A STUDY OF NOVEL MID-INFRARED OPTICAL DEVICES: WAVE PLATES AND TUNABLE FILTERS

BY

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THESIS

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ABSTRACT

The mid-infrared wavelength range is important for both molecular sensing and thermal imaging. However, many optical devices that are common in the visible range are not as accessible in the mid-infrared. In this thesis, we look to partially address this problem by proposing two novel structures using subwavelength gratings. First, we look at a wave plate design that uses a physical path length difference to impose a phase shift between the components of incident light as an alternative to costly birefringent crystals. Then, we look at a crossed grating structure that serves as a narrowband filter due to its extraordinary transmission. We also propose a way to make the filter structure actively tunable.
To my parents, Brian and Gail Taylor, for their love and support
I would like to thank Professor Daniel Wasserman for his direction and guidance through this process. His patience and accessibility as well as generous sharing of knowledge has had a significant positive impact on my research experience. I would also like to thank Dr. Stephanie Law for her constant support and advice on any and all topics. I have had the luxury of a fantastic research group, especially Lan Yu and Will Streyer, who were with me from the beginning and always had my back. Aaron Rosenberg, Gino Rooney, Tom Jacobs, Torin Kilpatrick, and Nish Nookala also had an impact on my time here.

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CHAPTER 1

INTRODUCTION

The mid-infrared (mid-IR) spectral range, which spans wavelengths from about 2 to 30 μm, is crucial for a variety of applications, including sensing and defense, as a result of several important characteristics. First, the fundamental absorption resonance of a significant number of molecules falls in the mid-IR. Every molecule has a distinct set of absorption lines, and this molecular fingerprint allows the presence and quantity of molecules of interest to be detected via optical sensing. Additionally, the peak black-body radiation of many biological and mechanical objects falls in the mid-IR. Black-body radiation is a type of electromagnetic radiation produced by a body held at constant temperature. The emitted spectrum is heavily dependent on the temperature of the object and is centered in the mid-IR for temperatures ranging from about 100 to 1500 K. As a result, the mid-IR is a vital wavelength range for defense technologies reliant on thermal imaging, such as night vision goggles and heat-seeking missiles.

There are a number of well-understood optical devices that are used to control, generate, or interact with light, from lenses to polarizers to lasers. Most such devices were designed and realized for the visible portion of the electromagnetic spectrum, because that is the light the human eye perceives. However, there has generally been less of a push to create these products for the mid-IR, even though they are necessary to conduct research in that spectral range. Historically, the research push in the mid-IR has lagged behind the visible and near-IR, but the mid-IR is becoming more important now due to new sources of mid-IR light that allow for compact and efficient sensors and systems [1]. In this thesis, we have created two structures that aim to improve the arsenal of mid-IR optical devices through innovative use of subwavelength gratings.
A diffraction grating is a well-understood optical component that uses a periodic structure to split an incident beam of light into several reflected or transmitted beams traveling in directions determined by the incident angle, wavelength, and periodicity. The reflected or transmitted angle of a given mode \( q \) can be determined by momentum conservation and is given by

\[
\sin(\theta_q) = \sin(\theta_i) + \frac{q \lambda}{\Lambda} \tag{1.1}
\]

or

\[
\theta_q = \sin^{-1}[\sin(\theta_i) + \frac{q \lambda}{\Lambda}] \tag{1.2}
\]

where \( \theta_i \) is the incident angle, \( \lambda \) is the wavelength, \( \Lambda \) is the grating periodicity, and \( \theta_q \) is the reflected or transmitted angle of mode \( q \) [2].

Subwavelength gratings are a type of grating with a period that is less than half the wavelength of light, namely \( \frac{\lambda}{\Lambda} > 2 \). Therefore, \( q \) must equal 0 in order to satisfy Equation 1.2, meaning only the 0th order mode exists. For normal incidence (\( \theta_i = 0 \)), the structure behaves as a subwavelength grating for \( \frac{\lambda}{\Lambda} > 1 \). Subwavelength gratings are used in a number of common optical devices, including wire-grid polarizers [3],[4], anti-reflection surfaces [5],[6], and graded-index components [7],[8]. These devices are used in a variety of applications such as imaging, spectroscopy, polarimetry, and integrated optics.

We have created two novel mid-IR optical devices that take advantage of subwavelength gratings to provide a specific useful function in this important wavelength range. First, we introduce a mid-IR wave plate, a device used to control the polarization of light. Wave plates are used in any application that requires control over polarization, including lasers, biomedicine, and aerospace, and in the mid-IR they are especially suited for sensing applications. Wave plates typically are made of birefringent crystals, which have a different refractive index between the two polarization axes. The different refractive index means the two polarization components propagate at different velocities, causing an effective path length difference between the orthogonal polarizations and leading to a phase shift as light passes through the crystal. Unfortunately, birefringent crystals are rare and expensive in the mid-IR. Instead, we have designed a wave plate that uses a subwavelength grating above a metallic ground plane to induce a phase shift due to a phys-
ical path length difference between the polarization components. This new design matches the performance of birefringent crystals at a fraction of the manufacturing costs.

The second device is a narrowband tunable filter that allows the spectral isolation of a specific wavelength, which is useful for (among others) molecular sensing. The filter can be tuned to a molecular resonance wavelength and will block all other light. The result is a signal that is either on or off depending on the presence of a particular molecule. The device consists of two gratings oriented perpendicular to one another, which yields an extraordinary transmission peak that can be tuned spectrally by adjusting the separation between gratings.

