specific processes and PECVD reactor used to deposit the materials in the Carleton University micro-fabrication facility. This information is essential to design of devices and interpretation of experimental results.
3. **Experimental Demonstration of All-dielectric Metasurface Thermal Emitter:** The thermal emitter structure was fabricated in the Carleton University micro-fabrication facility corresponding to SO_2 absorption. Emissivity of the structure was measured and the Q-factor of about 38 was achieved (expected 135 from numerical designs). In spite of various experimental tolerances and process variations, this measured Q-factor is more than 2 times larger than the state-of-the-art plasmonic based emitters. The large difference between the measured and designed Q-factors was found to be due to variations in the resonator structure, which were carefully studied and modeled in numerical simulators to predict the actual response. This demonstrates the viability of the silicon based metasurface emitter as a mid-IR source.

1.6 Thesis Organization

This chapter provided the motivation and summarized specific objectives of the thesis. Chapter 2 describes the theoretical background of some gas sensing techniques and other basic concepts related to the tailoring of mid-IR narrowband thermal emission. It also includes a detailed literature review on the thermal emitters based on both plasmonic as well as dielectric structures. Chapter 3 presents the design and simulation of plasmonic structures, loss mechanisms in a dielectric structure as well as the proposed all-dielectric metasurface design. The simulations demonstrate its absorption properties in the mid-IR range using full-wave analysis and provide further insights into its other properties. Chapter 4 discusses the characterization of optical constants of silicon and silicon dioxide in the mid-IR range as well as re-design and re-simulation of the dielectric structure based on the extracted optical constants for the two materials deposited using PECVD, and other fabrication limitations for this project. Chapter 5 highlights in detail the fabrication process to realize these structures. Chapter 6 reports the testing setup and emissivity measurement results for the narrowband thermal emitter. Finally, chapter 7 proposes recommendations to improve the device and future work that can be done using these structures.

Chapter 2 Background

The aim of this project is to design, fabricate and test a narrow-band metasurface thermal emitter suitable for use as a source for optical gas sensing. This chapter reviews optical gas sensing techniques and provides a brief comparison with other gas sensor technologies. This is followed by a summary of commonly available mid-IR sources. The theoretical background, working principle, and critical components required for a narrow-band thermal emitter are described. The chapter reviews work relevant to this topic that has been reported in the literature.

2.1 Types of Gas Sensing

The success of a gas sensing technology for a particular application depends on the performance of the technology measured in terms of cost, sensitivity, selectivity, repeatability, and response time. There is no single technology with ideal performance in all these areas. This section summarizes the most commonly used gas sensing technologies.

2.1.1 Metal Oxide Semiconductor (MOS) Based Sensors

Metal-Oxide Semiconductor (MOS) is one of the most widely used gas sensing technologies. MOS gas sensors are inexpensive to fabricate and are highly sensitive [45]. The operating principle is based on the change in the resistance of a metal oxide layer which is placed between two electrodes, as shown in Figure 2.1. Tin oxide is a commonly used metal oxide material in this type of sensor. The metal oxide is heated which results in a depletion region due to adsorption of oxygen on the surface of the metal oxide. The target gas (combustible reducing gas) reacts with the adsorbed oxygen present on the semiconductor surface, changing the free electron concentration on the MOS surface, thus resulting in a change in resistance of the device [46]. The sensitivity of the sensor is directly dependent on the surface area of the exposed metal oxide.

Most MOS sensors require high temperature to reduce the effect of humidity and to attain high sensitivity; therefore, they are attached to heating mechanisms such as membrane heaters or micro-hotplates. Although MOS sensors feature high sensitivity, their recovery following exposure to gas is slow. Thus they are not the right choice for rapidly changing gas concentrations [21]. After repeated use at high temperatures, the reactive surface was found to degrade, thus decreasing the sensitivity and precision over a period of time.

Figure 2.1 Typical assembly of MOS sensor sensor

2.1.2 Polymer Sensors

Polymer-based sensors exhibit a change in electrical conductivity with gas exposure, similar in behavior to MOS sensors. They are often used to detect volatile organic compounds that can't be identified using MOS sensors [47]. While the conductivity of pure polymers is low, the electrical conductivity of specialized polymers such as polypyrrole (PPy), polyaniline (PAni) and polythiophene (PTh) are known to be affected when they are exposed to certain gases. The operating temperature of polymer based sensors is around room temperature as compared to MOS based sensors that need a high temperature for detection.

2.1.3 Chromatography

Gas chromatography is another technology that is a typical laboratory setup where the separation between different constituents of gases is required. This technique is highly sensitive as well as selective [48]. While portable systems are available, this approach is impractical for compact, low cost, mobile applications.

2.1.4 Calorimetry

Calorimetry is also widely used for gas sensing. This approach is normally used for combustible gases or gases that have a significant difference in thermal conductivity relative to air. The procedure involves heating of the sample gas. As the gas heats up, it undergoes combustion, resulting in additional heat. The change in temperature is detected and attributed to different gases, using pre-calculated/pre-tested available data [49]. A standard implementation for this technique is the use of pellistor, which is a catalyst-loaded ceramic bead whose resistance changes in response to

temperature changes initiated by burning of the target gas at the device surface [50].

A drawback of calorimetry based gas sensing is catalyst poisoning that can take place due to various impurities present in the target gas. These impurities result in reduction of sensitivity as well as catalytic reaction of the gas with the catalyst.

2.1.5 Optical Gas Sensing

Optical gas sensors are based on spectroscopy. Their use is generally straight forward compared to other techniques. They are more sensitive, selective, stable, and repeatable as compared to other sensing techniques. They also exhibit long life and consistent performance after multiple uses. They have a fast response time, which makes them ideal for real-time gas sensing [21][51].

A considerable amount of work has been done on non-dispersive infrared sensing (NDIR) [21]. These sensors work on the principle of narrow-band infrared (IR) emission and molecular absorption spectroscopy [52]. Figure 2.2 shows the operating principle of a primary NDIR sensor. The source is a narrow-band emitter, emitting a specific wavelength that is strongly absorbed by the target gas. The light passes through a sample volume of gas, and the signal attenuation due to absorption is proportional to the concentration of the target gas.

Figure 2.2 Operating principle of an NDIR sensor

Even though sensors based on optical techniques have high sensitivity and repeatability, their use isn't as widespread as other gas sensing techniques due to system complexity and component cost. A simple, efficient and low cost light source has the potential to open new markets for optical gas

sensors.

2.2 Mid-IR Sources

An emitter is a key component of an optical sensing system. The choice of source for optical gas sensing systems depends on its emission characteristics, cost, size and power consumption. Mid-IR sources include narrowband band sources such as Quantum Cascade Lasers (QCL) and Interband Cascade Lasers (ICL) as well as broadband sources such as globars and MEMS microhotplates.

2.2.1 Quantum Cascade Lasers

Lasers are often used as sources for optical gas sensing systems when high output intensity is required and cost and operating conditions are not constrained. CO₂ based lasers have been widely used, but they are limited in terms of their emission bandwidth 27 THz - 33 THz (9 μ m - 11 μ m) as well as size [53]. Quantum Cascade Lasers (QCL) are becoming a well established source to produce mid-IR emission [54] [55] [56] [57]. A QCL has periodic layers of semiconductor materials which form multiple quantum energy wells (MQW) resulting in confinement of electrons to specific energy states. The MQW structure results in splitting of the permitted band of energies into discrete subbands. Electrons injected into the active region of the laser undergo a series of radiative transitions as they traverse the periodic structure. The layer thicknesses are engineered to create population inversion within these layers. The frequency of the emitted photons is dependent on the layer thicknesses rather than the material bandgap.

Commonly available QCL systems based on InGaAs/AlInAs and GaAs/AlGaAs produce emission limited to the range of 65 THz - 100 THz (3 μ m - 4.5 μ m) [53]. Various QCL materials have been explored to overcome the existing shortcomings, but they are still in a testing stage [53]. Moreover, the power consumption and fabrication cost of QCL laser sources is relatively high; this limits their use in low cost and portable sensor applications [58].

2.2.2 Interband Cascade Lasers

Interband Cascade Lasers (ICL) have been realized [59] [60] [61] and are now becoming commonly available. Like QCL's they use bandstructure engineering to emit multiple photons from each injected electron. However the photons are generated from interband transitions rather than intrasubband transitions used in QCL's. The longer lifetime of the excited states in ICL's enables population inversion and lasing to occur at lower electrical input powers than with QCL's. ICL's have been demonstrated in the range of 40 THz - 100 THz, however, they are highly sensitive to

operating temperature [53]. Due to high power density in operation, the active region heats up affecting the performance [53]. Moreover, like QCL's they have a relatively high cost of fabrication.

2.2.3 Globar, Microhotplate

A simple Globar (heated SiC rod) can reliably produce emission in the mid-IR range [62]. Sources based on thermal emission have been widely reported in the mid-IR region. Thermal emission in the temperature range of 200°K - 1000°K produces natural black body radiation which falls in the mid-IR range. A low thermal loss platform such as a MEMS micro-hotplate can be used as a source in the mid-IR while operating at low power. However, this is broad-band emission and high-Q narrow-band filters are required to convert the broad-band into a narrow-band source. The emitted power outside the frequency bands of interest is lost, reducing the source efficiency.

The emission spectrum from such a platform can be engineered into a narrow bandwidth by controlling temperature and fabricating unique physical features on the surface of the emitter. The following section describes the background and building blocks required to convert a broad-band thermal emitter into a narrow-band emitter.

2.3 Thermal Emission

Thermal emission is spontaneous emission of photons due to thermal motion of charges, and increasing temperature increases the energy and number of photons resulting in higher emission intensity. This is referred to as blackbody radiation, as described by Planck in 1900. Kirchoff's law of thermal radiation for black bodies states that "For a body of any arbitrary material emitting and absorbing thermal electromagnetic radiation at every wavelength in thermodynamic equilibrium, the ratio of its emissive power to its dimensionless coefficient of absorption is equal to a universal function only of radiative wavelength and temperature. That universal function describes the perfect blackbody emissive power"[63]. Absorption for different structures is calculated by measuring reflection and transmission, and by applying Kirchoff's law, "absorbance at a specific wavelength = emission at the same wavelength."

Materials that absorb all the wavelengths that are incident upon them are known as blackbodies or perfect absorbers. Very few naturally existing materials can be approximated to perfect absorbers. In 1900 Max Planck demonstrated that the irradiance from a body is directly dependent on its temperature. He also determined that materials at the same temperature will have the same brightness, irrespective of their chemical composition. According to Planck, blackbody radiation is described by;

$$B_{\lambda}(\lambda, T) = \frac{2 \cdot h \cdot c^2}{\lambda^5} \cdot \frac{1}{e^{\frac{h \cdot c}{\lambda \cdot \kappa \cdot T}} - 1}$$

where

B = spectral irradiance at each wavelength ' λ '

λ = wavelength of interest

h = Planck's constant

c = speed of light in vacuum

κ = Boltzmann's constant

T = absolute temperature of the body

Elevated body temperature will result in higher emission at all the wavelengths. As the temperature of the body increases the center peak wavelength (wavelength with the maximum emissivity) also becomes shorter. Wein's displacement law can be used to characterize the peak wavelength at a specific temperature:

$$\lambda_{max} = \frac{2898}{T} \cdot \mu\text{m.K}$$

Where 2898 $\mu\text{m.K}$ is a constant and T is the absolute temperature of the device. Figure 2.3 shows radiation intensity vs wavelength of a black body at different temperatures.

2.4 Broadband Emitters

Natural thermal emission from a material as described in the previous section covers a broad spectrum. Typical globars and microhotplates are broad-band thermal emitters. A thermal emitter based on a microhotplate can be fabricated by using CMOS compatible processes. The specific case of a thin structure supported at two ends is sometimes referred to as a microbridge. The suspended heating element can be designed to attain a high temperature with low input power due to small thermal conduction losses through the support arms [64] [65]. In addition, the small volume and low heat capacity of the structure can enable rapid temperature modulation which can be very useful for sensing applications. Use of a CMOS compatible microfabrication process enables integration of additional features [66]. Of particular interest in this work, the surface of the micro hotplate can be enhanced by addition of frequency-selective structures, enabling the inherent broad-band thermal emission to be converted to narrow-band emission.

Figure 2.3 Radiation intensity versus wavelength of a black body[1]

2.5 Tailoring the Emission Spectrum

There are several techniques that can be used to control the features of the emission spectrum. A simple technique is to place an IR filter in front of a broad-band source (or at the detector in a sensor) in order to pass only the desired frequency. In most configurations the energy at all frequencies in the filter's stopband is lost, thus lowering the efficiency. A related approach is to integrate the IR filter directly on the emitter surface using multiple layers of high index contrast materials, however the process of integrating these layers with a hotplate structure is relatively complex. Another possible technique to control emission is to fabricate frequency selective periodic resonant structures on the surface of the source. This should enhance emission at specific frequencies and increase the efficiency of the emitter, while adding only a few layers to the process. The following sections examine these techniques in more detail.

2.5.1 Quality Factor (Q-factor)

A good narrowband thermal emitter must have a high Quality factor (Q-factor). Q-factor is a dimensionless parameter which depends on the strength of the damping in an oscillating system. There are various methods to obtain the Q-factor. One approach is the comparison of the center

frequency of a system with the bandwidth of the system at FWHM (full width half maximum) as shown;

$$Q = \frac{f_r}{\Delta f}$$

where Δf = bandwidth at FWHM and, f_r is the resonant frequency. Another alternative way to define Q-Factor is in terms of energy:

$$Q = 2.\pi. \frac{\text{energy stored}}{\text{energy dissipated per cycle}}$$

The energy-based equation tells us that a high Q-factor can be achieved by using material with low losses. A high Q-factor is thus used as a figure-of-merit for the effectiveness of a narrow-band thermal emitter.

