Metasurfaces for photon sorting and selective absorption

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Metasurfaces for photon sorting and selective absorption

by

Isroel Mandel

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the requirements for the degree of Doctor of Philosophy, The City University of New York.

2015
Isroel Mandel

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This manuscript has been read and accepted for the Graduate Faculty in Physics in satisfaction of the dissertation requirements for the degree of Doctor of Philosophy.

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Abstract

Metasurfaces for photon sorting and selective absorption

by

Isroel M. Mandel

Advisor: Prof. David T. Crouse

Metamaterials are a recent discovery gaining much interest due to their promising applications to multiple devices in sensing, imaging, photovoltaics, nonlinear optics, heat conversion, sorters, and multitudes of other devices. These metamaterials are made of subunits called meta-atoms which take a role similar to that of atoms in bulk crystals. However, unlike their atom counterparts, these meta-atoms are macroscopic and can be engineered to respond to a driving field in a desired way. Metasurfaces, the 2-dimensional analog of metamaterials, have been shown to possess the ability to control light in novel ways. In this work, we investigate a particular type of metasurface namely a cavity array metasurface which consists of a metal film with an array of apertures which form the meta-atoms.

We will discuss methods for using such metasurfaces to develop innovative
forms of photon sorting and frequency selective absorption. The metasurface devices presented illustrate how, by designing the cavity meta-atoms, various desired global properties can be achieved. Among the devices we will demonstrate are a novel polarization sensing pixel implementing a 1-dimensional polarization sorting metasurface, a Stokes parameter sensor device implementing a novel 2-dimensional cavity array metasurface, a 2-dimensional perfect absorbing metasurface with subwavelength photon sorting in the microwave, a 2-dimensional transmitting metasurface with subwavelength photon sorting in the near-IR, and an actively tunable frequency selective perfect absorber using two 2-dimensional metasurface.
To my parents

שלום מנחמ נחום ואסתי מניחי הלוי

Thank you for the years of love, guidance, and laughter.
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Chapter 1

Introduction

Metamaterials are a new and exotic form of designed composite materials that enable an increased level of control of electromagnetic interactions. These metamaterials obtain their unique properties from subwavelength geometric patterns operating in conjunction with their composite material properties. These geometric elements are known as meta-atoms. In some cases, the meta-atom structure plays a significantly more important role that the materials it is made of i.e. the response of a split ring resonator will depend primarily on its circumference, width, and gap size and not on weather it is made of copper, gold, or silver even though these three metals have quite different dielectric permittivities.

In the past, most of the research in metamaterials was restricted mainly to the microwave frequency range. In this spectrum, subwavelength meta-atom elements can still be seen with the unaided eye, and fabricated relativity
easily via computer controlled cutting (CNC) machines, and printed circuit boards (PCB). In addition, metals can be very well approximated as perfect electric conductors in this range, which gives more control over the meta-atom design since damping can be added as an independent parameter. In recent decades the field of metamaterials has come to the forefront of photonics with advances in nanofabrication and optical materials. Meta-atoms are now designed and fabricated on nanometer scales for devices functioning in the IR, visible, and UV spectral ranges. These fabrication methods can be quite expensive however, requiring clean rooms and massive processing tools for methods such as photo lithography, electron-beam lithography, thermal evaporation, plasma enhanced vapor deposition, dry and wet etching, scanning electron microscopy, and multitudes of metrology tools. This emphasises the need for accurate prediction of a device before fabrication is undertaken. Thus electromagnetic simulations become both a necessary and powerful tool in order to correctly design complex devices.

Metamaterials have been developed to produced effects that have been predicted in theory but have been physically unreliable such as transformation optics[1], electromagnetic cloaking[2], negative-index materials[3], electromagnetic band gap materials[4], artificial magnetic conductors[5], hyperbolic materials[6], and many others. Metamaterials tend to have strongly
resonant responses which can have substantial dependencies on frequency, polarization, angle of incidence, and momentum and there is continuous re-
search into how to alleviate these dependencies.

The applications of metamaterials cover a wide field of potential de-
vices including photovoltaics, sensing, imaging, telecommunications, pho-
tonic computing, and biological and chemical analysis. Different classes of
metamaterials composed of specific meta-atoms may be best suited to par-
ticular devices. Metasurfaces are a class of metamaterial forming a surface or
sheet of meta-atoms[7]. Metasurfaces posses the ability to strongly interact
with and effect incident radiation and have been demonstrated for use in
multiple devices[8,9].