Chapter 2 details the motivation, design, and performance of the wave plate, while Chapter 3 does the same for the narrowband filter. Chapter 4 concludes the thesis.
2.1 Background

A wave plate is a well-understood type of optical device that alters the polarization of light. Polarization is a property of transverse waves that have more than one possible orientation. In the case of an electromagnetic wave, the polarization refers to the orientation of the electric field as the wave propagates through space. For a single photon, linear polarization is characterized by the electric field oscillating along a single transverse axis (Figure 2.1(a)), while elliptical polarization is characterized by the electric field rotating around the propagation axis. If the electric field has a constant magnitude as it rotates, the photon has a circular polarization (Figure 2.1(b)). If each photon in a beam of light has a different polarization, it is called unpolarized light, but if all the photons are the same, it is called linearly, elliptically, or circularly polarized light accordingly.

By breaking down the electric field into two components that make up the transverse plane, we can identify the type of polarization by the relative phase ($\Delta \phi$) between the components. The light is linearly polarized if $\Delta \phi = 0$ or $\Delta \phi = \pi$, and circularly polarized for $\Delta \phi = \frac{\pi}{2}$ or $\Delta \phi = \frac{3\pi}{2}$. Any other phase difference corresponds to elliptical polarization. A wave plate changes the relative phase by creating a path length difference between components as the light propagates. If the relative phase is changed by $\pi/2$, the device is called a quarter-wave plate (QWP). Quarter-wave plates convert linear polarization to circular and vice versa. If the relative phase is changed by $\pi$, the device is called a half-wave plate (HWP). Half-wave plates do not change the type of polarization, but do change the orientation of the linear polarization axis and the direction of rotation for circular or elliptical polarization.

Wave plates have application in virtually any field where the polarization
Figure 2.1: This figure shows the magnitude of a photon’s electric field as it propagates through space for linear (a) and circular (b) polarizations. The blue and green lines show the magnitude of the two transverse components projected onto their respective planes. The red line shows the magnitude and direction of the electric field. Images from commons.wikimedia.org.
of light needs to be controlled or analyzed, ranging from biological sensing [9],[10] to astronomy [11],[12]. Many applications involve polarimetry, which is the measurement and interpretation of the polarization of a wave. Polarimetry is especially useful in measuring waves that have somehow (via reflection, refraction, etc.) interacted with a material. The polarization of the resulting wave can be used to characterize the material. For example, research has been done analyzing the viability of using laser radar polarimetry to distinguish satellites from natural near-earth objects and man-made debris in space [13]. Essentially, polarization-controlled laser light is reflected off the object, and the returning wave is analyzed. Depending on how the polarization of the returning light has changed, the material properties of the object can be determined and the type of object can be identified.

Wave plates are a key element of many polarimetric systems. A generic polarimeter consists of two parts, one that generates light, and another that receives light. Light is generated with some form of (often unpolarized) source and passes through a polarizer to make linearly polarized light. One or more wave plates can then be used to convert that light to any desired incident polarization. After interacting with the target object, additional wave plates and polarizers are used to identify the resulting polarization.

In the visible spectrum, a wave plate is typically made using a birefringent crystal, which has interesting properties because it is an anisotropic medium, meaning the permittivity is rotationally dependent. Specifically, birefringent media are uniaxial, characterized by a permittivity (from [14]) of the form

$$\epsilon = \begin{bmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon_z \end{bmatrix}. \quad (2.1)$$

A wave propagating in the \(\hat{x}\) direction will experience a different refractive index in the \(\hat{y}\) and \(\hat{z}\) polarizations. In the \(\hat{y}\) direction, there is an ordinary wave with a wavenumber given by \(k_o = \omega \sqrt{\mu \epsilon}\) where \(\omega\) is the angular frequency of the incident wave and \(\mu\) is the permeability. In the \(\hat{z}\) direction there is an extraordinary wave with a wavenumber given by \(k_e = \omega \sqrt{\mu \epsilon_z}\). Since wavelength (\(\lambda\)) is inversely proportional to wavenumber (\(\lambda = \frac{2\pi}{k}\)), the \(\hat{y}\) and \(\hat{z}\) components have different wavelengths in the crystal and the relative phase is constantly changing as the light propagates. Therefore, varying the
thickness of the crystal allows control over the relative phase. For an incident wave given by

\[ E = \left( \hat{y} \frac{1}{\sqrt{2}} + \hat{z} \frac{1}{\sqrt{2}} \right) E_0 e^{i k x} \tag{2.2} \]

the wave upon exiting the birefringent material will have the form (ignoring reflection)

\[ E = \hat{y} \frac{E_0}{\sqrt{2}} e^{i k_o d} + \hat{z} \frac{E_0}{\sqrt{2}} e^{i k_e d} = \left[ \hat{y} + \hat{z} e^{i(k_e - k_o) d} \right] \frac{E_0}{\sqrt{2}} e^{i k_o d}. \tag{2.3} \]

As a result, the \((k_e - k_o) d\) term is the phase difference between the \(\hat{y}\) and \(\hat{z}\) components. A quarter-wave plate (phase difference of \(\pi/2\)) is defined by

\[(k_e - k_o) d = \left\{ \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots \right\} \tag{2.4}\]

\[d = \frac{(2m + 1)\pi}{2(k_e - k_o)} \quad m \geq 0 \tag{2.5}\]

and a half-wave plate (phase difference of \(\pi\)) is defined by

\[(k_e - k_o) d = \{\pi, 3\pi, 5\pi, \ldots\} \tag{2.6}\]

\[d = \frac{(2n + 1)\pi}{k_e - k_o} \quad n \geq 0 \tag{2.7}\]

where \(m\) and \(n\) are integers.

In the visible wavelength range, birefringent wave plates are well understood and easy to make, leading to affordable commercial products across the spectrum. However, the mid-infrared range presents a much more difficult challenge. In this range, birefringent wave plates exist but are both rare and excessively expensive. For example, Edmund Optics supplies quarter- and half-wave plates in the mid-IR range for a cost of $2,895.00 [15]. In this chapter, I will introduce a new reflective wave plate design that matches the performance of a birefringent crystal at a fraction of the cost.