2.5.2 2D Metamaterials (Metasurfaces)

Metamaterials are composites of different materials that are engineered to provide properties that are not exhibited by those materials naturally. These properties derive from the combination of physical properties and the spatial alignments of these materials. Metasurfaces are dimensional reduction of volumetric metamaterials and are composed of 2D periodic arrangement of sub-wavelength resonating structures made up of metals and dielectrics.

The working principle of the metasurface can be explained using established optical laws. As a plane wave traveling in a medium with refractive n_1 is incident at the boundary of materials with refractive index n_2 , part of it is transmitted (refracted) and part is reflected as shown in Figure 2.4. The reflection and transmission coefficients are dependent on the continuity of field components at the interface, and can be determined by Snell's law and the Fresnel equations. Introduction of an array of resonators at the interface will considerably change the boundary conditions resulting in the change in response of the surface. Incident electromagnetic waves are locally coupled to the surface to produce resonance at specific frequencies, and produce a desired macroscopic response [67]. The reflected and transmitted plane wave can have a phase variation that can vary from $-\pi$ to π depending on the wavelength of the incident wave and the periodicity of the resonators [68]. These changes in phase can be uniform or vary along the surface containing resonators, and can result in controlled propagation of the plane wave.

Optical surfaces and materials can be engineered to produce unique amplitude, phase, and polarization behavior of the incident light to generate a desired scattering response, which makes them an ideal platform for manipulating electromagnetic propagation [69] [70]. These unique proper-

ties of metasurfaces can be also used to control emissivity of surfaces where the sub-wavelength resonating structures act as narrow-band sources of light.

Figure 2.4 Plane wave incidence, transmission and reflection at homogenous boundary

A structure closely related to EM metasurfaces is a Frequency Selective Surface (FSS), which as the name suggests is used to select specific frequencies for perfect transmission, reflection or absorption. Frequency selectivity can be achieved by placing periodic resonant structures on a surface. To create an absorbing surface, lossy material can be incorporated in the periodic structures. Some typical applications of FSSs include reshaping of beams, stealth technology in aircraft, and frequency selective transmit antennas. 2D metasurfaces can thus be seen as a functional extension of FSSs, where more complex wave transformations and manipulations are possible. These might include signal re-direction or polarization control by introducing a diffraction grating or through guided mode resonances. A properly designed FSS on the surface of a broad-band thermal source can produce high Q-factor frequency selective emission. FSSs are typically periodic in nature as opposed to generally non-uniform array of particles in metasurfaces. Since in this work, the focus is on the uniformly periodic configurations, the resulting structures will be referred to as metasurfaces or FSSs, interchangeably.

2.5.3 Conductor Backed Frequency Selective Structure

One simple approach to achieve frequency selectivity is to use a two-layered cavity commonly known as a Salisbury screen. This structure has been conventionally used for absorbing specific

wavelengths while reflecting all the others. One layer is a thin ground plane that will reflect all the incoming plane waves incident on it. The second layer is made up of low loss dielectric. The third layer is a very thin conducting sheet. As an incoming wave is normally incident on the thin conducting sheet, part of it is reflected while part of it is transmitted into the lossless dielectric. The wave that goes into the low loss dielectric is reflected back from the ground plane. If the optical thickness of the low loss dielectric is $\approx \lambda/4$, there will be a 180° phase difference between the reflected wave and the wave that propagates in the low loss dielectric. This will result in a destructive interference between the two waves. This structure together acts as a Fabry-Perot cavity, as shown in Figure 2.5. Resonance occurs resulting in the reflection of all the frequencies except the resonant frequency [71], which is completely absorbed in the structure. While this is a simple technique, the frequency selectivity measured in terms of the Q-factor it not high.

Figure 2.5 Salisbury Screen, acting as a Fabry-Perot resonator, consisting of a cavity formed of a lossy media and a perfectly reflecting plane separated by $\approx \lambda/4$.

A large frequency selectivity can be achieved using the principle of Fig. 2.5 by fabricating alternating layers of high contrast materials, forming a thin film filter. The number of layers and their thicknesses can be modified to achieve sharp resonance at a specific design frequency. To obtain a narrow absorption band around the desired resonant frequency, the number of alternating layers can be increased. Although this is conceptually a simple technique to achieve high Q-factors, typically > 100 , the fabrication process can be challenging as thickness and stress of each layer must be accurately controlled for a large number of layers [72].

2.6 Review of Existing Narrow-band Thermal Emitters

A number of structures have been reported to produce narrow-band thermal emission. Many features of these devices have been reported, including Q-factor, power efficiency, emissivities approaching blackbody, ease and cost of fabrication, and CMOS compatibility. The majority of devices reported are based on plasmonic structures or all-dielectric structures. The following sections describe reported designs and their performance claims.

2.6.1 Plasmonic IR Emitters

Recently significant research work has focused on devising narrow-band thermal emitters based on plasmonic structures, also referred to as plasmonic metamaterials. In these structures, sub-wavelength metallic patterns are fabricated on top of a host dielectric. A plasmonic effect is produced due to the interaction of electromagnetic waves at the metal-dielectric interface, where the incident wave is coupled to electron oscillations and travels along the metal-dielectric interface. The optical resonances that are excited can be selected by carefully engineering the dimensions of the structure. Reported plasmonic structures include sub-wavelength gratings and resonator arrays.

Plasmonic effects have been exploited for a variety of applications, and have measured different quantities to predict emission and Q-factor. Some groups have measured the system absorbance and equated it with emissivity following Kirchoff's law. Others have directly measured the emissivity using FTIR spectroscopy.

Ikeda et al [73] fabricated 100 nm wide and 1000 nm deep Gold gratings. They achieved a polarized thermal emission in the range of $2.2\ \mu\text{m}$ - $5.5\ \mu\text{m}$ with emissivity values up to 94% of the black body for an angle of 5 degrees. They reported a Q-factor of around 4-7. Another group, Mason et al [2] reported periodic gold gratings on spin-on-glass as shown in Figure. 2.6 . They heated their device up to 160°C and reported a near unity emissivity at around $7.5\ \mu\text{m}$ with a Q-factor of about 4.

Various groups have reported metallic resonators instead of gratings on the dielectric. For example, Marquier et al [3] have proposed a plasmonic structure to achieve high thermal emission efficiencies. They simulated a 100 nm rectangular patch as the plasmonic unit cell made on top of a conductor-backed Silicon Nitride (SiN) as the dielectric, as shown in Figure 2.7. They achieved an absorption of 95% at a wavelength of $4.25\ \mu\text{m}$ for small angles.

Further, the same authors later reported a similar configuration but with platinum as the patch and tungsten as the substrate [74]. Due to the high melting point of tungsten and platinum, they were able to heat their structure to a temperature of 873°K . They measured the emissivity and found it to be in good agreement with their theoretical absorbance calculations. They reported a Q-factor of

Figure 2.6 Au gratings on spin-on-glass (SOG) [2].

Figure 2.7 Schematic of the rectangular patch shaped plasmonic unit cell on top of SiN layer backed by a Gold [3].

6.5 for a wavelength of $4.18\mu\text{m}$ and maximum thermal efficiency of 85% at an angle of 25° . Zhou et al [4] also reported similar plasmonic structures as Marquier et al [74]. They also used a variety of metallic nano-structure shaped antennas on top of a ground plane separated by a dielectric, as shown in Figure 2.8. All the structures have been designed for a wavelength of $4\mu\text{m}$. They reported a detailed analysis of these unit cells based on various geometrical parameters. The highest Q-factor that they have demonstrated from their different designs was approximately 8.

Chan et al further proposed methodical designs of metallic 2D photonic crystals for narrow-band thermal emission [75]. They outlined steps, performed numerical calculations, and reported that the periodicity of the metallic photonic crystals plays an essential role in determining the resonant wavelength, diffraction peaks, and surface plasmon modes. They compared the emissivity of a perfect black body, with a tungsten slab and a structure made up of tungsten photonic crystal in

Figure 2.8 Various geometrical shapes of conventional plasmonic thermal emitters such as patch, cross, hole and complementary bowtie aperture [4].

a range of 1000°K - 1200°K . The emissivity of the tungsten-based photonic crystal, was around 80 % of that of a black body around $2.9\ \mu\text{m}$, which was much higher than that of a uniform tungsten slab. Moreover, they also reported that their emissivity increased by a factor of 2.1 as they heated their structure from 1000°K to 1200°K . Similar works, such as by Alexander et al reported a CMOS compatible cross like metal-based thermal emitter in [5]. They fabricated a complete thermal system which acts as a narrow-band thermal emitter when heated. They fabricated an array of cross-like structures of copper on top of a metal-backed Alumina. These cross type structures have the same dimension in x - and y -direction, resulting in an unpolarized emission. The Q-Factor reported by them is 15.7 at the resonant wavelength of $3.96\ \mu\text{m}$, which they claim is higher than that of other metal-based thermal emitters due to an optimized resonator geometry. Moreover, their emissivity is close to 99 %. Their simulations show that the significant energy dissipation takes place in the top metallic crosses in the structure. Thus the Q-factor of the structure is dependent on the metal loss characteristics. Figure 2.9 shows the basic structure of the plasmonic cell. Based on the literature review, the design reported by Alexander et al. [5] has the highest Q-Factor of 15.7 for a metal-based emitter.

Figure 2.9 Physical structure of plasmonic/metallic thermal emitter structure and the unit cell configuration proposed in [5].

2.6.2 Dielectric Thermal Emitters

While plasmonic thermal emitters provide compact and sub-wavelength thermal emitting structures, they exhibit low Q-factors due to high metallic losses. Recently, novel all-dielectric resonating structures have been proposed in the context of high-performance metasurface structures, for advanced wave control, due to their low-loss characteristics [76] [77] [78]. Various research directions have been explored with all-dielectric structures for a variety of objectives, and are typically based on Multiple Quantum Well (MQW) and photonic crystals.

Zoysa et al proposed layered MQWs as narrowband thermal emitters with high Q-factors [6]. They claimed to recycle energy from all the unwanted wavelengths to the desired resonant wavelength. The quantum wells of GaAs are sandwiched between two layers of AlGaAs. Reported emissivity was 30% of the black body when the structure was heated to 373°K, as shown in Figure 2.10(a), and Q-factor was around 12.5. Furthermore, by combining the MQWs with photonic crystal concepts, they increased the emissivity from 30% to 80%. They were also able to heat their device to a much higher temperature for the same amount of input power, as shown in Figure 2.10(b).

Inoue et al [7] further proposed a MQW structure with an intricate square lattice of circular disks of two different diameters. The structure was heated to around 473 °K and a Q-factor of 107 at a wavelength of 9.1 μm was found. An emissivity of around 40 % of the blackbody radiation at 473 °K was reported. The MQW was fabricated by depositing 128 alternating thin layers of GaAs and AlGaAs. Figure 2.11 shows the two MQW structures that they fabricated and tested. While the MQW structures achieve high Q-factors, they are relatively complex to fabricate due to large number of dielectric layers required.

Figure 2.10 Thermal emission spectra of a MQW wafer at 373°K for different polarizations shown in (a), [6] and MQW combined with PhC that has a higher emission for the same amount of input power (b).

Asano et al [8] have also demonstrated an improvement in the efficiency of a thermal emitter in the wavelength range of around 900 nm by fabricating a photonic crystal structure with doped Silicon nanorods. The resonance due to band gap in the intrinsic Silicon is coupled with the resonance of the photonic crystal configuration of Silicon rods, producing a thermal emission of around 77% of the black body as well as a reduction in the background emission to less than 2%. Figure 2.12 shows the fabricated structure. The radius of the nanorods is 100 nm with a lattice constant of 500 nm.

O'Regan et al [9] reported an all-dielectric structure based on photonic crystals. Holes were etched in doped silicon to create a 2-D photonic crystal on Silicon on Insulator (SOI). The structure was heated by passing a current across their structure using contact pads. The device operated to around 1100°K and achieved a Q-Factor of around 18 at a wavelength of $1.5 \mu\text{m}$. The device can be seen in Figure 2.13.

Gesemann et al [79] also reported a 2D-3D photonic crystal design to achieve narrowband emission. The target wavelength was $9 \mu\text{m}$. Vertical holes were etched to form a triangular lattice on a silicon surface. It was possible to fine-tune the structure towards narrow-band emission by converting the 2D photonic crystal structure into a 3D photonic crystal structure. Cardador et al [80] reported 3D photonic crystal structures on amorphous silicon that could be used as a filter to filter a broad-band emitter to achieve narrow-band emission. Transmission of the desired wavelength ($4.6 \mu\text{m}$) was increased from 4% - 6% to 25% - 30% by reducing the thickness of the substrate by $160 \mu\text{m}$.

Figure 2.11 All-dielectric MQW structures as proposed by Zoysa and Inoue et al [7].

Figure 2.12 Silicon nanorods based photonic crystal structure [8].

Metamaterial based all-dielectric thermal structures are compact compared to structures based on photonic crystals due to their subwavelength dimensions [81]. Cole et al [82] reported a metasurface that comprises cylindrical structures of sub-wavelength sizes. Different materials were compared including, Silicon, GaSe, and Quartz for tuning of their structure. These structures were fabricated on a low-index medium. The aspect ratio of the cylinders was varied to match the electric and magnetic resonances of the structure and the structure was simulated to have an absorption of 99.5%, for a range of $200 \mu\text{m}$ - $1000 \mu\text{m}$ for use as a detector.

Liu et al [83] also reported metasurface absorbers. Simulated and fabricated cylindrical pucks of silicon on a dielectric showed strong absorption around 97% around their wavelength of interest ($285 \mu\text{m}$). The device could be used for thermal imaging techniques as well as sensing applications. Liu et al [84] also proposed an all-dielectric structure that could be used as a near perfect broadband reflector. A cross type structure of silicon on top of Silicon Dioxide was fabricated. The

Figure 2.13 Schematic of the thermal emitter using 2-D photonic crystals [9]

structure provided 97% reflection in the desired range of $1.3 \mu\text{m} - 1.5 \mu\text{m}$. Finally, Arbabi et al [85] reported a metasurface with cylindrical silicon pucks to control the polarization and phase of emission. The structure had variable sizes of silicon pucks on top of Silicon Dioxide, whereby manipulating the geometry and dimensions of the silicon pucks on the surface allowed control of polarization and phase.