This dissertation will focus on a particular kind of metasurface, the cavity
array metasurface, which consist of a metal film perforated with a periodic
array of dielectric filled cavities or apertures, and its application as a photon
sorter to novel polarization and hyperspectral sensors. The discussion pre-
sented is structured as follows: In Chapter 2 we will present and discuss some
of the basic theory of Maxwell’s equations relevant to cavity array meta-
surfaces: the basic structure of a cavity array metasurface, the effect of peri-
odicity on Maxwell’s equations, waveguide solutions to Maxwell’s equations,
and waveguide cavity modes. In Chapter 3 we present the Effective Cavity
Resonance (ECR) approximation for predicting the properties of cavity array metasurfaces which is based on the author’s published work in ArXiv[10] and Proc. SPIE [11] as well as a discussion of the rigorous coupled wave algorithm and finite element method used for simulating the designs. Chapters 4 and 5 present two applications of cavity array metasurfaces to polarization sensing and is based on the author’s work published in IEEE Sensors[12] and Proc. SPIE [13] respectively. Chapters 6 and Chapter 7 present frequency band selective photon sorting cavity array metasurfaces operating in the microwave and near-IR and is based on work submitted for publication in IEEE Tran, and published in APL[14] respectively. Finally in Chapter 8 we discuss the simulated results of a Fabry-Perot resonator implementing two metasurfaces for a continuously tunable hyperspectral microbolometer.
Chapter 2

Electromagnetic Theory

2.1 Maxwell Equations

2.1.1 Differential Maxwell Equations

Modern technologies and innovations can be attributed to advancement in the understanding of electromagnetic theory. Electromagnetism is the source behind electrical circuits, electrical motors, generators, speakers, radio communications, cellular phone communications, fiber optics, the global positioning system, the entire field of optics, and endless other technologies. All these systems are implicitly described by four equations. The fundamentals of the theory of electromagnetism as we are known today first became established when James Clerk Maxwell presented the four equations that govern all classical electromagnetic phenomena. These equations, now known as the Maxwell equations are given as:
CHAPTER 2. ELECTROMAGNETIC THEORY

\[ \nabla \cdot \mathbf{E} = 4\pi \rho \quad \nabla \cdot \mathbf{D} = 4\pi \rho_f \quad (2.1) \]

\[ \nabla \cdot \mathbf{B} = 0, \quad \nabla \cdot \mathbf{H} = 0 \quad (2.2) \]

\[ \nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J}_f + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} \quad (2.3) \]

\[ \nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \quad (2.4) \]

\[ \mathbf{D} = \varepsilon \mathbf{E} \quad (2.5) \]

\[ \mathbf{B} = \mu \mathbf{B} \quad (2.6) \]

where \( \mathbf{E} \) is the electric field, \( \mathbf{B} \) is the magnetic field, \( \rho \) is the charge density, \( \mathbf{J} \) is the current density, and \( c \) is the speed of light. These equations can be include the bulk properties of materials where \( \varepsilon \) and \( \mu \) are the bulk dielectric permittivity and permeability respectively of the material and \( \rho_f \) and \( \mathbf{J}_f \) are free charges and currents that are external to the materials i.e. not part of the charge-neutral material response to external radiation. These four differential equations determine how the electromagnetic fields interact with sources of charge and current, and propagate through matter. These the dielectric permittivity and permeability are an averaged response of the electrons, atoms, and molecules of the material to an external electric field.
CHAPTER 2. ELECTROMAGNETIC THEORY

2.1.2 The Wave Equation

In the electromagnetic systems of interest here, we will be investigating systems devoid of such free charges and currents. Including these conditions in Eq.2.1-2.4 and taking the curl of Eq.2.4 and using Eq.2.3 with Eq.2.5 we obtain a differential equation for the electric field alone which is given as:

\[ \nabla \cdot \mathbf{D} = 0 \] (2.7)

\[ \nabla \cdot \mathbf{H} = 0 \] (2.8)

\[ \nabla \times \nabla \times \mathbf{E} = -\frac{\epsilon \mu}{c^2} \frac{\partial \mathbf{E}^2}{\partial t^2} \] (2.9)

Using the curl identity:

\[ \nabla \times \nabla \times \mathbf{A} = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \] (2.10)

the equation for \( \mathbf{E} \) can be simplified to:

\[ \nabla^2 \mathbf{E} - \frac{\epsilon \mu}{c^2} \frac{\partial \mathbf{E}^2}{\partial t^2} = 0 \] (2.11)

This is the vector wave equation which together with the material boundary conditions describes electromagnetic radiation and its propagation in linear materials accounting for reflection, transmission, refraction, diffraction, and all other wave phenomenon. The boundary conditions at material inter-
faces can be given in condensed form as:

\[
\hat{n} \cdot (D_2 - D_1) = \sigma_f = 0 \tag{2.12}
\]

\[
\hat{n} \times (E_2 - E_1) = 0 \tag{2.13}
\]

\[
\hat{n} \times (H_2 - H_1) = K_f = 0 \tag{2.14}
\]

\[
\hat{n} \cdot (B_2 - B_1) = 0 \tag{2.15}
\]

where \(\hat{n}\) is the unit vector normal to the surface of the interface, \(\sigma_f\) is the free surface charge density, and \(K_f\) is the free surface current density, respectively. These interface boundary conditions, derived from Maxwell’s equations applied to infinitesimal elements at material interfaces, and the differential form of Maxwell’s equations form the fundamental mathematical description of electromagnetism.