2.2 Design

We have designed a reflective metal-dielectric structure that attacks the relative phase change problem in a unique and novel way. Instead of creating an
effective path length difference using refractive index, we create a physical path length difference between the two light components. This difference is achieved by placing a metallic grating (which serves as a wire-grid polarizer) above a fully metallic ground plane (see Figure 2.2). The component of the electric field parallel to the grating is reflected from its surface, while the perpendicular component passes through and reflects from the underlying metallic ground plane. The perpendicular component, therefore, takes a longer path. Both components are reflected back at the same angle and recombine, but a relative phase difference has been introduced due to the path length difference. This phase change can be tuned by changing the thickness of the dielectric spacer (d) to achieve a quarter-wave or half-wave plate.

![Reflective wave plate design](image)

**Figure 2.2: Reflective wave plate design.**

While the basic design can be applied to any wavelength range, it is more practical for longer wavelengths, both due to the inherent need for longer wavelength wave plates and because the device size scales with wavelength. In the terahertz, for example, it is a commonly used technique to place a wire-grid polarizer above a mirror to manipulate the relative path and create
a wave plate. In the visible range, the device dimensions are small enough to make fabrication impractical, but in the mid-infrared we find a scale at which we get both good performance and manufacturability.

There are two major design parameters that must be considered: the angle of incidence (Ω) and the wavelength of the incident light. A birefringent wave plate induces a phase shift on transmitted light that passes through the crystal, while our design reflects light. As a result, normal incidence is not a practical solution because it is difficult to access the reflected light. A beamsplitter would be required to separate out the incident and reflected light, which causes efficiency to drop by a factor of 4. Therefore, we chose a design angle of incidence of 45 degrees, in order to simplify application and optimize throughput.

The second important parameter is the wavelength. Like the angle of incidence, the wavelength is chosen prior to designing the physical parameters of the device. Namely, wavelength and incidence angles are chosen, and the physical device parameters are determined to accurately provide either a quarter-wave or half-wave plate at the given design parameters. We chose a wavelength of 3.3 µm, because that is roughly the center wavelength that Sandia’s M Squared Firefly-IR mid-IR laser can provide; however a device could be designed for any mid-IR wavelength.

Once the wavelength and incidence angle are selected, there are three physical parameters by which we can control the behavior of the device. The first two are the pitch (p) and duty cycle (w/p) that define the grating. The grating parameters are chosen to maximize the transmission of one component while minimizing the transmission of the other, and are determined via simulation. The third parameter is the separation (d) between the grating and the gold ground plane. This separation controls the total path length difference between the two components.

2.3 Simulation

In order to theoretically confirm the concept and to determine appropriate physical parameters, I did extensive simulations of this structure using the finite-difference time-domain (FDTD) method. FDTD is a method of solving electrodynamic problems using the finite difference method, which is
a mathematical process designed to solve differential equations by approximating the value of partial derivatives. To solve electromagnetic problems, FDTD discretizes the time-domain Maxwell’s equations space and time partial derivatives to create a problem where electric and magnetic field values can be solved given the fields in the previous step in space and time. The simulation region is broken spatially into a mesh, and a time-domain pulse containing the desired simulation wavelengths is introduced from a designated source plane. The simulation then discretely steps through time, solving the electric and magnetic fields in leapfrog fashion. Specifically, the electric field is solved across the mesh at a given instant of time; then, the magnetic field is solved at the next time step using the previous state. The simulation continues in this fashion until the total amount of field strength remaining in the region drops below a user-selected threshold.

The simulations were done using Lumerical FDTD Solutions [16], which provides a graphical user interface to simplify design and simulation. A three-dimensional structure consisting of a unit cell of the device (one strip of the grating (see Figure 2.3)) was used in the simulation. The width of the simulation area determines the periodicity of the grating, and the width of the strip relative to the simulation area determines the duty cycle. The separation between the grating and the ground plane is also defined. In addition to the structure to be modeled, a source needs to be present. In these simulations, the pulse entered the simulation region from above with a 45 degree incidence angle, per the design parameters. In order to accurately represent the full structure, as opposed to just the unit cell, Bloch boundary conditions were used on all four sides of the simulation region. Block conditions behave as periodic boundary conditions with an added phase shift to account for the angled incident field. So, the simulation is effectively simulating a structure with the unit cell repeated to infinity in all four directions in the XY plane. Finally, I placed a field monitor in the simulation area to determine how the electric field at a fixed point changes as the pulse propagates through the structure. The monitor was placed between the structure and the source, in order to capture both the incident and reflected waves. Both the monitor and source were many wavelengths away from the device to ensure an accurate simulation.

Because the simulations run in the time-domain, the input pulse is inherently a time-domain pulse. However, we want to specify the input electro-
Figure 2.3: Screen shot of Lumerical simulation. Orange and blue lines show the borders of the simulation region. Gold material is shown in yellow, silicon nitride in gray, and air in black.

magnetic wave at the design wavelength of 3.3 µm. The software takes the user selected wavelength or wavelength range and takes a Fourier transform to produce a time-domain pulse to be inserted into the simulation region. The result is a time-domain incident wave that oscillates as a sine function at the correct wavelength, and whose magnitude is represented by a Gaussian envelope function (see Figure 2.4). To identify the phase shift, we can look at the x and y components of the incident and reflected pulses, and determine how the two components behave.

In order to assess the suitability of a given parameter set, two key performance metrics were evaluated, namely the phase difference between the x and y polarization components and the efficiency. In order to understand the best method for calculating these values, we first looked at what data was available. Figure 2.5(a) shows the full monitor output for a half-wave plate (50% phase change) design. The first Gaussian envelope function contains the incident wave, while the second contains the reflected wave. Figures 2.5(b) and 2.5(c) show the incident and reflected waves contained by the envelope function.