Tab. 2.2 shows a comparison of all-dielectric structures, with their materials, design objective and measured performances. While the highest Q-factor reported for a plasmonic-based cell (relatively simple fabrication) was around 15.7, the highest Q-factor reported for an all-dielectric structure was about 100 (complex fabrication). All-dielectric structures offers much higher Q-factor, thanks to their low-loss characteristics which makes then an attractive candidate for generating narrowband thermal emission.

2.6.3 Proposed All-Dielectric Metasurface Frequency Selective Structure

While MQW based all-dielectric structures have been tested to produce a high Q-factor, the multi-layered structure is complex to fabricate and hence costly. On the other hand, some of the reported plasmonic structures have a simple fabrication process and have been proven to be CMOS compatible, but they have been tested to show a low Q-factor due to high losses in metal. This thesis undertakes a balanced approach between fabrication complexity and achieving relatively high Q-factors. Here we propose a conductor backed FSS formed using a low-loss dielectric resonator

(thus only two dielectric layers), consisting of a high permittivity Silicon resonator fabricated on top of low permittivity Silicon Dioxide, for instance, as shown in Figure 2.14. This structure uses common CMOS materials and can be fabricated by standard CMOS fabrication processing techniques. It will be shown that such a simple configuration is theoretically capable of achieving high Q-factors compared to MQW structures in spite of its simplicity.

Figure 2.14 Proposed all-dielectric metasurface thermal emitter consisting of a high permittivity Si resonator on top of a low permittivity SiO_2 host, backed by a metallic layer a) Periodic Silicon resonators, b) Single unit cell as simulated in HFSS

Table 2.1 Plasmonic Structures Comparison

Ref	Type	Structure	Lattice	Material	Wavelength	Claim	Measurement
[3]	Plasmonic	Gold patch on Gold substrate, SiN as di-electric	Square patch with a periodicity of $3\mu\text{m}$	Gold, SiN	$4.25\mu\text{m}$	Absorbance of 95% at $4.25\mu\text{m}$	Simulation
[74]	Plasmonic	Platinum patch on Tungsten substrate	Square patch with a periodicity of $3\mu\text{m}$	Tungsten, SiN, Platinum	$9.1\mu\text{m}$	$Q - F = 9.5$	Theoretical absorption
[4]	Plasmonic	Gold 4 designs on Silica and Al_2O_3	patch, cross, circular slit, bowtie	Gold-Silica/ Alumina	$4\mu\text{m}$	$Q - F = 8$	
[75]	Plasmonic	Tungsten photonic crystal	Circular Phc with a period of $3\mu\text{m}$	Tungsten	$2.9\mu\text{m}$	PHc has a higher emissivity than normal slab	Thermal Emission
[5]	Plasmonic	Copper resonator on top of copper ground plane	Copper cross- periodicity of $2.2\mu\text{m}$	Copper, Al_2O_3	$3.96\mu\text{m}$	$Q - F = 15.7$ Emissivity of 99%	Thermal Emission

Table 2.2 All-Dielectric (A-D) Structures Comparison

Ref	Type	Structure	Lattice	Material	Wavelength	Claim	Measurement
[6]	(A-D)	Multiple Quantum Well	Triangular lattice circular holes	GaAs-AlGaAs	10 μ m	Peak Emissivity 30% to 80% Q-F=12.5	Emission
[7]	(A-D)	Multiple Quantum Well	Photonic Crystal layered pucks	GaAs-AlGaAs	9.1 μ m	Q-F=107	Theoretical absorption
[9]	(A-D)	Silicon-Phc	2D square array of holes	doped-Si-SOI	1.5 μ m	Q-F=18 @ 1100K	Emission
[82]	(A-D)	Silicon-Phc	Cylinder-Sub Wavelength-PhC	Si-GaSe-Quartz	200 μ m-1000 μ m (0.3THz-1.9THz)	99% absorption in the bandwidth	Absorption
[79]	(A-D)	Silicon-Phc	2D-3D PhC heated resistively and passively	Si	9 μ m	Study of Thermal emission of 2D and 3D PhC	Emission
[80]	(A-D)	PhC-Macroporous Silicon	3D photonic crystals	Macroporous Silicon	4.6 μ m	Transmission increased from 6% to 29% going from 2D to 3D PhC for filtering	Transmission
[85]	(A-D)	Meta Surface	multi sized Si pucks on a single surface	Si	0.9 μ m	Polarization/ phase control	Transmission
[86]	(A-D)	SiC antenna meta-surfaces on Si	SiC antennas on Si post	Si-SiC	10 μ m - 12 μ m	50% of black body	Emission
[83]	(A-D)	Silicon on Silica	Si pucks on SOI	Si-SOI	250 μ m-500 μ m	97% absorbance	Absorbance
[84]	(A-D)	Silicon on Silica	Si cross on Silica	Si on SiO_2	1.3 μ m-1.5 μ m	98 % Broadband Reflectance	Reflection

Chapter 3 Proposed All-Dielectric Metasurface Thermal Emitters

Based on the literature review, two main configurations have been reported for thermal emitters. These configurations are either based on plasmonic structures or all-dielectric structures. Due to lower losses, dielectric based structures can produce a higher Q-factor emission. Some dielectric structures have been proposed incorporating complex multi-layered Multiple Quantum Well (MQW) structures. While the MQW structures have been shown to produce a Q-factor of about 100, their fabrication is complex and challenging as it involves deposition of 128 alternating layers of GaAs and AlGaAs. This research proposes a dielectric based metasurface structure for thermal emitter that has a Q-factor higher than that of the plasmonic devices, while remaining simple to fabricate. Silicon is known to be transparent in the mid-IR region upto $8\text{ }\mu\text{m}$ [87] [88]. Silicon has been used here as the dielectric resonator with silicon dioxide as the low permittivity host.

This chapter begins with the design and simulation of a thermal emitter based on a plasmonic structure. To show variation and control of the design of resonant structures, thermal emission at resonant frequencies of 74.65 THz ($\approx 4.05\text{ }\mu\text{m}$) and 41.5 THz ($\approx 7.2\text{ }\mu\text{m}$) have been simulated, which correspond to the absorption spectra of CO_2 and SO_2 respectively. As Q-factor is directly dependent on losses in the material, this chapter also describes through simulation the electromagnetic loss mechanism in dielectric structures. Finally, the design, simulation and analytical results of the proposed all-dielectric metasurface structure along with their characteristics are discussed.

3.1 Simulation Setup

The proposed metasurface was simulated using Ansys high-frequency structure simulator (HFSS) (Ver. 19.2). HFSS uses the finite element method (FEM) for a 3D full wave frequency domain electromagnetic solver. The proposed structure is a metasurface with periodic silicon resonators in both x - and y - direction. A single unit cell was designed in HFSS with a master/slave periodic boundary as shown in Figure 3.1. A layer of copper as a ground plane was created inside an air box. Silicon dioxide was used as a low loss dielectric and a silicon resonator on top of the silicon dioxide was designed within the air box of the unit cell. A Floquet port was used to launch a normally incident plane wave towards the conductor backed resonator. Floquet ports are a unique feature in HFSS that are exclusively used for periodic structures.

Figure 3.1 Unit cell simulation setup in HFSS

Figure 3.2 shows the typical solution frequency and the frequency sweep setup used in HFSS. The adaptive solution frequency was setup as 100 THz. This frequency is typically greater than or equal to the highest simulation frequency for the analysis. The number of passes was set as '12' and 'Delta S' was set as 0.001. The value for 'Delta S', the maximum change in S parameter magnitude between passes, was determined after successive frequency simulation. It was found that 12 passes gave consistent convergence for the simulation. The setup was done for a discrete frequency sweep from 40 THz to 100 THz. As the expected Q-factor was high, a step size of 0.01 THz was chosen, which ended up creating 7001 discrete frequency sweep points. Due to system limitations the sweep was done in 3 portions of 40 THz - 60 THz, 60 THz - 80 THz and 80 THz - 100 THz. The floquet port de-embed distance was set at 10 μm , which was more than the designed resonant wavelength for far-field results. S-parameters were used to determine the reflection and transmission coefficients. As the proposed structure was backed by a ground plane, only S_{11} (reflection) values were extracted to predict emissivity.

3.1.1 Determination of Thermal Emission by Simulation

The mid-infrared range for this work was from 3 μm - 7.5 μm , which corresponds to 40 THz (7.5 μm) - 100 THz (3 μm). During the design stage, the thermal emission of the proposed narrowband emitter was determined by Kirchoff's law of thermal emission. According to Kirchoff's law, for a body that is in thermal equilibrium, thermal emission at a given wavelength is the same as absorption at that wavelength, as given in the following equation:

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

Figure 3.2 Simulation and convergence setup used in Ansys FEM-HFSS.

Where,

$A(\omega)$ is spectral absorption,

$\mathcal{E}(\omega)$ is spectral emission,

$T(\omega)$ is spectral transmission and

$R(\omega)$ is spectral reflection across the structure.

The proposed structure has a metallic base that acts as a ground plane, hence $|T(\omega)| = 0$, and the emissivity expression reduces to $\mathcal{E}(\omega) = 1 - |R(\omega)|^2$. Therefore the structure should reflect all the incoming incident energy at all frequencies except the resonant frequency. Hence emissivity can be determined by determining the reflection coefficient. The reflection coefficient was extracted by S-parameters (S_{11}) using the floquet ports in HFSS.

3.1.2 Frequency Dependent Optical Constants

In the mid-IR high frequency region the permittivity of metals and dielectrics are dependent on frequency. A mid-IR drude model for copper was found in the literature [89] and was used for simulations as shown in (3.1a). The optical constants for silicon dioxide were available for material deposition done by a sputtering process [90] and (3.1b) were used to plot the frequency dependent data. No data for silicon was available in the mid-IR region. A Lorentz-Drude model for silicon was

available for the near-IR region [91], and this model was used to extrapolate the optical constants in the mid-IR region as shown in (3.1c). The frequency dependent models shown in (3.1a), (3.1b), (3.1c) are reported here in the same format as published in the literature, hence they have different units as shown. In the earlier stages of the project, the data available in literature was used to study the frequency dependent response of the metasurface in the mid-IR region.

$$\text{Cu: } \epsilon_r(\omega) = 1 - \frac{\Omega_p^2}{\omega(\omega - j\Gamma_0)} + \sum_{n=1}^m \frac{f_n \omega_p^2}{(\omega_n^2 - \omega^2) + j\omega\Gamma_n} \quad (3.1a)$$

$$\text{Silica: } \epsilon_r(\omega) = \epsilon_\infty + \sum_{n=1}^m \frac{\nu_{pn}^2}{(\nu_{0n}^2 - \nu^2) - j\nu_{\tau n}\nu} \quad (3.1b)$$

$$\text{Silicon: } \epsilon_r(\omega) = \epsilon_\infty + \sum_{n=1}^m \frac{\Delta\epsilon(\omega_n^2 - j\gamma'_n\omega)}{(\omega_n^2 - \omega^2) - 2j\omega\gamma_n}, \quad (3.1c)$$

The values of variables were taken directly from the literature and are shown in table 3.1. Exact frequency dependent material parameters were extracted for the materials that were used in the fabrication of this project using other deposition techniques. More discussion on frequency dependent Drude and Lorentz models will be done in Chapter 4.

Table 3.1 Material Parameters for Frequency Dependent Optical Constants

<p>Copper (3.1a), [89], $\Omega_p = 10.83\hbar \text{ eV}$, $\omega_p = 16.45 \text{ rad/s}$</p> <hr/> <p>$f_n \in [0.575, 0.061, 0.104, 0.723, 0.638]$</p> <p>$\Gamma_n \in [0.030, 0.378, 1.056, 3.213, 4.305]\hbar \text{ eV}$</p> <p>$\omega_n \in [0.000, 0.291, 2.957, 5.300, 11.18]\hbar \text{ eV}$</p> <hr/>
<p>Silica (3.1b), [90], $\epsilon_\infty = 2.09$</p> <hr/> <p>$\nu_0 \in [1046, 1167, 1058, 798] \text{ cm}^{-1}$</p> <p>$\nu_p \in [575, 288, 459, 415] \text{ cm}^{-1}$</p> <p>$\nu_\tau \in [1.55, 0.51, 10.57, 55.30] \text{ cm}^{-1}$</p> <hr/>
<p>Silicon (3.1c), [91], $\epsilon_\infty = 1$</p> <hr/> <p>$\Delta\epsilon \in [8.93, 1.855]$, $\omega_n \in [3.42, 2.72] \mu\text{m}^{-1}$</p> <p>$\gamma_n \in [0.425, 0.123] \mu\text{m}^{-1}$, $\gamma'_n \in [0.087, 2.678] \mu\text{m}^{-1}$</p> <hr/>

3.2 Plasmonic Thermal Emitter

As mentioned in chapter 2, a lossy structure backed by a reflector is a common structure used to achieve resonance. The resonant frequency can be modified by changing the layer thickness. The

resonance is also known to be enhanced further, by placing resonators on top of the ground plane separated by a dielectric. Metallic cross-dipole resonators on top of a ground plane are a common configuration used in RF frequency selective surfaces (FSSs) [71] to achieve strong resonance. Since the resonant energy is confined in the top resonator structure in the configuration, the Q-factor is directly dependent on the loss characteristics of the material of the resonator [5].