### 2.1.3 The Helmholtz Equation

The wave equation can be further simplified when the systems of interest are harmonic in time i.e. all the electromagnetic field components have time varying fields given as:

\[
I \propto e^{i\omega t} \tag{2.16}
\]

When this is introduced to the wave equation, we obtain:
\[ \nabla^2 \mathbf{E} + k^2 \mathbf{E}^2 = 0 \] (2.17)

\[ |k| = \sqrt{\frac{\epsilon \mu \omega^2}{c^2}} = n k_0 \] (2.18)

\[ |k_0| = \frac{\omega}{c} \] (2.19)

\[ n = \sqrt{\epsilon \mu} \] (2.20)

which is known as the Helmholtz equation where \( k \) is the wavenumber, \( k_0 \) is the free space wavenumber, and \( n \) is the refractive index of the propagating medium. The solution to the Helmholtz equation is in an infinite medium is the plane wave. It the primary description of an electromagnetic wave propagating in free space and is thus seen extensively in nature and known given by:

\[ \mathbf{E} = \mathbf{E}_0 e^{i k \cdot \mathbf{r}} \] (2.21)

\[ \mathbf{H} = \hat{k} \times \mathbf{E} \] (2.22)

\[ |k| = nk_0 = n \sqrt{k_x^2 + k_y^2 + k_z^2} = n \frac{\omega}{c} \] (2.23)

where \( \mathbf{E}_0 \) is the filed magnitude, \( \mathbf{k} \) is the wavevector, synonymous with the wave momentum and \( \mathbf{r} \) is the position vector. These equations can be analytically continued to allow complex components for the wavevector \( \mathbf{k} \) as long as Eq.2.23 holds. Plane waves with such complex wavevectors are called
evanescent waves, and the decay exponentially from a source plane. These allow for bounded modes that do not propagate energy in the decaying direction and can be a source of high intensity fields. For an infinite medium, this general solution includes all possible wavevectors satisfying these conditions, and in a finite medium, additional boundary conditions must be satisfied. There are plane wave solutions for anisotropic media as well but those will not be discussed here.

2.2 Meta-atoms, Metasurfaces, and Metamaterials

Electromagnetic metamaterials have been gaining much interest in recent years for their ability to produce novel behaviour not found in natural materials such as artificial magnetic conductors\cite{5}, cloaking\cite{15}, beam steering\cite{16}, photon sorting\cite{12,14}, altering radiative lifetimes\cite{17}, and multiple other phenomena that can be applied to various technologies. Metamaterials obtain these novel properties from engineered of sub-wavelength elements called meta-atoms\cite{7}. These meta-atoms are composed of multiple materials with varying dielectric and magnetic properties formed into engineered geometries. The geometry of these meta-atoms underly their physical response to electromagnetic fields.
These meta-atoms are usually designed to be subwavelength in dimension relative to the wavelength range of operation. This usually allows for a more controlled interaction of the meta-atom with a driving field with minimized scattering. It is the interaction of each individual meta-atom with a driving field as well as the coupling between these meta-atoms in an array that which determines the effective response of a metamaterial. Example of meta-atom structures are split-ring resonators[18], antennas[19], gratings[12,20], cavities[14,21], and other resonant and strongly responding geometries.

The primary meta-atom investigated in this work is the cavity, or inclusion, meta-atom that is arranged in a square periodic lattice in one or two dimensions to form a cavity array metasurface. An illustration of a cavity array metasurface is shown in Fig.2.1. It consists of a metal film of thickness $h$ perforated with a cavity filled with dielectric $\epsilon_c$ arrayed in a periodic lattice with periodicity $\Lambda$ in between a superstrate and substrate.
In this section we will begin by discussing periodic arrays used in many metamaterials systems and the effect periodicity has on Maxwell’s equation and its solution. In addition we will discuss various structures that will be implemented as cavity meta-atoms, particularly circular and rectangular waveguides which will exhibit waveguide cavity resonant modes.

2.2.1 Periodic Arrays

Periodic arrays have been known for hundreds of years, primarily in the form of the diffraction grating. The premise of periodic arrays is simple; they
are structures made of repeating identical elements or unit cells. However
this simple condition allows them to produce interesting and counterintu-
itive effects that is implemented in diffraction gratings, photonic crystals,
and metamaterials. Periodic arrays exhibit global effects arising from multi-
ple coupled unit cells operating in tandem resulting in phenomenon such as
diffraction and extraordinary optical transmission[22]. We will discuss the
theory behind periodic systems that will be used later in this work. Here we
will describe a 2-Dimensional periodic array. The equations can be readily
applied to 1-D arrays as well.