From these figures, it is clear there was a phase change between the two components after reflecting off the wave plate, as expected. The phase shift was calculated by first finding the two largest peaks in the x-component and
Figure 2.4: The incident wave. A sinusoidal function is contained within a Gaussian envelope function. Only the positive values are shown here to simplified the graphic. Both $E_x$ and $E_y$ are shown, but they overlap exactly in the incident pulse.
Figure 2.5: (a) Incident and reflected waves for a half-wave plate simulation (positive values only). (b-c) $E_x$ and $E_y$ overlap on the incident pulse, but $E_y$ is delayed after contact with the wave plate.
measuring the time-domain distance between them, given by $\Delta x$ (see Figure 2.6). We then identified the location of the nearby peak in the y-component, relative to the first x peak, and called the separation $\Delta y$. The phase shift can then be calculated using $2\pi \frac{\Delta y}{\Delta x}$. A half-wave plate, as is shown in Figure 2.5, will have a phase shift of approximately $\pi$.

![Figure 2.6: Measuring the phase shift.](image)

To determine the efficiency, the peak value in the reflected wave was divided by the peak value in the incident wave for each component. The overall efficiency was important because it was important to maintain signal strength and limit losses. However, the ratio of the x efficiency to the y efficiency was also important to consider. If the ratio differed from the desired 1:1, the beam, regardless of polarization, would become distorted. Specifically, circularly polarized light would become slightly elliptically polarized with the major axis aligning with the stronger polarization component. Likewise, linearly polarized light would no longer be angled at 45 degrees, and would instead tilt in the direction of the weaker polarization. Figure 2.7 demonstrates this phenomenon.

The pitch, duty cycle, and separation parameter spaces were simulated to determine the combination that provided the desired phase change with limited losses. Specifically, we were looking to design both a quarter-wave plate ($\Delta y/\Delta x = 0.25$) and a half-wave plate ($\Delta y/\Delta x = 0.25$). With a constant pitch and duty cycle, the separation controlled the phase shift without having a large impact on efficiency and could therefore be used to tune the phase shift. As a result, pitch and duty cycle were chosen to maximize efficiency. This choice was made by designing the grating to exhibit polarizer-like behavior, ideally reflecting 100% of one polarization while passing 100% of the other. Simulating that parameter space gave a pitch of 220 nm and a metal
width of 70 nm as the ideal parameters to both maximize efficiency and balance the $x$ and $y$ polarizations. Given these values, varying the separation resulted in a gap of 340 nm for a quarter-wave plate (94.4% efficiency) and 465 nm for a half-wave plate (92.8% efficiency). The half-wave plate result is shown in Figure 2.5.

Given a device design, we then sought to understand how each of the five parameters impacted the behavior of the wave plate by running simulations varying each parameter (wavelength, incidence angle, pitch, duty cycle, and separation) from the half-wave plate design specifications while keeping the other parameters constant (see Figure 2.8). Pitch, duty cycle, and separation are fixed once the sample is fabricated so the data only matters so far as determining ideal parameters, but there are several interesting characteristics of this trend data. First, changing the grating pitch without changing duty cycle has minimal impact on the phase shift, while the separation has a significant impact (Figure 2.8(a)). In fact, changing the separation by about 25% in either direction results in a $\pi/2$ or $3\pi/2$ phase shift, which is our quarter-wave plate design. However, the grating pitch experiences a
Figure 2.8: Phase shift (a) and efficiency trend (b) graphs for incidence angle, wavelength, duty cycle, pitch, and separation.
Figure 2.9: Phase shift and reflection efficiency as a function of wavelength (a) and incidence angle (b). The parameters vary from a phase shift of $\pi$ at the design parameters of 3.3 $\mu$m wavelength and 45 degree incidence. The limited variation in efficiency means these parameters can be used to change the phase shift as necessary.
significant drop-off in efficiency once it reaches a threshold size, caused by the grating size being too large to act as a good polarizer (Figure 2.8(b)). The result is that a polarization will have some percentage reflection and some percentage transmission at the grating. Since light that reflects off the ground plane experiences an additional $\pi$ phase shift, the result is destructive interference between the light the grating reflects and the light it passes, hence a drop in efficiency.

The wavelength and incidence angle, on the other hand, can be altered post-fabrication and have a significant impact on the magnitude of the phase shift (see Figure 2.9). Both parameters were able to tune the phase shift in either the positive or negative direction depending on how they deviated from the design value without significantly altering efficiency. This property was useful for two reasons. First, any slight deviation from the ideal device geometry in fabrication could be compensated for by varying one or both parameters. Second, a positive shift due to changing wavelength could be compensated for with a negative shift in incidence angle. As a result, the device was tunable over a wavelength range of several hundred nanometers.

2.4 Fabrication

The devices were fabricated by cleanroom staff at Sandia National Laboratories using a gold grating and ground plane and a silicon nitride buffer. The grating was patterned with e-beam lithography because the features were too small to fabricate with photolithography. The first devices to be fabricated had a period of 220 nm, line width of 70 nm, and separations of 340 nm and 465 nm, as the simulations predicted. However, there were problems with the nitride deposition process, leading to an absorption peak at a wavelength of 3.2 $\mu$m, which falls in our desired performance range. As a result, the deposition method was altered to avoid the absorption peak, leading to a change in the SiNx refractive index. As a result, the samples were fabricated with a separation of 400 nm after new simulations were performed.
2.5 Testing

The test setup (see Figure 2.10) was built around an M Squared Firefly-IR optical parametric oscillator laser with a tunable wavelength range of 2.4 to 3.6 µm. First, the output power is significantly attenuated by a neutral density filter such that it will not damage any of the supporting devices. The initial laser beam is vertically polarized, so we use a wire grid polarizer angled at 45 degrees to balance the vertical and horizontal components. The beam then passes through an iris aperture to limit the beam diameter such that it is only incident on the relatively small patterned area. After striking the sample at 45 degree incidence, the light passes through another polarizer in a rotating mount. A Kolmar Technologies InSb photodiode is used to capture the light. We also used a lock-in amplifier to minimize the impact of noise, with a 650 Hz chopper in the beam path. In order to account for fluctuating laser output power, there is a beamsplitter prior to the first grating that sends half of the light to a ThorLabs pyroelectric power meter. The entire setup is controlled automatically by a LabVIEW program.