Figure 3.3(a) shows a typical plasmonic resonant structure which was designed and simulated to achieve resonances at 41.4 THz and 74.65 THz by varying the structural dimensions. The cross-dipole metallic resonator has been placed on silicon dioxide (which is a low loss dielectric) on top of a metallic layer made up of copper that acts as an infinite ground plane. The cross-shaped structures are known to achieve resonant wavelengths four times the optical length of each side [71]. The structure in Figure 3.3 has a copper cross with a length $\ell = 1 \mu\text{m}$, the thickness of 10 nm, $s = 0.2 \mu\text{m}$, unit cell size is $\Lambda = 1.5 \mu\text{m}$ and the dielectric spacing between the cross and the back reflector is $h_s = 0.25 \mu\text{m}$ to achieve a resonant frequency of 74.65 THz. Unpolarized emission can be achieved if the cross-dipole structure is symmetric along the x - and y -directions as shown in Figure 3.3(b).

The plasmonic cell was simulated using Finite Element Method (FEM) in HFSS using Floquet port with periodic boundary conditions along x - and y - direction. The incident wave is considered to be normal. As the proposed application is in the mid-IR range, frequency-dependent optical properties of the materials have been used in the simulations. Frequency-dependent data in the mid-IR for Silicon dioxide [90] and Copper [89] was used from the literature, as discussed above. The Q-factor (Q) for this emission can be calculated as: $Q = f_0/\Delta f$, where $f_0 = 74.65 \text{ THz}$ is the resonant frequency, $\Delta f = 7.5$ is the Full-Width-Half-Maximum (FWHM), so that $Q \approx 10$. While a slightly larger Q has been reported in the literature for a plasmonic unit cell, the simulated Q-factors are comparable to these reported ones. The dimensions were modified to $\ell = 1.95 \mu\text{m}$, $\Lambda = 2.5 \mu\text{m}$ and $h_s = 0.54 \mu\text{m}$ to achieve a resonance of 41.4 THz (corresponding to SiO_2 absorptions) as shown in Figure 3.3(c). The Q-factor for this emission is found to be approximately 9.

Figure 3.3 Typical plasmonic unit cell emitter based on frequency selective metallic cross structure. a) The unit cell configuration [10]. b) FEM-HFSS simulated emissivity response. The structure dimensions are: $\Lambda = 1.5 \mu\text{m}$, $h_s = 0.25 \mu\text{m}$, $\ell = 1 \mu\text{m}$, $s = 0.2 \mu\text{m}$ and thickness of copper base is $1 \mu\text{m}$ to achieve a resonance at 74.65 THz (corresponding to the CO₂ absorption). c) emissivity response of a plasmonic cell for resonant frequency $f_2 = 41.4$ THz (corresponding to SO₂ absorption).

Significant dissipation of energy takes place in the top resonator, and since metal has high dissipation losses in the mid-IR frequencies, as $Q \propto E_{\text{stored}}/E_{\text{dissipated}}$, Q becomes low. To demonstrate the losses in the plasmonic structure, the emissivity response was re-simulated for resonant $f_1=74.65$ THz, and the top metallic resonator was replaced with a lossless material. Figure 3.4 shows that the emissivity falls from around 1 to below 0.02 for f_1 . This confirmed the hypothesis that the resonant energy is mostly confined in the top metallic resonator.

Figure 3.4 Simulated emissivity response for a lossless metallic resonator

3.3 Proposed All-Dielectric Metasurface Thermal Emitter

This research focuses on design, simulation, and fabrication of a narrowband all-dielectric metasurface thermal emitter. A structure with a cylindrical Silicon resonator on top of a Silicon Dioxide layer with ground plane as the backing structure was designed. Figure 3.5(a) shows the unit cell for the proposed structure, where Λ is the unit cell length, h_{gnd} is the thickness of the ground plane, h_s is the thickness of the host substrate, h_{res} is the height of the resonator and r_{res} is the radius of the resonator. The metasurface was assumed to be periodically repeated in the x- and y- direction

The frequency-dependent optical constant data for Silicon Dioxide and Copper in the mid-IR range was available in the literature and was thus used in all HFSS simulations. However, the data for Silicon in mid-IR was not available in the literature. Some Lorentz-Drude models for Silicon were available for the near-IR range. For this chapter, the near-IR frequency-dependent model was extended to mid-IR, and the extrapolated optical constants were used for simulations in HFSS.

As mentioned earlier, dielectric resonators are better than plasmonic resonators in terms of Q-factor due to their low loss properties. An all-dielectric metasurface structure, as shown in Figure 3.5(a) has been simulated in HFSS to have an emission at a resonant frequency of $f_0 = 74.65$ THz. The dimensions of the structure for this resonance are $\Lambda = 2.75 \mu\text{m}$, $h_s = 1.9 \mu\text{m}$, $r_2 = 0.6 \mu\text{m}$, $h_{Si} = 0.8 \mu\text{m}$. Similar to the simulation of plasmonic structures earlier, this simulation was done using Floquet port periodic boundary conditions. This results in an unpolarized emission, since the cylindrical structure is symmetric in both x - and y - direction, as shown in Figure 3.5(b).

Figure 3.5 All-dielectric unit cell. a) A periodic all-dielectric metasurface unit cell, with a high permittivity resonator on top of low permittivity host substrate, backed by a ground plane. Unpolarized emission response of all-dielectric metasurface unit cell with circular puck unit at a resonant frequency of b) 74.65 THz for possible detection of CO₂ and c) for 41.4 THz for possible detection of SiO₂ (Q-factor of 520). Λ is the unit cell length, h_{gnd} is the thickness of the ground plane, h_s is the thickness of the host substrate, h_{res} is the height of the resonator and r_{res} is the radius of the resonator

The Q-factor (Q) for this emission can be calculated as, $Q = f_0/\Delta f$, where $f_0 = 74.65$ THz is the resonant frequency, $\Delta f = 0.12$ THz is the Full-Width-Half-Maximum (FWHM), so that $Q \approx 600$. Near unity emission is achieved, with a high Q-factor of about 600 for f_0 , primarily due to low loss material properties of Silicon in mid-IR range. A strong concentration of H-field is present in the Silicon resonator as shown in Fig. 3.6 at the resonant wavelength where the overall structure can be assumed to be matched to free space for maximum absorption. To further demonstrate control of resonant frequency, the structure of Figure 3.5(a) was re-designed and re-simulated with modified dimensions to have a new resonant frequency at $f_0=41.4$ THz as shown in Figure 3.5(c).

As expected the simulated Q-factor was high, around 520. It confirms that the dimensions of the unit cell can be modified to achieve a resonant frequency for the detection of the target gas.

Figure 3.6 H-field distribution at the resonant frequency $f_0=74.65$ THz, inside all-dielectric unit cell showing the dominant field concentration inside the dielectric resonator [10].

The circular Silicon resonator can be replaced with an elliptical structure, as shown in Fig. 3.7(a) to produce a polarized thermal emission [85]. As in the previous cases, the structure was simulated with a normal incident plane wave excitation with Floquet port periodic boundary conditions. The structure will emit dominant polarized radiation depending on ellipticity parameter τ , which is the ratio of the minor radius with the major radius. Fig. 3.7(b) shows one example for the case of $\tau = 0.9$, where the structure now operates in two distinct bands emitting narrowband thermal emissions with orthogonal polarizations and negligible cross components. Remarkably, large Q-factors, as well as near unity emissivities, are maintained for both emission bands. The ellipticity parameter can be modified according to emissivity requirements.

Dielectric based resonant structures will have a higher Q-factors than the plasmonic counterparts due to lower losses. A simple unit cell structure was designed and simulated to understand and verify the dissipation loss mechanism. This analysis was done on a small frequency range of interest. Hence both the dielectric materials have been considered frequency-independent for simplicity in

Figure 3.7 Polarized emission: a) All-dielectric metasurface cell structure with elliptical resonator. b) Emission response of an elliptical-cylindrical cell ($\tau = 0.9$) for polarized radiation, in two separate bands. The emission resonant frequency of the two bands are 75.65 THz and 76.65 THz.

simulation, $\epsilon_{r,Si} = 11.85$ and $\epsilon_{r,Silica} = 1.9$. Moreover, the ground plane was replaced by a perfect electric conductor (PEC).

The losses in a material are modeled using imaginary component of the permittivity. For simulation, HFSS requires the real permittivity and the loss tangent ($\tan \delta = \epsilon''/\epsilon'$) (where ϵ'' is the imaginary part of permittivity and ϵ' is the real part of permittivity) to calculate emissivity response. To study the effect of losses on the emissivity and Q-factor, the loss tangent was varied, as shown in Fig. 3.5(a). Simulations show that an increase in losses results in a significant decrease in peak emissivity as well as broadening of the bandwidth at the resonant frequency. Fig. 3.8(b) shows the simulated Q-factors with varying $\tan \delta$. As can be seen from the figure, the Q-factor goes down with an increase in losses. However, the lowest value of Q-factor (due to relatively high losses) was still larger in comparison to a typical plasmonic cell, proving that all-dielectric emitters are expected to perform better than plasmonic emitters in terms of Q-factor.

3.4 Working Principle of the All-Dielectric Structure

Periodic dielectric resonators proposed in this project have been known to exhibit magnetic as well as electric resonances [92]. Assuming a standalone resonator configuration in free space, a Huygen's source configuration is formed as the two resonances become spectrally overlapped. This configuration eliminates any backscattering from the structure, i.e. it is impedance-matched to free-space [82]. Compared to the standalone resonator in free space, the all-dielectric unit cell considered here includes a back-reflecting ground plane.

Figure 3.8 Q-factor characteristics with varying losses

A unit cell has been simulated for a resonant frequency of $f_0 = 74.65$ THz, and Figure 3.9 shows the magnetic and electric field distributions within the structure for a specified polarization. The top row shows a strongly confined magnetic field distribution in the dielectric puck at resonance whereas the electric field has a null at the center of the dielectric puck. Moreover, the electric fields are known to circulate the H-fields, which is a typical behavior of such resonator configurations [5][86].

As the magnetic resonance is confined in the top dielectric puck, this configuration can be further explained with the image theory. The fields can be considered to be a magnetic resonant dipole radiating on top of a perfect reflector (ground plane). According to this theory, the magnetic fields will be optimized for a host substrate thickness $h_{\text{base}} \approx \lambda/2$ [93], while the electric fields will be optimized for $h_{\text{base}} \approx 3\lambda/4$. This fact is further confirmed as can be seen in Figure 3.10(a) where the emissivity becomes maximum when $h_{\text{base}} \approx \lambda/2$, at the resonant frequency of 74.65 THz. Which is due to the magnetic dipole and its image leading to constructive interference at the puck location when the Silicon Dioxide thickness is approximately $1.9\mu\text{m}$.

The emissivity of the resonant frequency is dependant on the angle of incidence. Simulations done so far were for normal incidence condition. Angular dependence of the unit cell was simulated and the emission response of the all-dielectric unit cell is shown in Figure 3.10(b) in the $x - z$ plane with E_y field polarization. The half-power angular range of the absorption is found to be $\approx 16^\circ$ at the resonance frequency, f_1 .

Figure 3.9 E- and H-f distribution at the resonant frequency f_0 of the structure, consisting of a Silicon puck on top of Silicon Dioxide host layer, backed by a ground plane. Results are computed in FEM-HFSS using Floquet periodic boundaries, and fields are shown for y -polarized plane-wave excitation [10].

Figure 3.10 The variation of the emissivity of the all-dielectric unit cell structure of Figure 3.5(b) with a) the height of the host Silicon Dioxide substrate, h_{base} , and b) the angle of incidence. [10].

Figure 3.11 Comparison between the emission spectrum of the plasmonic unit cell of Figure 3.3 and the proposed all-dielectric metasurface unit cell of Figure 3.5 from 50 THz to 100 THz.

3.5 All-Dielectric vs Plasmonic Emitters

Figure 3.11 shows the comparison between the emissivities of the dielectric unit cell with the plasmonic unit cell. While the all-dielectric metasurface cell offers a highly selective emission peak at the desired resonant frequency, it is also accompanied by few extra emission peaks including an additional resonant peak at around 95 THz of similar Q-factor characteristics. The two strong peaks at resonant frequency $f_1 = 74.65$ THz and $f_2 = 95$ THz are due to the concentration of H-Field and E-Field in the Silicon resonator puck and are at a location corresponding to a magnetic and electric dipole on a ground plane as predicted by image theory. This is further verified in Figure 3.12 which shows the concentration of E- and H- fields for the two resonant frequencies.

Figure 3.12 Concentration of E-Fields and H-Fields in the Silicon puck at resonant frequencies of $f_1 = 74.65$ THz and $f_2 = 95$ THz.

There are some additional peaks between the two resonant frequencies. These are due to complex

Figure 3.13 Emission spectrum for thin silicon dioxide layers $h_{\text{base}} = 480$ nm from 50 THz to 100 THz.

interactions of the fundamental and higher-order electric and magnetic dipolar moments associated with the dielectric resonator and the metallic reflector present at the base of the structure. These peaks were successfully removed by reducing the thickness of silicon dioxide to a few hundred nanometers, as shown in Figure 3.13. For this specific structure, reducing the thickness to 480 nm completely removes the additional resonances. For such small thicknesses, the silicon resonator comes very close to the ground plane, and acts as a magnetic dipole placed on top of a ground plane where the dipole and its image radiate with constructive interference.

Figure 3.14(a) shows the emission peak at the designed resonant frequency of 41.45 THz for a structure with a thin layer of silicon dioxide. Figure 3.14(b) shows the concentration of fields in the silicon resonator at the resonant frequency, which appears similar to field concentrations for a structure with a thick layer of silicon dioxide. Figure 3.14(c) shows the Poynting vector simulation in HFSS. It can be seen that the energy flux density has a high magnitude in the top silicon resonator.

3.6 Summary

It has been demonstrated that the significant resonant energy is confined in the top resonator and thus having a resonator made up of a dielectric instead of metal results in a higher Q-factor due to relatively low losses in the dielectric. An all-dielectric metasurface thermal emitter can be made by fabricating high permittivity Silicon pucks on a metallic ground plane, separated by a low permittivity Silicon Dioxide to enhance resonance that results in near-unity emissivity. The resonant

Figure 3.14 Device design for the thermal emission using measured optical constants of Cu, Si and SiO_2 by ellipsometry. a) The emissivity. b) H-Fields at the resonant. c) Poynting vector inside the structure.

frequency of the emission can be manipulated by changing the dimensions of the top resonator along with tuning the Silicon Dioxide thickness. Moreover, polarized emission can be achieved by adjusting the ellipticity parameter of the elliptical resonator.