An electromagnetic periodic array consists of a dielectric structure with
the following property:

$$\epsilon(x + m\Lambda_x, y + n\Lambda_y) = \epsilon(x, y) \quad m, n = 0, \pm 1, \pm 2$$ (2.24)

where $m, n$ a integers and $\Lambda_x$ and $\Lambda_y$ are the length of the periodicity on the
$x$ and $y$ directions respectively. This means that for any integer translation
of $\Lambda_x$ and $\Lambda_y$ the dielectric function remains unchanged. When this dielectric
is introduced into the Helmholtz equation 2.20, it can be shown[23, 24] that
the wave solutions are of the form:
\[ \Psi(x, y) = u(x, y) \exp^{i(k \cdot r)} \]  
\[ k = k_x \hat{x} + k_y \hat{y} \]  
\[ u(x, y) = \sum_{i,j} u_{ij} \exp^{iK_{x,m}x} \exp^{iK_{y,n}y} \]  
\[ K_{x,m} = m \frac{2\pi}{\Lambda_x} = mK_{0,x}, \; m = 0, \pm 1, \pm 2... \]  
\[ K_{y,n} = n \frac{2\pi}{\Lambda_y} = nK_{0,y}, \; n = 0, \pm 1, \pm 2... \]  

These are known as Bloch waves in solid state physics, or more commonly as Floquet modes in mechanics and optics. The wavenumbers \( K_{0,x} \) and \( K_{0,y} \) are the reciprocal lattice vectors associated with the periodic lattice and form the quanta of momentum that the lattice can add or subtract from an incident beam. The function \( u(x, y) \) has the same periodicity as the dielectric function as is evident from the Fourier expansion above where \( u_{ij} \) are the Fourier coefficients. Furthermore the wavevectors \( k_x \) and \( k_y \) are only unique in the first Brillouin zone where \(-K_{0,x}/2 < k_x < K_{0,x}/2 \) and \(-K_{0,y}/2 < k_y < K_{0,y}/2 \) since translating the wavevector by a multiple of the reciprocal lattice vector does not change the function. The phase factor as well as the periodic constraint on the solution wavefunction has profound effects on the interaction of a periodic dielectric with incident radiation.

Diffraction is one of the most elementary yet profound effects of this pe-
riodicity. This occurs when an incident beam from a uniform dielectric, such as air or vacuum, strikes a periodic dielectric: the scattered and transmitted beams then must contain a multiple of the lattice momentum. This results in discreet propagating and surface bound scattering channels or modes that are frequency dependant. These have multiple uses, the most obvious being frequency filtering. The exact shape and material of the diffraction grating determines how much energy is contained in each diffraction mode. The diffraction modes in the superstrate above the grating are given as plane waves as in Eq.2.21 but with the constraint composed by Eq. 2.30 as follows:

\[
E = E_0 \exp \left( i (K_{x,m} + k_x)x \right) \exp \left( i (K_{y,n} + k_y)y \right) \exp K_{z,m,n} z
\]

(2.30)

\[
K_{x,m} = k_x + mK_{0,x}
\]

(2.31)

\[
K_{y,n} = k_y + nK_{0,y}
\]

(2.32)

\[
K_{z,m,n} = \sqrt{n k_0^2 - K_{x,m}^2 - K_{y,n}^2}
\]

(2.33)

These discreet modes become evanescent when \(K_{z,m,n}\) is imaginary which occurs when the added lattice momentum is greater than \(k_0\) i.e. \(nk_0^2 - K_{x,m}^2 - K_{y,n}^2 < 0\). These allow for high fields and strong coupling between elements on the scattering surface. These propagating and evanescent diffraction modes will be discussed in greater detail in Sec.3.1.3 where it will be used to develop
2.2.2 Waveguides and Waveguide Cavity Modes

An essential element of electromagnetic systems is a system used to guide electromagnetic waves. These systems can be constructed from dielectrics and metal materials or a combination of both. When these waveguides have a finite thickness they obtain cavity-like resonant behavior and exhibit waveguide cavity modes (WCM). These discreet structural elements will form the basis of the meta-atoms we will be implementing in the photon sorting meta-surfaces investigated here. To analyze this element we first consider a system consisting of a hollow metal waveguide filled with a uniform isotropic dielectric material. Such waveguides have been used extensively to transfer power between various components in microwave and other RF components. Some waveguides with fixed cross sections and infinite length (into the page) are illustrated in Fig.2.2. Waveguides of finite length will be discussed after we present the theory of waveguides constructed with perfect conductors.

The solution method to solving the waveguide problem is taken from Jackson[25] and is general for all waveguides with either dielectric or metal cladding around a dielectric core. The electric and magnetic fields are split into field components along the waveguide and field components transverse
Figure 2.2: Cross-sectional view of a square waveguide (left) a rectangular waveguide (middle) and a circular waveguide (right). All waveguides exhibit the properties of a cutoff frequency, light channeling, light confinement, and dispersion. The square waveguide is defined by the edge length $a$, the rectangular waveguide has two parameters $a$ and $b$ for the two sides, and the circular waveguide is defined by its diameter $D$.