![Figure 2.10: Test setup diagram.](image)

The efficiency was also measured using this setup. To measure total efficiency, the second polarizer was removed and the total signal reflecting off the sample is background-adjusted to the total signal reflecting off a flat gold-coated substrate. To measure the efficiency of the polarization components individually, the same experiment was performed with the second polarizer
oriented to pass either vertical or horizontal light. As described above, it is important for the two polarizations to have similar efficiencies because an unbalanced ratio of vertical to horizontal light will skew the resulting wave.

To determine the phase shift, we measured the angle dependence of transmission through the second polarizer. Specifically, we rotated the polarizer 180 degrees in steps of 5 degrees and measured the transmission at each angle. This allowed us to identify if the light was linearly, elliptically, or circularly polarized. If the light was circularly polarized, the electrical field would be balanced amongst all 360 degrees and would therefore appear as a straight horizontal light on the intensity vs. angle plot (see Figure 2.11). Linear polarization, on the other hand, would pass 100% of the light at one polarizer angle while passing 0% of the light at another. For elliptical polarization, the shape would be somewhere in between, depending on the shape of the ellipse. Given that the incident light was linearly polarized, we expected a quarter-wave plate to produce circularly polarized light and a half-wave plate to produce linearly polarized light.

![Figure 2.11](chart.png)

(a) Cartesian  
(b) Polar

Figure 2.11: Anticipated intensity plots as a function of the second polarizer angle. The expected shapes for linear, elliptical, and circular polarizations are plotted in both Cartesian (a) and polar (b) coordinates. We should be able to compare our results to these charts to determine the type of polarization.
2.6 Results

The results described in this section were obtained with the 400 nm separation wave plates created after I left Sandia National Labs, so I was not involved in the testing, and the data does not match the simulations described above. However, the simulation and testing processes fit with what was ultimate done to achieve these results.

The wave plates behaved as expected, demonstrating a clear change in polarization. The samples tested were designed as half-wave plates, and achieved a strongly linear polarization rotated 90 degrees from the incident beam, as shown in Figure 2.12(a). The measure efficiency was in the 88% to 90% range, which is on par with commercial birefringent wave plates. The wave plate was also shown to be highly tunable, over a range of about 300 nm in wavelength, by adjusting incidence angle.

Additionally, the wave plate was used to demonstrate both half- and quarter-wave retardation at an incidence angle of 25 degrees, as shown in Figure 2.12(b). At a wavelength of 2.4 µm, the wave plate induces a roughly \( \frac{\pi}{2} \) phase shift, while at 3.3 µm wavelength the wave plate induces a \( \pi \) shift. In all, the wave plate clearly demonstrated the behavior predicted by simulation and showed its viability as an alternative for birefringent plates.

2.7 Next Steps

Given that the material cost is minimal, we believe these devices can be mass produced at a significantly more affordable rate compared to the competition. The current cost-limiting factor is the need for e-beam lithography. If mass produced, nanoimprint lithography (NIL) may provide a cheaper substitute. NIL uses a mold containing the desired topological features that is pressed into an imprint resist to transfer the pattern. The resist is then cured, and selective etching is done to transfer the features to the underneath material. The process has been used to make gratings with pitches in the tens of nanometers [17], so there would be no resolution issues with our gratings. There is a larger up-front cost with NIL due to the need to make a mold, but since the mold is reused it becomes economically viable at large throughput. Additionally, tunability in both wavelength and incidence angle may allow
Figure 2.12: Wave plate results. (a) Intensity vs. angle at 45° incidence and varying wavelength. The results clearly show strong linear polarization, meaning the half-wave plate worked as designed. (b) Intensity vs. angle at 25° incidence and varying wavelength. The results show a clear change in polarization across the laser’s wavelength range from 2.4 µm (roughly circular) to 3.3 µm (linear), confirming the tunability of the wave plate and demonstrating the viability of a quarter-wave plate.
for commercial products that are tunable in wavelength.

We have successfully demonstrated the viability of quarter- and half-wave plates in the mid-infrared. The efficiency is on par with existing birefringent wave plates in the same wavelength range. Overall, we believe this mid-IR wave plate design is a significant improvement on existing technology because it provides comparable performance at a lower price point.
CHAPTER 3
TUNABLE FILTERS

3.1 Background

The second mid-infrared optical device we have looked at is a narrowband tunable filter for the mid-IR. Filters have a wide variety of useful applications, but one of the most important for this wavelength range is sensing. As discussed in the introduction, the mid-IR contains a molecular resonance wavelength for a vast number of molecules. The ability to selectively permit transmission of a given wavelength, therefore, allows for the creation of a molecule-specific detector (such as carbon monoxide or ozone). Furthermore, the ability to tune the transmitted wavelength would allow the user to detect multiple molecules with the same device.

The mid-IR is also home to the majority of black-body radiation for objects with temperatures ranging from about 100 to 1500 K. While sensing an object in a room, for instance, is not feasible due to all of the objects being at about the same temperature, black-body radiation detection is important in other remote sensing fields, such as astronomy [18]. While stars are too hot to fall in this wavelength range, there are interesting interstellar objects such as dust clouds and planets that are best sensed in the mid-IR.

Given that most black-body emission for terrestrial temperatures occurs throughout the mid-IR, tunable filters are also useful in their ability to vary transmission at a fixed wavelength. For example, an object radiating at some wavelength could be cloaked and uncloaked by setting the transmitted wavelength at or far from that wavelength. As a result, filters are potentially applicable in security and defense as well as sensing.
3.2 Design

We have created is a tunable filter designed by placing two polarizer-like gratings perpendicular to each other with narrow separation (Figure 3.1). At large separation, two crossed polarizers will block 100% of incident light, due to the inherent nature of a polarizer. However, at separation much smaller than the wavelength, some amount of light does in fact pass through the structure, as demonstrated by simulation and experimentation described below.