These simulation results suggest it is worthwhile to fabricate and evaluate the dielectric metasurface emitter structure. However mid-IR optical constants for PECVD silicon and silicon dioxide available in the Carleton University Microfab are required to accurately predict the emitter behavior. Frequency dependent optical constants for both the materials in mid-IR range can be extracted using ellipsometry. In addition, an existing lithographic mask with features close to the requirements of the project was available for use in the micro-fabrication facility. Optical constant measurements and fixed mask geometry were therefore incorporated in a revised design.

Chapter 4 Frequency-Dependent Optical Properties for Materials in the Mid-IR

The all-dielectric metasurface thermal emitter described in this project is designed to operate in the mid-infrared (mid-IR) or terahertz frequency range. To complete the design, the frequency-dependent optical properties for each of the materials: copper, silicon, and silicon dioxide were required. Device design and simulations in chapter 3 were completed using available frequency-dependent data in the literature. Frequency-dependent models for silicon and silicon dioxide have been reported in the literature [90] [91]. While optical property data for silicon dioxide was available in the mid-IR range, no data was found for silicon.

The data reported for silicon dioxide was obtained by depositing thin layers of material using the sputtering deposition technique. The device for this project was fabricated at the Carleton University microfabrication facility, and plasma enhanced chemical vapor deposition (PECVD) was used to deposit both silicon and silicon dioxide layers. To better understand and accurately model the device performance, optical properties for copper, silicon, and silicon dioxide were measured in the frequency range of interest. The fabricated metasurface device was implemented using an existing photolithographic mask with a unit cell of periodicity $6\ \mu\text{m}$ and with a square opening of $3.2\ \mu\text{m}$. The device emission spectrum was re-simulated with these constraints on the geometry.

This chapter begins with a brief discussion of optical dispersion in materials, followed by a description of the key measurement tool, ellipsometry. The measured frequency dependent properties are presented and discussed, with particular attention to features related to the materials and deposition process. The last part of this chapter describes the redesign and re-simulation of the all-dielectric metasurface thermal emitter based on mask constraints and extracted permittivity values.

4.1 Frequency-Dependent Materials: Lorentz & Drude Oscillator Model

Electrons in a material in an electromagnetic equilibrium state are considered to form a symmetric cloud around the nucleus. As an electric field is applied, the positively charged nucleus is pushed in one direction while the electron cloud in the other direction. This movement of charges creates a variation in the fields in the vicinity of the charge resulting in a dipole moment. At low frequencies of changing electrical fields, the material properties can be approximated to a constant value as the change in the field is very slow, but at high frequencies due to continuous back and forth oscillation of electrons, material properties become a function of frequency.

The application of electric fields and the inherent restoring force on the atoms can be modeled as a mass-spring-damper system. This model can be applied to metals as well as dielectrics. The

Lorentz model describes the motion and response of dielectrics to fast-changing fields [94] while the Drude model describes the response of metals to the changing dipole moments [95]. However, some materials are described by a combined Lorentz-Drude model (LD model).

The Lorentz oscillator model describes the effect of an applied electric field on a dielectric. Real materials can exhibit multiple resonances, which can be due to the electron cloud shifting or due to molecular bonds twisting or stretching. To have an accurate model, the response of all of these resonances should be included when determining material parameters. The equation below shows the frequency dependent relative permittivity of a material at each resonant frequency:

$$\tilde{\varepsilon}(\omega) = 1 + \frac{\omega_p^2}{\omega_o^2 - \omega^2 - j\omega\Gamma} \quad (4.1)$$

where ω_p = plasma frequency, ω_o = resonant frequency, ω = frequency and Γ = damping coefficient. The Drude oscillator model approximates the motion of electrons specifically in metals where charges are free to move. The Drude model has similarities to the Lorentz model, but since the electrons aren't bound, there is no resonant frequency, so that

$$\tilde{\varepsilon}_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + j\omega\Gamma}. \quad (4.2)$$

Permittivity obtained by the Lorentz and Drude models is a complex quantity. Both the imaginary and real parts of the permittivity contribute towards losses in the material. To get an accurate value of these losses, the refractive index should be determined by taking the root of the product of material permeability and permittivity:

$$\tilde{n}(\omega) = \sqrt{\tilde{\varepsilon}_r \tilde{\mu}_r} \sqrt{\varepsilon_0 \mu_0}, \quad (4.3)$$

where $\tilde{n}$ = complex refractive index, $\tilde{\varepsilon}$ = complex permittivity, $\tilde{\mu}$ = complex permeability; for non magnetic materials $\tilde{\mu}_r=1$, $\tilde{n} = \sqrt{\tilde{\varepsilon}}$, since $\tilde{\varepsilon}$ is complex, refractive index n is also complex, therefore $\tilde{n}=n+j.\kappa$, where, n = refractive index and κ = extinction coefficient.

4.2 Ellipsometry

Ellipsometry was used to measure frequency dependent optical properties for copper, silicon and silicon dioxide in the mid-IR region. This is a non-destructive optical characterization technique that can measure film thickness and optical properties of thin films with high precision. It utilizes the property of change in polarization of light upon reflection from a thin film surface to determine the dielectric properties of the thin film material.

Light is an electromagnetic wave, and its electric field defines its polarization state. As light is reflected off a surface, a plane of incidence is formed, which is defined by the direction of the incident and reflected light. Light with electric field direction in the plane of incidence is p-polarized light, whereas the light with electric field perpendicular to the plane of incidence is referred to as s-polarized light. Assuming single interface reflection and transmission, the Fresnel equations describing p- and s- field quantities of the transmitted and reflected light can be described as follows [96];

$$r_p = \frac{E_{rp}}{E_{ip}} = \frac{n_t \cos \theta_i - n_i \cos \theta_t}{n_t \cos \theta_i + n_i \cos \theta_t}, \quad t_p = \frac{E_{tp}}{E_{ip}} = \frac{2n_i \cos \theta_i}{n_t \cos \theta_i + n_i \cos \theta_t} \quad (4.4a)$$

$$r_s = \frac{E_{rs}}{E_{is}} = \frac{n_i \cos \theta_t - n_t \cos \theta_i}{n_i \cos \theta_t + n_t \cos \theta_i}, \quad t_s = \frac{E_{ts}}{E_{is}} = \frac{2n_i \cos \theta_i}{n_i \cos \theta_t + n_t \cos \theta_i} \quad (4.4b)$$

Where n_i and n_t are the complex refractive index of the two mediums, θ_i and θ_t are the angles of incidence and transmission (refraction) respectively.

In an ellipsometric system, unpolarized light from a light source is passed through polarizers to produce a p- and s- polarized light. This light is then reflected off the surface of the thin film at the same time. p- and s- polarized light reflect differently. This difference in reflection ends up producing elliptically polarized light and is the central concept behind ellipsometry measurements. The system measures and analyzes the complex reflectivity ratio of the p- and s- polarized light before and after reflection as shown in the equation below:

$$\tan \psi = \frac{|r^p|}{|r^s|}, \quad \Delta = \delta_1 - \delta_2 \quad (4.5)$$

where r^p and r^s are the fresnel reflection coefficient, and Δ is the phase difference between the s- and p- polarized light. The equations are analyzed together in the system as:

$$\tan \psi e^{j\Delta} = \frac{r^p}{r^s} \quad (4.6)$$

For materials with frequency dependent optical properties, software fits the measured data to dispersion relations and oscillator models. For transparent materials, a dispersion relation is used to fit the data, whereas, for lossy materials, different oscillator models such as Lorentz, Drude, Gaussian and harmonic models are used to obtain frequency dependent optical properties. The data obtained are consistent with Kramers-Kronig to ensure the principle of causality. To improve confidence in the measured data, the measurements are repeated at multiple angles closer to the Brewster angle,

and the optical properties are matched for each iteration.

4.3 Material Preparation & Measured Optical Properties using Ellipsometry

The optical parameters were measured by ellipsometry at Polytechnique Montreal, Department of Engineering Physics. The materials were prepared at the fabrication facility at Carleton University. For copper, a 1 μm layer was deposited on a silicon substrate by e-beam evaporation in a Balzers evaporation system. As copper is reflective, it was used as a base material for characterization of the silicon dioxide layer. 1.6 μm of silicon dioxide was deposited on copper in a Trion PECVD system. The optical constants for silicon dioxide were extracted by modeling a two-layered system of silicon dioxide on copper. Deposition of silicon directly on copper can lead to the formation of alloys at the copper-silicon interface, therefore a three-layer model, i.e., silicon on silicon dioxide on copper was modeled, with previously extracted values of copper and silicon dioxide used in the calculation.

Copper was the first layer to be characterized. 1 μm of copper was deposited by e-beam evaporation in the Balzers system on a 2 inch wafer. The ellipsometry measurements were taken at the center of the sample. Fig. 4.1(a) shows the real and imaginary permittivity of copper. As expected, copper's negative permittivity shows that it is a good reflector material for the ground plane.

A thin layer of silicon dioxide was deposited on copper in the Trion PECVD system on a 2 inch wafer. The center of the wafer was used for measurement. Fig. 4.1(b) shows the ellipsometry determined real and imaginary permittivity of silicon dioxide. There are two points where internal material resonance can be seen from the figure. These are at 67.7 THz and 101.5 THz. The resonance at 67.7 THz is due to the stretching of Si-H bonds [97] [98] [99], which are formed due to Silane SiH_4 which is used in the PECVD deposition of silicon dioxide. The other resonance at 101.5 THz is due to N-H-N stretching [100], also formed due to the interaction of gases during the PECVD process.

Finally, a thin layer of silicon was deposited on silicon dioxide, on copper by PECVD. The extracted frequency-dependent permittivity for copper and silicon dioxide were fed into the three-layered model available in the software to enable calculation of parameters for silicon. Once again the center most part of the wafer was used for measurement purposes. Fig. 4.1(c) shows the extracted data for silicon. A strong material resonance is observed at approximately 60 THz. This is due to stretching of Si-O bonds which happens during PECVD due to the use of SiH_4 mixture [101].

Mid-IR frequency dependent optical property data for silicon was not available in the literature. However, a Lorentz-Drude model was available for the near-IR range. That model was used to calculate and extrapolate optical properties for silicon in the mid-IR which were then used to simulate

Figure 4.1 Extracted real and imaginary permittivity obtained by Ellipsometry: a) copper, b) Silicon Dioxide (SiO₂), and c) Silicon (Si). The measurement was taken at the center of the 2 inch wafer.

resonant structures for CO_2 and SO_2 in chapter 3. A comparison of the extrapolated model from the near-IR was made with the actual ellipsometry derived data, as shown in Fig. 4.2(a). The actual real permittivity of silicon is slightly lower as compared to that of the extrapolated model from the literature, and as mentioned before there is a resonance at around 60 THz, which is specific to the PECVD process. The imaginary permittivity of the ellipsometry derived data is considerably lower beyond a frequency of 65 THz.

Figure 4.2(b) shows the permittivities of silicon dioxide, including ellipsometry data and data available in the literature. The silicon dioxide data from the literature was from material produced by sputter deposition, whereas for this project PECVD was used to deposit material. The real permittivity was slightly different for the two processes. The imaginary permittivity for the two processes was similar for the two cases with the exception of the additional material resonances attributed to process gases incorporated during PECVD deposition.

4.4 Device Redesign and Simulation

The optical property values found by ellipsometry for PECVD deposited layers were different from those reported for sputtering process and extrapolated from literature, prompting an iteration of the simulation and design of the metasurface structure. In addition, the geometry of the photolithographic mask available for this project needed to be taken into account. The mask had square openings of $3.2\ \mu\text{m}$ per side with a pitch of $6\ \mu\text{m}$, as shown in Fig. 4.3. The metasurface had an area of $8\ \text{mm} \times 8\ \text{mm}$, which makes 1333 resonators in x – as well as y –direction. The total number of resonators in an area of $8\ \text{mm} \times 8\ \text{mm}$ is approximately equal to 1.77 million.

The square openings meant that the fabricated resonant structures after lithography would be square of approximately $3.2\ \mu\text{m}$ each side, and the unit cell size (periodicity) will be $6\ \mu\text{m}$, as shown in Fig. 4.3. The resonant wavelength for the all-dielectric metasurface thermal emitter had to be longer than $6\ \mu\text{m}$, which corresponds to a frequency lower than 50 THz. This gave a workable frequency range of 40 THz to 50 THz for the resonant frequency from the structure as silicon dioxide has a cutoff for frequencies lower than 40 THz. Moreover, after several fabrication runs, it was found that the silicon resonator structure would undercut during etching, such that the top of the silicon resonator was approximately $0.1\ \mu\text{m}$ smaller than the base of the resonator. Due to these project limitations in terms of unit cell size, resonator size and frequency cut-off for materials, the structure was re-designed and simulated. The redesigned cell had a square Silicon resonator with a lengths of $3.2\ \mu\text{m}$ at the base and $3.1\ \mu\text{m}$ at the top of the resonator.

The dimensions of the modified unit cell were chosen to produce a resonant frequency around 41.6 THz, which was close to an absorption line of SO_2 [102] [103]. The thickness of the Copper

Figure 4.2 Comparison of the the extracted permittivity obtained using ellipsometry and Drude model extrapolated from near-IR for a) Silicon, and b) Silica (data from literature where Silica was deposited using another process (sputtering)).

Figure 4.3 Microscopic image of lithographic mask available for the project.

h_{gnd} was $0.6 \mu\text{m}$, thickness of the Silicon Dioxide $h_s = 0.39 \mu\text{m}$ and the height of the Silicon resonator was $h_{Si} = 1.05 \mu\text{m}$. The periodicity and the resonator size were fixed at $6 \mu\text{m}$ and $3.2 \mu\text{m}$ by the mask layout. Fig. 4.4(a) shows the redesigned structure for the all-dielectric metasurface thermal emitter.