to the guide with a propagation phase dependance on $z$ given as:

$$E = E_t + E_z$$  \hspace{1cm} (2.34)$$

$$B = B_t + B_z$$  \hspace{1cm} (2.35)$$

$$E(x,y,z) = E(x,y)e^{\pm ik_z z}$$  \hspace{1cm} (2.36)$$

$$B(x,y,z) = B(x,y)e^{\pm ik_z z}$$  \hspace{1cm} (2.37)$$

where $E_t$ ($H_t$) is the transverse electric (magnetic) component and $E_z$ ($H_z$) is the longitudinal electric (magnetic) field component, with $z$ being the axis along the direction of the guide. Using this in Eq.2.20, it can be shown that the transverse components $E_t$ and $B_t$ can be expressed entirely on $E_z$ and $B_z$ as:
\[
\mathbf{E}_t = \frac{i}{\gamma} [\pm k \nabla_t E_z - \omega \hat{z} \times \nabla_t B_z]
\]
\[
\mathbf{B}_t = \frac{i}{\gamma} [\pm k \nabla_t B_z + \mu \omega \hat{z} \times \nabla_t E_z]
\]
\[
\gamma = \sqrt{\mu \varepsilon \omega^2 - k^2}
\]

Where the longitudinal components, symbolized by the function \(\psi\), satisfy the eigenvalue equation:

\[
\nabla_t^2 \psi + \gamma^2 \psi = 0
\]

Where \(\nabla_t\) is the transverse derivative and \(\gamma\) is the eigenvalue. This eigenvalue equation has to be solved with the right boundary conditions on the cladding walls. For perfect electrical conductors the tangential components of \(E\) must be zero on the walls, thus these boundary conditions are given as:

\[
\psi|_s = 0 \text{ for } E_z \text{ defining TM modes} \tag{2.42}
\]
\[
\frac{\partial \psi}{\partial n}|_s = 0 \text{ for } B_z \text{ defining TE modes} \tag{2.43}
\]

The fields can then be separated into transverse electric (TE) and transverse magnetic (TM) modes by treating \(E_z\) and \(B_z\) individually. The resulting eigenfunctions form a complete basis set in the waveguide and can there-
fore be used as an expansion basis for any field distribution in the waveguide.

The propagation constant in the $\hat{z}$ direction is then given as:

$$ k_z = \sqrt{\epsilon k_0^2 - \gamma^2} $$

(2.44)

where $\epsilon$ is the dielectric in the waveguide.

**Rectangular Waveguide**

The eigenfunctions that are the solutions of Eq.2.41 for a rectangular waveguide of width $a$ and height $b$ are:

for TM $E_z = \psi_{m,n}^{TM} = I_{m,n}^{TM} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi y}{b}\right)$

(2.45)

for TE $B_z = \psi_{m,n}^{TE} = I_{m,n}^{TE} \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi y}{b}\right)$

(2.46)

$m, n = 0, 1, 2...$

(2.47)

These modes have a cutoff frequency where $k_z$ becomes imaginary and waves no longer propagate. The eigenvalue $\gamma_{mn}$ and the associated cutoff frequency of the guide is given by:

$$ \gamma_{mn} = \pi \sqrt{\left(\frac{m}{a}\right) + \left(\frac{n}{b}\right)} $$

(2.48)

$$ \omega_{mn} = \frac{\pi}{\sqrt{\mu \epsilon}} \sqrt{\left(\frac{m}{a}\right) + \left(\frac{n}{b}\right)} $$

(2.49)
The longitudinal field profiles for the TE and TM modes are shown in Fig. 2.3 and Fig. 2.4.

![Field profiles for $B_z$ for TE modes](image)

**Circular Waveguides**

The solution for a circular waveguide of radius $R = a/2$ is given by:

$$
\psi_{mn}(\rho, \phi) = I_{mn}(x_{mn}\rho)e^{im\phi} \quad m = 0, 1, 2, \ldots \quad (2.50)
$$

$$
x_{mn} = \frac{\gamma_{mn}}{R} \quad (2.51)
$$

where $J_m(\gamma_{mn}) = 0$ for TM and $J'_m(\gamma_{mn}) = 0$ for TE \quad (2.52)
Figure 2.4: Field profiles for $E_z$ for TM modes

Figure 2.5: Circular waveguide field profiles for TE modes
2.2.3 SIBC Boundary Condition

The above descriptions for waveguide modes were for perfect conductors. However, for frequency ranges in IR and higher, metals can no longer be well approximated as perfect conductors. However, below the near-IR, metals can be approximated well by using impedance boundary conditions. This incorporate loss into the metal surface with the field still assumed zero inside the metal. We will describe the waveguide modes for impedance approximated metals for gratings.
The waveguide modes for an aperture of width $a$ starting at a distance $d$ from the origin and filled with a dielectric $\epsilon_{l,m}$ in a metal with impedance $Z_l = \sqrt{\frac{\mu}{\epsilon}}$, is given by:

\[
|\phi_{l,m,n}^{\pm}\rangle = f_{l,m,n}(x)e^{\pm ik_{y,l,m,n}} \tag{2.53}
\]

\[
f_{l,m,n}(x) = \cos(\alpha_{l,m,n}x) + \eta \sin(\alpha_{l,m,n}x) \quad \text{for TM} \tag{2.54}
\]

\[
f_{l,m,n}(x) = \eta \cos(\alpha_{l,m,n}x) + \sin(\alpha_{l,m,n}x) \quad \text{for TE} \tag{2.55}
\]

\[
k_{y,l,m,n} = \sqrt{\epsilon_{l,m}k_0^2 - \alpha_{l,m,n}^2} \tag{2.56}
\]