![Tunable filter design](image)

Figure 3.1: Tunable filter design. Two gold gratings with pitch $p$ and metal width $w$ are encased in silicon nitride, separated by a distance $d$ and oriented perpendicular to each other.

It is important to note that it is not broadband light that is transmitted. In fact, there are various spectral peaks in the 2 to 12 $\mu$m wavelength range that allow these structures to behave as filters. The location and shape of the peaks is altered by adjusting any of the three parameters that define the structure, namely grating pitch, grating duty cycle, and, most importantly,
separation between the gratings. This property leads to the possibility of a tunable filter because an electrically tunable separation would lead to the ability to selectively choose a transmission wavelength.

The physics behind the transmission peaks are not well understood. Simulation has shown there is clear coupling between the two gratings, as would be expected given the enhanced transmission. One possible explanation comes from extraordinary optical transmission (EOT), demonstrated by Ebbesen et al. through a two-dimensional subwavelength hole array in metal [19]. Transmission significantly exceeded what was predicted by traditional aperture theory. This phenomenon has since been demonstrated in the mid-IR [20]. Extraordinary transmission has also been demonstrated through metal gratings placed parallel (instead of perpendicular as in our structure) with a subwavelength separation [21],[22]. In both cases, surface plasmons are thought to assist transmission through the structures. It is therefore a reasonable prediction that enhanced transmission through our cross grating structures results from some form of surface plasmon assistance.

In principle, the structure can be modulated using some kind of MEMS device, as described in Section 3.7. However, the first step, which is in fact the end goal of this thesis, is to demonstrate the extraordinary transmission peak physically, in addition to demonstrating it via theory and simulation. In order to successfully do so, we designed a structure consisting of gold gratings suspended in a silicon nitride film. Silicon nitride, which in our case is thin enough to have minimal absorption, provides physical structure and allows the gratings to be suspended in air to achieve symmetry.

3.3 Simulation

The cross polarizer structures were simulated using Lumerical FDTD at Sandia National Laboratories. The goal of the simulation was to explore the parameter space of period, duty cycle, and grating separation and to identify the combinations that give the best results. The process is similar to the simulation detailed in Section 2.2, so elaboration is not needed about the mechanics of the FDTD or Lumerical here. The key differences between the wave plate simulation and the tunable filter simulation will be discussed.

The first key difference is clearly the basic device structure, but the simu-
lations also differ in the ultimate objective. Instead of measuring reflection at a given incidence angle, the goal is to determine transmission properties at normal incidence. As a result, the monitor (which detects electric field strength) was placed on the opposite side of the structure from the source (see Figure 3.2(b)). Additionally, the sides of the simulation region used periodic boundary conditions instead of Bloch boundary conditions since we no longer need a phase change to account for angled incident light. Since the structure is symmetrical through both vertical planes, symmetry was used to shorten the simulation time by a factor of 4.

There is also a significant change in the source output and how we read the data. In the wave plate simulation, we wanted a specific wavelength input, and we cared about the time-domain phase properties. However, we want the cross polarizers to behave as a filter, and therefore we want to input broadband light and measure the frequency-domain transmission spectrum. Ideally, we are looking for a peak somewhere in the 2 to 12 $\mu$m wavelength range that is tunable with our three parameters, pitch, duty cycle, and separation.

In order to optimize the device parameters, a script was used to simulate the three-dimensional parameter space. Grating period data was taken from 2 to 5 $\mu$m in increments of 1 $\mu$m, metal width was taken from 0.8 to 2 $\mu$m in increments of 0.2 $\mu$m, and grating separation was taken from 0 to 600 nm in increments of 150 nm. From there, the period/metal width combinations that
did not have a peak with more than 50% transmission were taken out, and the simulations were rerun with separation from 0 to 600 nm in increments of 100 nm to get better resolution on how the peaks shifted with varying separation. Data was taken for polarizations both with and against the first grating.

Several important observations came to light after running simulations. Using a monitor in Lumerical, a video was taken to show how light propagates through the medium. The video showed clear coupling between the two gratings, because a non-negligible amount of energy was trapped between the gratings. Additionally, there was no polarization dependence, as predicted by time-reversal symmetry.

The spectrum itself is somewhat unpredictable. Across the 2 to 12 $\mu$m range, each spectrum has multiple large peaks and various other spectral features. However, isolating a specific peak allows for the demonstration of our desired spectral tuning. Figure 3.3 shows the $p = 3$ $\mu$m, $w = 0.8$ $\mu$m grating pattern for $d = 400$ nm, $d = 500$ nm, and $d = 600$ nm. Each spectrum has multiple peaks with over 50% transmission, but by focusing on a narrower wavelength range, a clearer picture emerges. The transmission peak clearly shifts over the range shown in Figure 3.3(b) while the separation is varied.

For the purpose of making a narrowband filter, the key features are the width of the peak and the strength of the peak relative to the noise. The three peaks shown in Figure 3.3(b) have full-width at half-maximum (FWHM) values of 450 nm, 400 nm, and 320 nm, respectively, giving them Q-factors (Peak wavelength/FWHM) of 13.2, 15.8, and 20.8, respectively, which puts them in the range of narrowband filters.