Figure 4.4 Modified unit cell configuration due to limitation in mask size and fabrication issues. a) Unit cell, and b) Simulated emissivity of the modified unit cell for a resonant frequency of 41.6 THz. $\Lambda = 6 \mu\text{m}$, $h_s = 0.39 \mu\text{m}$, and $h_{Si} = 1.05 \mu\text{m}$.

Figure 4.4(b) shows the simulated emissivity of the modified unit cell. The Q-factor for the modified device is approximately 135. This is lower than the Q-factor simulated in chapter 3. A possible reason for the decrease in Q-factor is the measured permittivity includes higher losses in silicon

around the resonant frequency of 41.6 THz when compared with the model used in the previous design. Another possible reason for the decrease in Q-factor was the under-cut in the silicon resonator during RIE etching. After several fabrication runs, it was determined that the minimum amount of under cut after optimizing all the other parameters of the etching process resulted in the top of silicon resonator being $0.1 \mu\text{m}$ smaller than the base of the resonator, resulting in a wider resonance. This redesigned structure will next be fabricated and measured.

Chapter 5 Fabrication

5.1 Fabrication of Structure

To achieve a narrow-band thermal emission in the mid-IR region, the frequency selective periodic resonant structures have dimensions on the order of a few microns. Structures of this size have been made possible by using standard lithographic processes used for CMOS. To fabricate the all-dielectric metasurface thermal emitter, a Silicon wafer was selected as the substrate. A ground plane consisting of $0.75\ \mu\text{m}$ of copper was deposited using e-beam evaporation. This process was followed by deposition of $0.39\ \mu\text{m}$ silicon dioxide as the low permittivity host and $1.05\ \mu\text{m}$ of silicon as the high permittivity resonator for the emitter. The layers of silicon dioxide and silicon were deposited by Plasma Enhanced Chemical Vapor Deposition (PECVD). The thin film stack was then patterned and the top silicon layer was etched using RIE to produce silicon resonators separated from a copper ground plane by a thin film of silicon dioxide. Figure 5.1 shows the fabrication process flow for the entire process. This chapter describes the fabrication process in detail, followed by some significant fabrication issues and choices made during the process.

5.1.1 Substrate

A standard 2 inch Silicon wafer was selected as the substrate. It was RCA cleaned to remove any ionic, organic, and particle contamination. This process was of critical importance as multiple thin layers will be deposited during the fabrication process at temperatures of up to 350°C . The resonators are around $3.2\ \mu\text{m}$ in size in a high density array, and any particle contaminants can present a serious risk to the operation of the final device.

5.1.2 Copper Deposition (E-beam Evaporation)

A reasonably thick layer of copper is required to form a good ground plane, and the target thickness was chosen as 750 nm. Copper was deposited using e-beam in the Balzers evaporation system. To improve adhesion of copper to the Silicon substrate, 50 nm of Titanium was deposited at a deposition rate of 0.1 nm/s on the substrate followed by the Copper deposition at a deposition rate of 0.1 nm/s.

Figure 5.1 Illustration showing the Fabrication process flow for the all-dielectric metasurface thermal emitter.

5.1.3 Silicon Dioxide Deposition (PECVD)

Silicon dioxide was used as the low permittivity dielectric between the silicon resonators and the copper reflector. 0.39 μm of silicon dioxide was deposited using a Trion Plasma Enhanced Chemical Vapor Deposition (PECVD) system. The deposition rate was found to be uniform at the center of the holder at 3.57 nm/sec. The deposition rate became lower outside a 1.1 cm diameter region at the middle of the holder, therefore the sample was placed in the holder as shown in Figure 5.2. An important precaution was taken to cool down the holder before placing the substrate with copper on it to avoid oxidation of the thin layer of copper due to hot holder. The process conditions were as follows:

ICP Triode Power: 81 Watts

Gas Flow:

SiH_4 : 21 SCCM

N_2O : 355 SCCM

N_2 : 110 SCCM

Pressure: 1000 mTorr

Temperature: 350°C Time: 110 secs

5.1.4 Silicon Deposition (PECVD)

The top resonator structures were made up of high permittivity silicon. To realize the structure, a thin layer of silicon was deposited in the Trion PECVD system. Similar to silicon dioxide deposition, the substrate was placed in the center of the holder to achieve uniform layer thickness. The thickness of the silicon was 1.05 μm , deposited at a rate of 0.8148 nm/sec. The process conditions were as follows:

RF Power: 39 Watts

Gas Flow:

SiH_4 : 25 SCCM

Ar: 50 SCCM

Pressure: 900 mTorr

Temperature: 350°C

Time: 1289 secs

Figure 5.2 Device loading on center of holder in Trion PECVD for uniform deposition rate at the center of wafer

5.1.5 UV Photolithography (Silicon Resonators)

Photolithography was a multi-step process. This turned out to be one of the most critical process during the fabrication of the device. A metal liftoff technique was used to deposit a periodic array of chromium features with each structure the size of $3.2\ \mu\text{m} \times 3.2\ \mu\text{m}$ square. These features were used as masks during subsequent RIE etching to realize the silicon resonators. The following steps describe the various steps followed in this stage of the fabrication process:

1. **Lithographic Mask** The mask available used for this project was described in Chapter 4. Due

to variation of deposition rate across the 2 inch substrate, a special precaution was taken to align the mask with the substrate. It was placed in such a way that one complete 8 mm x 8 mm active area (one complete thermal emitter) on the mask was aligned perfectly with the center of the substrate to ensure layer thickness uniformity across the device.

2. **Lift-Off for Chromium Mask:** A lift-off process was used to create openings for chromium hard-mask deposition on the top silicon layer. HMDS was used to enhance adhesion of lift-off resist (LOR) to the silicon layer. It was applied at spin speeds of 1000 rpm and 4000 rpm followed by a soft bake at 115°C for 1 minute. Next, a 100 nm layer of LOR-1A was deposited at spin speeds of 1000 rpm and 1500 rpm followed by a bake at 190°C for 5 minutes. This bake helps in control of undercut during the lift off process. Finally a 100 nm layer of S-1811 photoresist (PR) was applied at spin speeds of 1000 rpm and 4000 rpm. The wafer was again soft baked at 115°C for 1 minute.
3. **Exposure and Development:** After the application of all the PR layers, the structure with the mask on top was exposed under ultraviolet (UV) light for 22 sec on Karl-Suss MA6 mask aligner using contact printing. The UV exposed wafer was then developed in MF-321 for 50 seconds to produce square shaped opening, as shown in Figure 5.3. The development time in MF-321 varied between 45 seconds – 55 seconds depending on the age of the developer and visual inspection of the device during the development process.

5.1.6 Metal Mask (Chromium) Deposition and Lift-Off

The next step was to deposit Chromium in the openings created in the photoresist layers following development. An O₂ descum was done for 1 minute at a power of 100 watts and a pressure of 300 mT in the Technics Etcher. This was to ensure removal of any left over PR residue in the openings after the development stage. 30 nm of Chromium was evaporated in the Balzers system at a deposition rate of 0.1 nm/sec. Once the chromium was deposited, the bi-layer structure was immersed in PG remover to etch and remove the unwanted LOR/Chromium. Two baths of PG remover at 80°C were used in this process. The first bath, lasting 10 minutes at 80°C, removed most of the LOR-1A with the chromium on top. The second clean bath under the same conditions removed smaller sections of LOR and chromium left behind. The PG remover was followed by a 10 second ultrasonic bath to ensure complete removal of any remaining particles.

5.1.7 RIE Etching

The device was etched in a MRC Reactive Ion Etching (RIE) system. The device was placed at the center of the system wafer chuck as shown in Figure 5.2(b). Filler silicon wafers were placed on the

Figure 5.3 Multi-layered structure after lithography

sides to ensure uniform etching. The etching was done in two steps of 8 minutes and 7 minutes. The etch depth was measured after the first etch, and the time for second etch was adjusted accordingly to ensure precision. The total thickness of top silicon resonator was 1050 nm, out of which only 1020 nm was etched in the MRC RIE etcher. The remaining 30 nm of Silicon was etched away in a polysilicon wet etch solution for 7 seconds. This was done to ensure that the underlying Silicon Dioxide layer was not exposed during RIE dry etch, as previous fabrication attempts resulted in the formation of grass like structure on the silicon dioxide surface after RIE etching. Polysilicon wet etch solution's etch rate for silicon dioxide was considerably slower compared to that of silicon. Hence the silicon dioxide layer acted as an etch stop for the silicon etches. The exact process condition for MRC RIE etch were as follows:

RF Power: 350 Watts

CF_4/O_2 : 50 SCCM

Etch Pressure: 80 mTorr

Temperature: 350° C

Figure 5.4 Placement of device for RIE etching. Silicon filler wafers were placed on the sides for even etching

5.1.8 All-Dielectric Metasurface Thermal Emitter

A layer of chromium oxide was formed around the silicon resonators during RIE etch. After verification of the etch depth after RIE and polysilicon etch, the device was dipped in Transene chrome wet etch at an elevated temperature of 80°C for 5 minutes to remove chromium mask. High temperature nichrome etchants are known to speed up the etch [104] as well as to remove the chromium oxide layer formed during RIE etch. Figure 5.5(a) shows 3 columns of fabricated silicon resonators. Figure 5.5(b) shows the SEM image of a single silicon resonator.

5.2 Fabrication Choices and Issues

During the fabrication process, several issues and challenges were faced. Some material/processes were tested and ruled out to obtain the best possible result with available equipment. Some initial processes were modified after fabrication failures and defects. This section discusses the major issues and choices made after various failures, and these should be avoided for future fabrication

(a)

(b)

Figure 5.5 SEM images of fabricated Silicon resonators. a) Array of resonators. b) Various measured dimensions of a single resonator.

runs to save time and resources.

5.2.1 Copper Deposition

Initially, the copper was deposited at a rate of 0.5 nm/s. This deposition rate resulted in spits of molten copper ejected from the source being deposited on the wafer surface. These defects weren't clearly visible under the microscope due to the highly reflective surface, but they resulted in pinholes following the high-temperature deposition of Silicon and Silicon Dioxide layers. These holes became visible after the last step of the process, during the chromium etch. Transene chrome etch was initially used to remove the chromium mask, but it is known to etch away copper as well. It entered defects in the film surface and could etch away the underlying copper as shown in Figure 5.6. A slower deposition rate of copper (0.1 nm/s) significantly improved the quality of the copper layer and minimized the defects. Another issue related to copper deposition was the adhesion to the substrate. A tape test confirmed that the copper did not strongly adhere to the underlying silicon substrate. Adhesion was improved by depositing a layer of 5 nm of titanium on the substrate before depositing copper [105].

Figure 5.6 Pin holes in layers due to Copper defects

5.2.2 Top Silicon Resonator Structures

Three possible fabrication processes were explored to fabricate silicon resonator structures on top of the silicon dioxide layer. The mask available for the project had square holes of $3.2\ \mu\text{m} \times 3.2\ \mu\text{m}$,

which meant that the structures could either be made by depositing the silicon layer, followed by a photoresist mask and then etching away the unmasked areas. Second explored possibility was to deposit a metal mask using lift-off technique followed by an etch. The third option that was explored was to use lift-off technique to open $3.2\ \mu\text{m}$ windows after deposition of silicon dioxide layer and then evaporate silicon in the Balzers system. The following processes were explored but not pursued due to fabrication issues were as follows

1. **Evaporation of Silicon for Resonators:** A process was explored to fabricate the silicon resonators directly by lift off, and thereby eliminate the RIE etch step from the process. Following the deposition of the silicon dioxide layer in the Trion PECVD system, 1800 nm of LOR 10 A was deposited at a spin speed of 1000 rpm. This was followed by deposition of S-1811 photoresist at 1500 rpm. The lift-off resist structure was exposed and developed as previously described. Silicon was then e-beam evaporated onto the patterned wafer in Balzers system [106]. Unfortunately this process resulted in poor adhesion of silicon to the underlying layer of silicon dioxide. A possible reason for this was the stress mismatch between the PECVD deposited silicon dioxide and the e-beam evaporated silicon. A number of silicon resonator structures were removed from the surface during the lift off and drying stages. Figure 5.6(b) shows the final structure after the evaporation of silicon.

Figure 5.7 Adhesion issues due to evaporation of silicon resonators on silicon dioxide

2. **Photoresist Mask:** For a simple develop and etch process, both negative and positive photore-

sists were available. Since the mask had square holes, a negative photoresist was an option to deposit ($3.2\ \mu\text{m} \times 3.2\ \mu\text{m}$) regions of photo resist on top of thin film silicon, which would be further used to etch away unmasked silicon area to form resonator structure. However the PR would not hold up to the RIE etch through the full thickness of silicon.

5.2.3 PECVD Thin Film Deposition

It was found out that the deposition of silicon and silicon dioxide was not uniform on the 2 inch substrate in the PECVD Trion. The center region had a thickness different than the outer regions. To have consistent layer thickness for the device, the fabricated thermal emitter at the center of the wafer was considered for testing. Another issue faced during thin film deposition by PECVD, was the difference in deposition rates for shorter and longer deposition times. The deposition rate for silicon dioxide was $3.57\ \text{nm/sec}$ for film thicknesses lower than $500\ \text{nm}$ and was $3.4\ \text{nm/sec}$ for film thicknesses greater than $1\ \mu\text{m}$. Similarly silicon also had a variation in the deposition rates for shorter and longer deposition times.

5.2.4 Mask Loading in Aligner Plate

The mask used in this project was on a 5 inch plate whereas the target substrate was 2.5 inch. Since the mask plate was 5 inch, the aligner mask holder with either 4 inch or 2 inch opening could have been used during exposure, as shown in Figure 5.8. With the mask loaded on the holder with the 4 inch opening, much larger than the substrate diameter, the contact was imperfect and produced inconsistent feature size across the device substrate. When the mask holder with the 2 inch opening was used, contact appeared to improve and irregularity in the feature size was removed.