with $f_{l,m,n}(x)$ satisfying the SIBC impedance boundary condition:

\[
E_{\parallel}(x = 0) = Z\hat{n} \times H_{\parallel}(x = 0) \tag{2.57}
\]

\[
E_{\parallel}(x = a) = Z\hat{n} \times H_{\parallel}(x = a) \tag{2.58}
\]

where $\hat{n}$ is the normal of the metal wall, which is in the $\pm \hat{x}$ for the gratings investigated in work. For TM modes where $\overline{H} = H_z = H_{\parallel}$ and $E_{\parallel} = E_y$ this becomes:

\[
E_y(x = 0) = -ZH_z(x = 0) \tag{2.59}
\]

\[
E_y(x = a) = ZH_z(x = a) \tag{2.60}
\]
and for TE modes it becomes:

\[
E_z(x = 0) = Z H_y(x = 0) \quad (2.61)
\]

\[
E_z(x = a) = -Z H_y(x = a) \quad (2.62)
\]

Inputting Eq. 2.54 into Eq. 2.57 and matching the conditions for the TM polarisation gives:

\[
- \frac{1}{ik_0 \epsilon} \eta \alpha_{l,m,n} = -Z \quad (2.63)
\]

\[
- \frac{1}{ik_0 \epsilon} (-\alpha_{l,m,n} \sin (\alpha_{l,m,n}a) + \eta \alpha_{l,m,n} \cos (\alpha_{l,m,n}a)) = Z (\cos (\alpha_{l,m,n}a) + \eta \sin (\alpha_{l,m,n}a)) \quad (2.64)
\]

\[
\rightarrow \tan (\alpha_{l,m,n}a) = \frac{2iZ \alpha_{l,m,n} k_0 \epsilon}{\alpha_{l,m,n}^2 + (Z k_0 \epsilon)^2} \quad (2.65)
\]

\[
= \frac{2\gamma^s \alpha_{l,m,n}}{\alpha_{l,m,n}^2 - (\gamma^s)^2} \quad (2.66)
\]

with \( \gamma^s = iZ k_0 \epsilon \). For the TE polarization gives:

\[
\tan (\alpha_{l,m,n}a) = \frac{2\gamma^p \alpha_{l,m,n}}{(\alpha_{l,m,n} \gamma^p)^2 - 1} \quad (2.67)
\]

with \( \gamma^p = \frac{Z^2 k_0}{\eta \epsilon} \). The roots of these transcendental equations give the eigenvalues for the TM and TE modes as well as the eigenvectors of the
waveguide modes, which allow the fields and propagation constants to be determined.

### 2.2.4 Plasmonic Waveguide Modes

At higher frequencies the metal dielectric function decreases in magnitude. Close to the near IR-visible it is still negative, but the SIBC condition no longer gives a good approximation of the aperture modes and resonant behaviour. At these frequencies the field penetration into the metal walls of the aperture become significant. Metals can be reasonably well approximated in this regime with the Drude plasma model which gives the metal dielectric as

\[ \epsilon(\omega) = 1 - \omega_p^2 / (\omega(\omega + i\gamma)) \]

where \( \omega_p \) is the metal’s plasma frequency and \( \gamma \) is the electron collision frequency. To obtain the field profiles and dispersion properties of waveguides in the frequency range we make use of the MIM solutions for a dielectric waveguide bounded by metal. These solutions include coupled plasmonic modes and waveguide modes. This is done by considering a single aperture in an infinite metal film as shown in Fig. 2.7.

We assume two types of modes, plasmonic waveguide modes and dielectric waveguide modes. These are treated by expanding the fields into different functional forms in each region and applying the boundary conditions. For the plasmonic approach the following anzats is used:
$H_z = Ae^{k_1^I x} e^{i k_y y}$ for Region I with $x < -a$ \hspace{1cm} (2.68)

$H_z = Be^{k_1^I x} e^{i k_y y} + Ce^{-k_1^I x} e^{i k_y y}$ for Region II with $-a < x < a$ \hspace{1cm} (2.69)

$H_z = De^{-k_1^I x} e^{i k_y y}$ for Region III with $x > a$ \hspace{1cm} (2.70)

$k_1^I = \sqrt{k_y^2 - \epsilon_1 k_0^2}$ \hspace{1cm} (2.71)

$k_2^{II} = \sqrt{k_y^2 - \epsilon_2 k_0^2}$ \hspace{1cm} (2.72)

where the $k_y$ is the plasmon propagating momentum, and the fields are assumed to be exponentially decaying from the interfaces in all regions. The magnetic (H) fields are continuous across the boundaries since there are no free currents and the tangential electric field are continuous across the boundaries. Thus for $x = -a$: 