All three peaks have more than 65% peak transmission, which is strong considering the classically expected transmission. For an actively tunable filter, the key characteristic is the ON/OFF ratio at a given wavelength. This ratio shows the ability of the filter to control transmission of a specific wavelength. In this measure, the simulations perform well. At a wavelength of 6.4 $\mu$m, the ratio between the 500 nm spectrum and the 400 nm spectrum is almost 75. Therefore, light at that wavelength can be selectively transmitted simply by varying the separations between gratings.
Figure 3.3: Spectral shift demonstrated by varying the separation between gratings, $d$. The grating parameters are $p = 3 \ \mu m$, $w = 0.8 \ \mu m$. The spectrum spanning 2 to 12 $\mu m$ is shown in (a), while (b) shows a targeted portion of the spectrum where the best shift occurs.
3.4 Fabrication

The cross polarizers were fabricated in the Micro and Nanotechnology Laboratory (MNTL) cleanroom located at the University of Illinois at Urbana-Champaign. The materials were deposited epitaxially on an indium phosphide (InP) substrate, which was ultimately removed to leave a thin film containing the structure. The gratings were made of gold and structurally supported in a film of silicon nitride such that the device could stand alone. The detailed process is described in this section (see Figure 3.4).

![Diagram of fabrication steps](image)

Figure 3.4: Tunable filter fabrication steps.

The devices were deposited onto a rectangular sample approximately 7 to 9 mm on a side that was taken from a dummy-grade 3 inch indium phosphide wafer purchased from InPact. The electrical and optical properties of the substrate were unimportant, but a polished surface with minimal defects was essential. The first layer was a 200 nm thick SiNx film deposited using an STS plasma-enhanced chemical vapor deposition (PECVD) tool (Figure 3.4(a)). This layer is an outer boundary of the silicon nitride film.

Next, the first grating layer was created through a multi-step process (Figure 3.4(b)). A layer of AZ5412 photoresist was spun on at 7000 rotations per minute for 30 seconds, leaving a layer that was approximately 1 µm thick. The edge bead was removed using a wooden dowel dipped in acetone and carefully moved along the edges of the sample. This step was necessary in
order to ensure a totally flat surface to achieve the best possible contact. A Karl Suss MJB-3 aligner was used to pattern a periodic grating pattern 3 mm by 3 mm in size. There were a number of mask patterns, with differing periods and duty cycles to choose from. An exposure time of 5 seconds was used with a bulb wavelength of 320 nm. In order to get the best possible contact, and therefore the straightest photoresist sidewalls, the exposure was done in vacuum mode using a vacuum chuck. The pattern was developed using AZ 327 developer, leaving strips of photoresist that correspond to the gaps in the grating. A Cooke evaporator was used to deposit 10 nm of titanium (Ti), followed by 50 nm of Au, via e-beam evaporation. The Ti was necessary because gold does not attach well to SiNx. The photoresist was removed by placing the samples in acetone and sonicating for 20 seconds on 40% power.

Another layer of SiNx was applied to provide a buffer layer between the two gratings (Figure 3.4(c)). The process was identical to the first SiNx deposition, excepting the thickness of layer. This thickness can be controlled to determine the separation between the two gratings, which is a key parameter for the design. Then, the second grating was added in the same fashion as the first (Figure 3.4(d)). Alignment markers were used to place the second grating at 90 degrees with respect to the first layer, creating the cross grating structure. Finally, a 200 µm SiNx layer was deposited to form the film’s other outer boundary and create symmetry (Figure 3.4(e)).
After the cross grating structure was fully fabricated, the substrate was removed to leave a thin (<1 µm) film floating in air. The sample was attached with crystal bond to a 1 inch diameter brass disk (Figure 3.4(f)). The disk had a 2.5mm hole in the center, over which the cross polarizer structure was positioned. The disk and sample were placed in a beaker of hydrochloric acid, which efficiently etches InP, and heated at low temperatures using a hot plate to remove the substrate (Figure 3.4(g)). After 45 to 60 minutes, the InP substrate had been sufficiently etched to expose the film covering the hole. At that point, there was a free-standing film of SiNx containing two crossed gratings separated by a process-dependent distance. Figure 3.5 shows a photograph through a microscope objective of a completed cross grating structure.

3.5 Testing

The cross polarizers were tested using a Bruker V80V Fourier transform infrared spectrometer (FTIR) in combination with a Bruker mid-IR microscope. Light produced by a mid-IR source exits the FTIR and is fed into the optical input channel of the microscope, optionally through a polarizer. The internal optics of the microscope route the light and focus it onto the sample using a reflective objective. The light is then collected on the opposite side of the sample, and is fed to a mercury cadmium telluride detector that is internal to the microscope. The output signal of the detector is fed back into the FTIR and the spectrum is produced using the FTIR’s Opus software.

The mid-IR microscope is useful because it allows the user to measure transmission (or reflection) through a region as small as tens of microns. Using just the source and focusing optics, this accuracy is difficult to duplicate. In fact, prior to the acquisition of the microscope, a complicated setup to measure transmission was built, but we were unable achieve a beam spot small enough to get reliable results. However, the microscope does have an important flaw in that because it uses a reflective objective, none of the light is incident normally on the structure (see Figure 3.6). Instead, all of light is incident at some angle, by as much as 20 degrees. Since transmission through gratings is inherently angle dependent, the microscope is unable to precisely replicate simulation conditions and therefore is unable to exactly
match simulation results.

In addition to slightly non-normal incident light, the cross grating itself does not sit perfectly flat relative to the test setup. During the fabrication process, silicon nitride was deposited on indium phosphide. Since the two materials are not lattice matched, strain occurs between the film and the substrate. When the substrate is removed, the strain is released and the film becomes wavy (Figure 3.7). As a result, is impossible to precisely control (or measure) the incidence angle for a given measurement, which leads to uncertainty in the results.

3.6 Results

The first device we fabricated and tested had a grating period of 4 µm, a metal width of 1.4 µm, and a grating separation of 150 nm. Figure 3.8 shows the unpolarized experimental data overlaid with the simulation data for this structure. At wavelengths below 5 µm, the results diverge somewhat, but between 5 and 10 µm wavelength both simulation and experiment show dual peaks at about the same spectral location.

While the experimental data does in fact show extraordinary transmission and displays two peaks that match the simulation, the results are by no means a perfect match. There is a significantly reduced efficiency, with one peak dropping from 60% transmission down to 40%, and the other dropping from 75% down to 33%. Additionally, the results only fit well for the 5 to 10 µm range.