5.2.5 Exposure Times

The feature size on the mask was approximately $3.2\ \mu\text{m} \times 3.2\ \mu\text{m}$. To obtain accurate pattern transfer to the substrate, various exposure times were tested. A 22 sec exposure time produced features very closely replicating those on the mask. Increasing the exposure time resulted in the square features converting into round-edged squares as shown in Figure 5.9. These round shaped features were of inconsistent size across the device.

5.2.6 RIE Etching

The silicon resonators were etched in MRC RIE. Initially, a $30\ \text{nm}$ of Aluminum (Al) was used as the etch hard mask. During the plasma RIE etch, the Al mask was found to have a micro-masking effect [107] [108], resulting in rough grass-like structures in the area between etched

Figure 5.8 Aligner plate options for mask loading for lithography. Plate on the left is for mask for a 2.5 inch wafer and on the right for a 4 inch wafer.

Figure 5.9 Round openings after development in photolithography due to over exposure.

silicon resonators as shown in Figure 5.10(a). To eliminate this rough area around the resonator structures, chromium was chosen as a mask material in place of aluminum. Chromium is known to stand up during etch [107] and reduce micro masking.

Figure 5.10 Various issues related to RIE etching. a) Rough grass like structures due to Al micro-masking. b) Undercuts below the Chromium mask.

During the RIE etch a problem was observed when the underlying silicon dioxide was exposed during etching of the silicon resonators. This resulted in grass like structures in the fields around resonators. To avoid this defect, the silicon wasn't completely removed in the RIE. Approximately 30 nm of silicon was left during RIE etch, and this remaining thin layer of silicon was removed by dipping the RIE-etched device in polyetch for 7 seconds. Polyetch is known to etch away silicon approximately 15 times more than it etches oxide [109]. This process cleared out the remaining silicon and slowed down the etch considerably as soon as it hit the underlying oxide layer.

Another issue related to etching in RIE was the undercut of the resonator structure during etching. This resulted in the fabricated resonators having a non-ideal profile as shown in the SEM image in Figure 5.10(b). Undercut was reduced by varying the process parameters of the RIE etch, specifically reducing the etch pressure from 130 mTorr to 80 mTorr [110] [111].

5.2.7 Wet Etching vs Dry Etching for Resonators

There was an option for wet etch to fabricate the silicon resonators. However, wet etch processes are generally isotropic [112] [113]. Simulations showed that for a high Q-factor in a narrowband thermal emitter it was essential to have the top and the bottom of the Silicon resonator as close as possible in size. Therefore dry etching was preferred.

5.3 Summary

In Summary, the metasurface emitter structure is a fairly simple design with common CMOS materials and easily attainable dimensions. However to achieve accurate dimensions and geometry suitable for a narrow-band thermal emitter in a small-volume prototype required considerable process development. After several iterations, an array of $3.2\ \mu\text{m} \times 3.2\ \mu\text{m}$ silicon resonators on a $6\ \mu\text{m}$ pitch and covering an $8\text{mm} \times 8\text{mm}$ active area were successfully fabricated on a copper-backed silicon dioxide dielectric layer. The spectral response of this device will now be measured next.

Chapter 6 Testing and Results

The aim of this project is to design and test a mid-infrared (mid-IR) thermal emitter that can be used for optical gas sensing applications. Common industrial and hazardous gases such as SO_2 and CO_2 are known to have mid-IR absorption peaks at 41.6 THz and 74.65 THz respectively. Due to material frequency cut-off limits and the dimensions of the available mask for this project, the workable spectral range for selective emissivity is 39 THz – 50 THz. The thermal emitter has been designed to have a peak emission at 41.4 THz. The frequency dependent emissivity and the bandwidth of emission peaks are important characteristics of the emitter. In simulations the emissivity is determined using Kirchoff's Law of thermal emission. For a device backed by a ground-plane, the emissivity is given by: $\mathcal{E}(\omega) = 1 - |R(\omega)|^2$, where $\mathcal{E}(\omega)$ is spectral emission, $R(\omega)$ is spectral reflection across the structure.

In the physical device, the emissivity is measured by heating the fabricated device to 80°C and measuring the emission spectrum by Fourier Transform Infrared spectroscopy (FTIR). To find the emissivity of the device the FTIR spectrum is compared with a blackbody reference at the same temperature. The bandwidth of an emission peak is typically described by the Q factor of the peak. This chapter begins with the description of FTIR testing and the emissivity measurement setup, followed by a detailed description and analysis of the results.

6.1 FTIR Emission Spectroscopy

6.1.1 Fourier-transform infrared spectroscopy (FTIR)

Fourier-transform infrared spectroscopy (FTIR) is used to measure the radiated spectrum of the emitter. Standard FTIR systems use an interferometer with a variable path length to measure spectral absorption/transmission. For measuring the absorption, an internal IR source generates radiation, that passes through the interferometer then through the target material and then reaches the detector. The mirror in one arm of the interferometer moves at a known rate. The signal on the detector is a function of time as the mirror moves. This can then be converted to a function of frequency through a Fourier Transform. This approach allows fast and sensitive collection of spectra when compared with diffractive spectrometers. Typically a sample absorbs specific frequencies depending on the chemical structure of the sample.

This project required the mid-IR emissivity measurement of the fabricated thermal emitter. For emissivity measurement, the internal IR source of a standard FTIR transmission system is disconnected [114]. An optical path is created with the sample acting as the source. The energy from the

(a)

(b)

Figure 6.1 FTIR Emission Spectroscopy. a) FTIR spectrometer setup for thermal emissivity measurement. b). FTIR equipment used to measure emissivity at Stony Brook University.

heated sample is guided through multiple mirrors into the interferometer and to the detector. The schematic for the system is shown in Figure 6.1(a).

6.1.2 Emissivity Measurement Setup

The emissivity was measured at Geo Sciences department at Stony Brook University SUNY. It was measured on a Thermo Scientific Emissivity Spectrometer as shown in Figure 6.1(b). The actual size of the fabricated thermal emitter on the wafer was a square of the size of 8 mm x 8 mm, after cleaving the size reduced to approximately 7.8 mm by 7.8 mm. The sample was placed flat on the circular holder, as shown in Figure 6.2(a). The holder was placed in the heating cabinet for 30 minutes, so that it was heated evenly. The temperature set inside the heating cabinet was maintained at 80°C. The holder was painted black and made up of a dense material to maintain the temperature while it was transferred from the heating cabinet to the sample chamber. The holder with the sample on it was then placed on top of a heater inside the sample chamber. The purpose of this heater was to keep the sample holder at a constant temperature.

This emission measurement setup gives the emissivity of the sample compared to that of a black body at the same temperature. Before collecting the measurement, the systems measures emissivity of a blackbody source at 70°C and 100°C and generates an error correction function which is then applied to the actual emissivity measurement of the sample, which is measured at a fixed temperature of 80°C. While there was an option to heat the sample to a different temperature, the built-in black body source was fixed at 80°C for emissivity measurements. Emissivity at higher temperature can reduce the background emission as well as giving a higher intensity for better measurements. The minimum possible sample size for accurate emissivity measurements on this instrument is 1 cm² due to limitations in the aperture size. A sample smaller than the recommended size will result in light collected from the sample as well as the holder on which the sample is placed. For repeatability, the sample should be heated at 80°C multiple times and the emissivity should be measured and compared. As this is a frequency selective metasurface thermal emitter, its power consumption cannot be measured using this setup. For this specific instrument the measurement relies on the built-in heater that heats up the sample. To enable a power consumption study the metasurface emitter should be fabricated on top of a MEMS micro-hotplate and the the emissivity setup should be modified with the sample as a stand alone source.

6.2 Measured Thermal Emission

The spectral emissivity of the heated thermal emitter was measured and processed with reference to a perfect black body at 80°C. The sample is placed flat on the holder as shown in Fig. 6.2(a), which

has been painted black to have an emissivity closer to a perfect blackbody. The measured thermal emission from the sample and holder is shown in Figure 6.2(b). There is an emission peak at the resonant frequency of 41.6 THz as designed for the thermal emitter. There is background signal such that the entire emissivity graph appears shifted up with a base of the spectrum at approximately 0.55. The emissivity value at the resonant frequency of 41.6 THz is about 0.35 from the base of the spectrum. As expected, there are additional emission peaks beyond 50 THz and a frequency cut-off below 38 THz.

The recommended area for emissivity testing based on the aperture size was 1 cm^2 . The size of the fabricated thermal emitter was $0.8 \text{ cm} \times 0.8 \text{ cm}$. After cleaving the thermal emitter from the wafer, the size was reduced to $0.75 \text{ cm} \times 0.75 \text{ cm}$, which was approximately equal to an area of 0.55 cm^2 . This meant that the thermal emissivity measurement included light from both the sample surface and the holder. The actual emissivity of the metasurface was extracted by using the measured emissivity of the sample and holder together as shown in Fig. 6.2(b) and the emissivity of the holder only as shown in Figure 6.2(c). The thermal emissivity of the holder is approximately 0.95, as it is painted black to have emissivity approaching a black body.

(a)

(b)

(c)

Figure 6.2 Thermal emission measurement. a) Fabricated thermal emitter on top of the holder, b) Measured thermal emissivity of the fabricated thermal emitter and the holder, and c) Measured thermal emissivity of the holder.

Figure 6.3 Thermal emission measurement. a) Combined thermal emissivity of two regions with areas a_1 and a_2 , b) Extracted thermal emissivity of the fabricated thermal emitter.

To extract the metasurface emissivity, consider an FTIR emissivity measurement of a general surface composed of two regions as shown in Figure 6.3(a). For an instrument aperture opening of total area a , the measured total emissivity is from two regions, one contained inside other with two different thermal emissivities $\mathcal{E}_s$ and $\mathcal{E}_h$, respectively. The inner surface has an area of a_1 and that of the second surface is $a_2 = (a - a_1)$. The total emissivity of such a surface can be calculated by ;

$$\epsilon(\nu) = \frac{B_s(\nu)a_1 + B_h(\nu)a_2}{B_\nu(a_1 + a_2)}, \quad (6.1)$$

where $B_s(\nu)$, B_h and B_ν are spectral radiance ($\text{W} \cdot \text{m}^2 \cdot \text{sr}^{-1} \cdot \text{nm}^{-1}$) of the device sample, holder and an ideal black body radiation, at the frequency ν , of the same area, respectively. According to FTIR emission testing, $\mathcal{E}_1$ was the measured emissivity of the holder without the sample i.e. $a_1 = 0$;

$$\mathcal{E}_1(\nu) = \frac{B_h(\nu)}{B_\nu} \Rightarrow B_h(\nu) = \mathcal{E}_1(\nu)B_\nu. \quad (6.2)$$

Next, the total emissivity of the sample with holder was measured, and is given by the following expression;

$$\mathcal{E}_2(\nu) = \frac{B_s(\nu)a_1 + \mathcal{E}_1(\nu)B_\nu a_2}{B_\nu(a_1 + a_2)}, \quad (6.3)$$

leading to

$$B_s(\nu) = \frac{\epsilon_2(\nu)B_\nu(a_1 + a_2) - \epsilon_1(\nu)B_\nu a_2}{a_1}. \quad (6.4)$$

Finally, the emissivity of device sample of area $(a_1 + a_2)$ is given by

$$\epsilon_s(\nu) = \frac{B_s(\nu)}{B_\nu} = \left\{ \frac{\epsilon_2(\nu)(a_1 + a_2) - \epsilon_1(\nu)a_2}{a_1} \right\}. \quad (6.5)$$

The extracted thermal emissivity of the metasurface thermal emitter shown in Figure 6.3(b) indicates a peak emissivity of 0.78 for the designed resonant frequency.

6.2.1 Extra emission peaks

Extra emission peaks were observed at 50 THz, 60 THz and 67 THz in the thermal emissivity measurements. Two of these resonances are introduced during the thin layer deposition in PECVD. Figure 6.4(a) shows the imaginary permittivity of silicon and silicon dioxide and the thermal emissivity measurements. The emissivity peak at 60 THz corresponds to stretching of Si-O bonds which occur due to the SiH_4 mixture during the PECVD deposition of silicon [101], and the resonance at 67 THz is due to stretching of Si-H bonds which are deposited during PECVD deposition of silicon dioxide once again due to SiH_4 mixture [97]. The cut-off for Silicon Dioxide can also be seen in the imaginary permittivity plot at a frequency of 38 THz.

The additional resonant emissivity peaks at 60 THz and 67 THz can be removed by using sputtering instead of PECVD. The sputtering method uses a source from which the pure material is sputtered to the substrate typically in a noble gas background. The deposited material has the same properties as the source. In PECVD, precursor gases react chemically to produce silicon dioxide which gets deposited on the substrate. Optical properties of silicon dioxide deposited by sputtering are available in literature, as shown in Figure 6.4(b). There is no resonance in the range of 40 THz-140 THz. While optical property data for sputtered silicon isn't available from literature, silicon can be deposited by using sputtering to remove the additional material resonance at 60 THz.

There are multiple peaks that occur between 50 THz and 55 THz. The unit cell size of the periodic structure is $6 \mu\text{m}$ which corresponds to 50 THz; there are multiple resonances for frequencies above 50 THz (wavelength below $6 \mu\text{m}$) as can be seen in Fig. 6.4(c). These individual peaks above 50 THz combine to make a broad peak. Variable resonator dimensions may also contribute

Figure 6.4 Contributing factors to extra emission peaks in the measured spectrum. a) Measured thermal emissivity and Imaginary permittivity of Si and SiO₂, b) Optical constants for SiO₂ by sputtering.

to this, and will be discussed later in this chapter.