![Figure 2.7: Exact metal solution](image)
\[
A e^{-k^I_x a} = B e^{-k^I_x a} + C e^{k^I_x a} \quad (2.73)
\]
\[
\frac{k^I_x}{\epsilon_I} A e^{-k^I_x a} = \frac{k^I_x}{\epsilon_{II}} B e^{-k^I_x a} + \frac{-k^I_x}{\epsilon_{II}} C e^{k^I_x a} \quad (2.74)
\]
for \(x = a:\)
\[
B e^{k^I_x a} + C e^{-k^I_x a} = D e^{-k^I_x a} \quad (2.75)
\]
\[
\frac{-k^I_x}{\epsilon_{II}} B e^{k^I_x a} + \frac{k^I_x}{\epsilon_{II}} C e^{-k^I_x a} = \frac{k^I_x}{\epsilon_I} D e^{-k^I_x a} \quad (2.76)
\]
\[
\frac{\epsilon_I k^I_x + \epsilon_{II} k^I_x}{\epsilon_{II} k^I_x - \epsilon_I k^I_x} = e^{-2ak^I_x} \quad (2.79)
\]
Solving these sets of equations give an eigenvalue equation for the propagation vector:

This can be reduced to odd and even modes:

\[
\tanh k^I_x a = -\frac{k^I_x \epsilon_{II}}{k^I_x \epsilon_I} \quad \text{odd } E_y (\text{Even } H_z \text{ and } E_x) \quad (2.80)
\]
\[
\tanh k^I_x a = -\frac{k^I_x \epsilon_I}{k^I_x \epsilon_{II}} \quad \text{even } E_y (\text{odd } H_z \text{ and } E_x) \quad (2.81)
\]
for the odd \(E_y\) mode, \(H_z\) is even and \(A = D, B = C,\) and \(B = \frac{A e^{-k^I_x a}}{e^{k^I_x a} + e^{-k^I_x a}}.\)
for the even \(E_y\) mode, \(H_z\) is odd and \(A = -D, B = -C,\) and \(B = \frac{A e^{-k^I_x a}}{e^{k^I_x a} - e^{-k^I_x a}}.\)
The odd mode has a cutoff frequency whereas the even mode does not, thus
there is always an even TM coupled plasmon mode[26]. The dispersion curve for the primary M-I-M plasm mode for an air core with silver cladding is shown in Fig. 2.8a for multiple core widths. The $H_z$ fields are shown in Fig. 2.8b for two such widths. The rapid change in field is evident at the metal boundaries, and the fields are symmetric.

Figure 2.8: a) Dispersion curves for M-I-M plasmon modes in drude silver for various core widths. b) Magnetic field profiles for the primary M-I-M plasmon modes in drude silver for air core widths of 25 nm and 50 nm.

### 2.2.5 Waveguide Cavity Modes

Thus far we have discussed infinite dielectric waveguides with a metal cladding where the metal surface can be approximated as either a perfect electric conductor, an impedance boundary, or as a Drude plasma. The dispersion curves for these waveguide modes describe the effective index of light traveling in the guide. When the waveguide terminates, the light experiences an index mismatch between the guide and free space causing some of the light to be
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reflected back into the guide with an additional phase which is dependent on the exit interface. For a finite waveguide, there are two such terminals, resulting in light reflecting at both exit interfaces and retracing its path; this ultimately produces a resonance structure since, at specific resonant frequencies, the light remains in phase with its previous traversal in the guide giving rise to a constructive interference effect. This is a waveguide cavity mode resonance, it behaves similarly to a cavity mode in that it is bounded yet behaves as a waveguide and allows power to pass through it. In the following chapter we will discuss these modes in greater detail, particularly when these finite waveguide meta-atoms are in a periodic array.
Chapter 3

Effective Cavity Approximation and Simulation Methods

In this chapter we will present a novel theoretical approach for modeling the resonant properties of transmission through subwavelength apertures penetrating metal films. We show that cavity mode theory applies to an effective resonant cavity whose dimensions are determined by the aperture’s geometry and the evanescent decay lengths of the associated diffracted waves. This method suggests a concrete physical mechanism for the enhanced transmission observed in periodic aperture arrays, namely it is the evanescently scattered light, localized in the near field of the metal surface, which couples into the apertures. Furthermore, it analytically predicts the frequencies of peaks in enhanced transmission, the quality factor of the peaks, and explains their dependence on variation in the hole radius, periodicity, and the film thickness over a wide range of geometries. This model demonstrates strong
correlation to simulation and existing results with a high degree of accuracy. We then discuss the rigorous coupled wave method for numerically solving cavity array structures.

3.1 Effective Cavity Resonance

Enhanced optical transmission (EOT) through a periodic array of subwavelength apertures in a metal film was first reported by Ebbesen in 1998[22]. Since then, many theories have been proposed for the underlying physical mechanism for this effect. The most common approach asserts that surface plasmon excitations on the periodic surface of one or two-dimensional arrays coupling through the apertures are the mechanism that enables EOT[27–31]. This approach explains the role that structure periodicity plays in EOT. However, it does not account for the variation in EOT due to aperture shape[32, 33]. Furthermore, EOT has been demonstrated with PEC structures, as well as non-metallic materials where SP contributions are nonexistent[34–36].