There are a few reasons why the experimental data does not perfectly

![Ray diagram of a reflective objective](image-url)

Figure 3.6: Ray diagram of a reflective objective. Courtesy of www.jpsalaser.com.
Figure 3.7: Image of sample after substrate removal. The film section that is unsupported by the copper disk becomes wavy.

Figure 3.8: Experimental cross grating data with simulation data. The separation between gratings is 150 nm.
match simulation. First, the incidence angle does not match, as discussed in Section 3.5, which would explain a slight drop in transmission and potentially a shift in the spectral shape. Additionally, there is potential for variation in the silicon nitride. Important characteristics like refractive index and losses are heavily dependent on the chemical makeup and frequency of lattice defects in the silicon nitride, which is in turn dependent on the deposition method. The material properties used in simulation were measured by staff at Sandia National Labs from silicon nitride grown using their deposition techniques, while the actual devices were fabricated at the University of Illinois. As a result, there is uncertainty over the material properties of the nitride, which helps explain deviation by the experimental results from the simulation.

Another major difference between the simulation and experimental results is the polarization dependence. According to the device design, there are two ways the structure can be oriented relative to the incident light; namely, it can interact with the horizontal grating or the vertical grating first. However, due to time-reversal symmetry, the device will produce the same transmission spectra for light traveling forward and backward through the structure. Since light will encounter the opposite orientation moving backwards from forwards, transmission is not dependent on which grating is encountered first, and the structure is not inherently polarization dependent. The simulations confirm the intuitive physics explanation.

However, the experimental results show a strong polarization dependence (Figure 3.9). The polarization dependence indicates that the two gratings are fundamentally different; namely, the polarization that orients with the vertical grating behaves fundamentally differently than the one that orients with the horizontal grating. Time-reversal symmetry still holds, as it does not matter in which order the gratings are encountered, but the polarization is not rotationally symmetric.

We used a scanning electron microscope (SEM) to obtain high resolution images of the gratings in order to identify how the gratings were different. It was clear that the second grating was not flat across the surface of the sample (Figure 3.10). After the first grating was deposited, the surface of the sample was no longer flat. The subsequent silicon nitride deposition did not planarize the surface as we had hoped, and therefore the second grating was deposited on an uneven surface.
Figure 3.9: Experimental horizontal and vertical polarizations through a cross grating structure.

Figure 3.10: SEM image of the cross grating structure. The top grating is wavy due to an uneven deposition surface.
The second structure we made kept the same period (4 \( \mu \text{m} \)) and metal width (1.4 \( \mu \text{m} \)), but had a separation of 100 nm. The goal of this experiment was to demonstrate a spectral shift of one or both peaks. There is a distinct shift in the peak around 7.5 \( \mu \text{m} \), and maybe a shift in the other peak as well (Figure 3.11). Neither shift is enough to clearly demonstrate spectral control, but they do indicate that the structure may be tunable.

We have demonstrated extraordinary transmission through the cross grating structure that exceeds the results predicted by classical physics and approximately matches the spectral shape predicted by simulation. These results show the potential for a narrowband filter in the mid-IR. We have also demonstrated a shift in the transmission peaks due to variation of grating separation, which shows potential for the structure to be tunable.

### 3.7 Next Steps

Although we confirmed the existence of extraordinary transmission through the structure, we have not yet conclusively demonstrated spectral shifting due to grating separation. The first step is to create samples with incremental
increases in separation to see how the transmission spectrum changes. With more data points, the potential for tuning can be better understood.

The following step is to create a structure that can control the separation in real time, which will allow for an actively tunable filter. The ability to electrostatically collapse and reform a thin gold film has been demonstrated by Keum et al. at the University of Illinois [23]. By controlling a gate voltage, they have been able to manipulate control over the air gap between a sub-micron thick gold surface and a silicon dioxide buffer layer. In theory, this result can be expanded to control the separation between two gold gratings with a buffer layer in between (Figure 3.12), which would create an actively tunable narrowband filter.

In this chapter, we have introduced a novel narrowband filter design for the mid-IR. A passive structure was simulated and fabricated, and both extraordinary transmission and tunability were demonstrated. Additionally, the potential for making the device actively tunable was explored.
CHAPTER 4

CONCLUSION

In this thesis, we have proposed two new optical devices for the mid-infrared wavelength spectrum using subwavelength gratings.

First, we proposed novel half-wave and quarter-wave plate structures that serve as an alternative to birefringent crystals (Chapter 2). A subwavelength metal grating is placed some distance above a metallic ground plane. For light incident at an angle, one polarization will be reflected at the grating while the other is reflected at the ground plane. After recombining, the two polarizations will have experienced different path lengths and, therefore, will have a different relative phase. The path length difference – and, therefore, the change in phase – is controlled by the separation between the grating and the ground plane. We presented simulations and experimental data that confirm the presence of a half-wave plate with an efficiency that is on par with birefringent equivalents. Additionally, the wave plate is tunable by adjusting the wavelength and incidence angle of the light.

Next, we introduced a narrowband filter for the mid-IR (Chapter 3). These devices use a cross grating structure with submicron separation that has an extraordinary transmission peak not predicted by classical physics. In this thesis, we showed simulation and experimental results that demonstrated the presence of an extraordinary peak in a passive structure. In addition, we presented simulation results that predict the ability to spectrally tune the peak location by altering the separation between gratings. Experimental data was presented that indicates the presence of this spectral shift, but more data is needed for conclusive verification. A passively tunable peak leads to the potential for an actively tunable filter using an electrostatically controlled separation.

The mid-infrared is an important wavelength range because of its importance for remote sensing and the presence of black-body spectra for a wide temperature range. However, the cost of doing research in this wavelength
range is excessively high, due in part to the lack of affordable optical devices. While there is still much work to do, the devices presented in this thesis show the potential to expand functionality and bring costs down in this exciting field.
REFERENCES