6.3 Measured Emissivity vs Simulation

The emissivity simulations for the unit cell were focussed in the spectral window of 40 THz-50 THz. The unit cell dimensions were designed to have an emission peak at 41.6 THz, with a Q-factor of 135. The emission intensity for this resonant frequency was simulated to be approximately 0.95 compared to a black body. The thermal emissivity measurements show an emission peak at 41.6 THz according to the design, however the Q-factor was 38 with an emissivity of 0.78. To understand this difference, the fabricated thermal emitter was carefully examined under the microscope, and a variation in the resonator dimensions was found. Fig. 6.5 shows a specific variation as seen on the

microscope with a zoom of $100\times$. The red arrows on the figure point to faint lines that appear as irregular sized resonators across the y -directions of the resonator array. This irregularity is periodic as has been marked by red arrows. A detailed analysis was done to determine the different size of resonators that were present and their frequency of occurrence for re-simulation purposes.

Figure 6.5 Variation in resonators as seen under microscope zooming factor $100\times$.

6.3.1 Variation in resonator size

Examination of the resonator array revealed that the resonator size remained consistent along the x -direction, but it changed along the y -direction. Each region between successive red arrows as shown in Fig. 6.5 was $180\text{ }\mu\text{m}$; there were a total of 44 regions, with each region having 30 rows of resonators. The last two rows of resonators in each region were slightly smaller than the other 28 rows. The size of the resonators changes periodically along y -axis. The first region had an average feature size of $3.10\text{ }\mu\text{m}$ whereas the last region had an average feature size of $3.40\text{ }\mu\text{m}$. A sample of resonator dimensions was taken across the y -directions and recorded, as shown in Table 6.1.

The resonator size was measured on microscope with $100\times$ zoom; some resonators are shown in Fig. 6.6(a). The uncertainty of the microscopic measurements is $0.02\text{ }\mu\text{m}$. This uncertainty is visible when an image is captured on the microscopic camera and measured on the computer screen. This uncertainty can change the resonator size range from $3.1\text{ }\mu\text{m}$ - $3.4\text{ }\mu\text{m}$ to $3.08\text{ }\mu\text{m}$ - $3.42\text{ }\mu\text{m}$, which does not result in a significant change in the location of the emission peak or its value (confirmed in FEM-HFSS).

S.No	Resonator Size	Frequency
1	3.10 μm - 3.15 μm	10
2	3.15 μm - 3.20 μm	10
3	3.20 μm - 3.25 μm	11
4	3.25 μm - 3.30 μm	14
5	3.30 μm - 3.35 μm	22
6	3.35 μm - 3.40 μm	23

Table 6.1 Variable resonator size and frequency

The variation in resonator size influences the emission spectrum for the thermal emitter. The resonant frequency, the corresponding value of emissivity and Q-factor is unique for each resonator size. The resonator dimensions were fine-tuned in the design section such that with the silicon resonator size of 3.2 μm , resonator height of 1.05 μm and the silicon dioxide separation of 0.39 μm , the maximum emissivity of approximately 1 is at a resonant frequency of 41.6 THz with a Q-factor of 135. However, the variation in resonator size would result in different emissivity values at different frequencies as shown in Fig. 6.6(b). The emissivity is '1' for a resonant peak of 41.6 THz. The emissivity decreases for frequencies around 41.6 THz. The emissivity is negligible for resonators size of 3.35 μm and 3.4 μm . Table 6.1 shows that the maximum occurrence of resonators is for the resonator size of 3.35 μm and 3.4 μm . The thermal emitter was thus re-simulated to predict the response of the fabricated device, taking into account these predicted variations in the dimensions.

Figure 6.6 Variable resonators measured under microscope with zoom 100 $\times$ shown in (a) along with simulated emissivities for variable resonator sizes in (b).

With further inspection, it was determined that the variation in the resonator size was transferred from the lithographic mask, as mask feature sizes were consistent with the fabricated silicon resonators sizes. The mask was supposed to have a uniform features of size of 3.2 μm x 3.2 μm ,

however there was a variation in the feature size from $3.1\ \mu\text{m}$ to $3.4\ \mu\text{m}$. Conventional laser written masks have a typical critical dimension resolution of $0.25\ \mu\text{m}$, so for a feature size of $3.2\ \mu\text{m}$, this is approximately 8%. The mask used in this project was made using a laser system and the variation found in the mask was within 8%. The feature size can be made consistent by using an Extreme Ultraviolet (EUV) or Electron beam (E-Beam) technique to create small resonators. EUV [115] [116] and E-Beam [117] [118] lithographic systems are known to have consistency for feature sizes as small as a few nanometers.

6.3.2 Variation in RIE Etch Rate

A variation in the RIE etching of Silicon was found across the wafer. After the fabrication of the final device, profilometer readings showed that the underlying silicon dioxide has etched more on the sides of the wafer than at the center of the wafer as shown in Figure 6.7(a). The oxide thickness at the edge of the wafer after RIE etch was $0.36\ \mu\text{m}$ as compared to $0.39\ \mu\text{m}$ at the center of the wafer over a length of 21.4 mm. This meant that the oxide etch thickness changed $0.0014\ \mu\text{m}$ per mm. According to these calculations, the edge of the center most array of silicon resonator will have a variation of silicon dioxide thickness of $0.005\ \mu\text{m}$ going from the edge of the array to the center ($0.385\ \mu\text{m}$ to $0.39\ \mu\text{m}$). Simulation in HFSS was done to verify if this variation would cause a change to the emissivity or the Q-factor. Figure 6.7(b) shows that the emissivity for the two thicknesses of silicon dioxide hardly changed the emissivity or the Q-factor. This proved that this change in the RIE etch rate will not have any considerable effect in the measured thermal emissivity.

6.3.3 Fabrication Tolerance Modeling

The thermal emitter was remodeled in simulation to incorporate the variation in resonator size in the emissivity response. An array of 30 resonators with varying sizes was designed. The dimensions of the resonator in the simulation were set according to Table 6.1. The weight of each resonator size was calculated and set in the 30 resonator array, as shown in Figure 6.8(a). The device was re-simulated in HFSS with periodic boundary conditions. Figure 6.8(b) shows the comparison of the simulated emissivity of the multi-cell array after incorporation of the variations in the structure sizes and the measured emissivity.

Figure 6.7 Variable etch rate of Plasma RIE and its impact on thermal emissivity a) Illustration showing the nonuniform etching of Silica (figure not to scale), b) Emissivity for variable Silicon Dioxide thickness.

Figure 6.8 Redesigned thermal emitter with 30 multi-sized resonators, weighted according to Table 6.1. a) Simulation configuration and its b) Measured emissivity vs simulated emissivity with fabrication tolerance modelling

A good match between the two emissivities is obtained, both in terms of the location of the emissivity peak and its frequency bandwidth. These simulation results suggest that the variation in the resonator sizes is a prominent cause of lower Q-factors. The different resonance peaks combine as a single emission peak, which results in broadening of the bandwidth thus reducing the Q-factor, as compared to, emission peak from a single sized resonator. While the region above 50 THz isn't a perfect match, a more uniform variation in the resonator size will likely result in the combination of these multiple peaks into a single feature. The variation in the resonator sizes also leads to lower emissivities, as is clearly visible in Figure. 6.6(b). The variation in the resonator size can be improved through use of better mask making systems to provide uniform features across the entire metasurface.

6.4 Proposed Gas Sensor Assembly

The fabricated all-dielectric metasurface thermal emitter can be used as a source for an optical gas sensing system. A high Q-factor will enable the source to emit radiation of the desired resonant frequency and hence can be used without the aid of additional optical filters, which would require extra components to be fabricated/aligned in the optical gas sensing system. While the fabricated all-dielectric metasurface thermal emitter was not tested for power consumption, literature shows that MEMS based thermal sources having a narrow band emission generally operate at a relatively low power due to very low emission at frequencies other than at resonance. For this device to be incorporated in an optical gas sensing system, a gas cell along with a detector will be required. For a proof of concept experiment the emitter and the source can be placed in close proximity to each other as suggested by [5]. This can eliminate additional optical assemblies that may be required to collimate the emission from the source. A thermopile with lock-in amplification can be used as a detector. A lock-in amplifier system uses amplitude modulation of the sensor signal at a known frequency to reject noise and interference signal[119]. The cited example uses a Stanford SR830 lock-in with a thermopile detector with a sensitivity of 500 mV and a time constant of 3 seconds. This enabled detection of 400 ppm of CO₂. The source developed in this thesis will improve the cited device through increased Q factor leading to increased source efficiency.

While the designed thermal emitter emits a frequency corresponding to 41.6 THz due to mask restrictions, the metasurface can be re-designed to emit 71.2 THz for detection of CO₂. Figure 6.9 shows a typical assembly that can be used for CO₂ detection. The configuration has a narrowband emitter that will emit a radiation specific to the target gas (CO₂). The proposed gas cell will be approximately 10 cm with a silicon thermopile detector (HMS-J21, Heimann Sensor) to give a detection limit of 50 ppm as it has been demonstrated in the literature [120]. There will be another channel for the source without going through the sample for reference (not shown in figure). The

detected signals can be compared according to Beer-Lambert principle to evaluate the concentration of the target gas.

Figure 6.9 Proposed gas sensor assembly with all-dielectric metasurface thermal emitter as the source.

6.5 Conclusion

The emissivity of the fabricated metasurface emitter was measured and a narrowband thermal emission peaks was successfully obtained. However lower peak emissivities and larger bandwidth compared to ideal design simulations were observed. Inspection of the fabricated resonator array revealed variations in the resonator sizes, which appeared to originate with the photomask. When this size variation is included in numerical simulations, the measured Q-factor and frequency dependent emissivities were successfully recreated around the region of interest. With process improvements, particularly mask fabrication, these results indicate that it is feasible to fabricate a narrow-band metasurface thermal emitter at the desired frequencies with high Q-factors and large emissivities.

Chapter 7 Summary and Future Work

A state-of-the-art, all-dielectric metasurface thermal emitter has been designed, fabricated, and tested which can be used for different applications in mid-IR spectroscopy, specifically for optical gas sensing. This thermal emitter has a relatively simple standard CMOS fabrication process as compared to other reported dielectric based designs and offers a Q-factor higher than the conventionally used plasmonic-based thermal emitter. The design and simulation of two unique resonant frequencies of around 41.4 THz and around 74.65 THz corresponding to the absorption band of SO_2 and CO_2 respectively has been demonstrated. The thermal emitter can be re-designed for other gases having molecular absorption in the mid-IR, by simple tuning of the geometrical features of the metasurface unit cells.

The frequency dependent optical properties for silicon in the mid-IR region were missing from the literature. This thesis fills this gap by providing these optical constants. PECVD was used to deposit thin layers of silicon and silicon dioxide and no credible data for optical constants for both the materials were found for PECVD process. Hence their optical constants have been characterized using ellipsometry and reported. The ellipsometry data showed that silicon has a molecular resonance at 60 THz, and silicon dioxide at 67.7 THz and 101.5 THz. These resonances are introduced due to SiH_4 , that was used in PECVD to deposit these layers. The spectral range for this project was limited to 40 THz - 50 THz due to the periodicity of silicon resonators on the mask and the cut-off frequency of silicon dioxide. This range can be increased by decreasing the periodicity of the resonators, as demonstrated in Chapter 3.

The fabricated thermal emitters have been tested for thermal emissivity using FTIR. While, the resonant frequency of the emissivity matched with that of the design, the measured Q-factor and emissivity were lower than expected. The designed Q-factor was 140, whereas the measurements showed a Q-factor of approximately 38. Even though this is low, it is still higher than what has been reported by any plasmonic-based thermal emitter. The designed emissivity was 0.95, whereas the measured emissivity was 0.38. The drop in Q-factor as well as emissivity was attributed to the variable size of the periodic resonators in the mask that were transferred to the fabricated thermal emitter. The device was re-modeled in numerical simulator by incorporating the variable size resonator and both the measured Q-factor and peak emissivities were successfully reconstructed in the region of interest.

7.1 Future Work

This thesis showed for the first time the feasibility of using all-dielectric structures for achieving narrow-band thermal emission in the mid-IR region, with Q-factors larger than typically reported plasmonic structures, using a simple CMOS compatible configuration. While various challenges and issues were faced in this work, several steps and future works may be undertaken to remedy and improve the thermal emission characteristics and functionalities.

1. The spectral range for this project was limited to 40 THz - 50 THz due to the periodicity of feature size on the mask available for with work and the cut-off frequency of silicon dioxide. The spectral range can be increased by adjusting the periodicity of the resonators and modifying the mask. For example, a periodicity of $2.75\ \mu\text{m}$ as demonstrated in chapter 3 can increase the spectral range to 100 THz, making it suitable for CO_2 gas sensing which has wide-spread practical applications. However, the lower cut-off will be 40 THz due to the cut-off in silicon dioxide.
2. The ellipsometry data showed that silicon has a molecular resonance at 60 THz, and silicon dioxide at 67.7 THz and 101.5 THz. These resonances are introduced due to SiH_4 , used in PECVD to deposit these layers. These resonances are not ideal for thermal emitter designs between 40 THz and 100 THz. However, this can be resolved by using sputtering instead of PECVD to deposit Silicon Dioxide. Data available in the literature showed no internal resonance peaks in Silicon Dioxide.
3. The main performance limiting feature of the reported designs here has been the variations of the resonator dimensions following the laser-written masks. The Q-factor, as well as emissivity, can be significantly improved by using e-beam written mask instead of laser written mask. E-beam masks have a better uniformity in terms of feature size, albeit at a cost of higher fabrication costs. This could be the most practical way of achieving the high Q-factors as predicted by the numerical simulations.
4. Silicon Dioxide has a cut-off at 39 THz, which puts a lower limit on the spectral range. Other Dielectric materials can be explored to increase the frequency range of the thermal emitter with lower cut-offs and better electrical characteristics.
5. Only uniform all-dielectric metasurfaces has been demonstrated here. However, a non-uniform distribution of resonant features may be used to engineer and tailor the thermal emission. This may include multi-spectral emission with directional radiation, for instance, along with achieving polarized emissions at the desired frequencies.

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