Approaches which consider the waveguide modes of the apertures as the physical mechanism for EOT have also been investigated[37–41]. These arguments assert that incident light can only propagate through the metal film and contribute to EOT in a manner which satisfies a waveguide condition along the length of the aperture similar to a Fabry-Perot resonator. These
approaches capture some limitations that the individual cavity structures place on allowed frequencies which demonstrate EOT, but do not directly explain the effect of periodicity on EOT.

Efforts combining these two approaches include a generalization of Bethe’s theory for a single, extremely small hole through an infinitely thin perfect electric conducting (PEC) film\cite{42}, to account for periodic arrays\cite{43}, and finite thicknesses\cite{44}. However, these approaches are limited to extremely small holes and perfect conducting metals, two situations which are not typically realized.

EOT has been studied extensively through use of a semi-analytical coupled wave analysis\cite{31,45–48}, as well as by many different finite element or finite difference numerical simulation approaches\cite{49,50}, and experimentally\cite{27–32}. These methods all empirically shed light on the dependence of EOT on structure periodicity and cavity shapes, but do not provide an intuitive, or fundamentally clarifying approach toward the mechanisms of EOT. Furthermore, these approaches are often computationally and experimentally expensive to carry out.

Thus, a complete first-principles approach to explain the effect of EOT through two-dimensional arrays of subwavelength holes in metal films is desirable. We develop an approach which analytically and intuitively explains
the physical mechanism of EOT, and completely explains the aforementioned
dependence on structure periodicity and cavity shape. The theory is accu-
rate over an extremely broad range of geometrical configurations. In this
approach, we extend the idea of waveguide dispersion analysis to account for
finite film thicknesses[10].

For a finite film, an impedance mismatch between the superstrate, i.e.
the material above the film, and the metal at the top and bottom of the
cavities introduces a restriction on the wavelengths that exhibit resonant be-
behavior along the $z$-direction. It is at these resonances, where light is strongly
coupled into and through the apertures, where peaks in EOT are mani-
fest. There have been some successful studies of cavity-type resonances for
one-dimensional gratings, under limited geometrical conditions:[48,51–53] we
extend this approach to two-dimensional arrays and a larger range of geome-
tries.

Our goal is to describe an effective resonant cavity which has resonant
properties that match that of the actual aperture array. It should be em-
phasized that this is not an actual cavity resonance, i.e. the fields do not
demonstrate standing-wave behavior and there is a flow of energy along the
aperture, but an effective cavity resonance (ECR) where the physical extents
of the equivalent cavity are determined by the material’s structural and ma-
CHAPTER 3. ECR AND SIMULATION METHODS

3.1.1 Effective cavity resonance solutions

Here we discuss cylindrical apertures of radius $a$, filled with dielectric $\epsilon_c$ embedded in a metal film of thickness $h$, arranged in an infinite square periodic lattice of period $\Lambda$, with a dielectric, $\epsilon_s$, above and below the film, see Fig. 3.1. The approximation of an infinite lattice is valid in practice as long as the size of an complete hole array is significantly larger than the wavelength of incident light, where we can neglect edge effects[24]. We additionally neglect any magnetic effects, taking $\mu = 1$ for all materials, and assume an implicit $\exp[-i\omega t]$ harmonic time dependence.

Considering an infinitely-long aperture, the dispersion relation of light within these structures is given in Eq.2.44. The transverse wavevector $\gamma_{mn}$ is found by evaluating boundary conditions at the cavity’s metal walls. For cylindrical apertures embedded in a PEC film, its values are the $\gamma_{mn}$ satisfying the conditions in Eq.2.52. We can approximate real metals using the skin depth boundary condition (SDBC) discussed in detail by Lansey et al[41] which modifies $\gamma_{mn}$ as follows

$$\gamma'_{mn} = \left( \frac{1}{1 + \xi} \right) \gamma_{mn}, \quad (3.1)$$

where $\xi \equiv \delta_m/a$, and $\delta_m$ is the skin depth in the metal. Another approach to
(a) A top-down view of the structure under consideration.

(b) A cross section view of the structure under consideration.

Figure 3.1: A schematic of periodic cylindrical channels in a thin film is shown from top down a and in cross section b. The gray region represents the metal, the light blue regions are the dielectric-filled apertures, and the white is the superstrate and substrate.

modeling real medals is via the impedance boundary condition as discussed in Sec.2.2.3. Note that Eq.2.44 captures the dependence of the cavity shape and dielectric, as well as metal properties, but does not yet account for any properties of the superstrate or periodicity.

The remainder of this work involves determining an appropriate restriction on $k_z$ due to the finite film thickness and periodicity of the structure. If the restriction forces $k_z$ to take discrete values, it changes the allowed $\omega$ in Eq.2.44 from a smoothly varying range of values to distinct resonance frequencies. Again, we note that this ECR is not an actual cavity resonance, but
there are still spatial restrictions which introduce a buildup in field strength within the apertures which can be modeled as an effective resonant cavity.

### 3.1.2 The Fabry-Perot model

We first investigate a simple, Fabry-Pérot (FP) model for a restriction on $k_z$ which sets up a resonance condition, which we will study in greater detail in Section 3.1.3, and serves to illustrate our general approach. It is worthwhile noting that, due to its simplicity of form, this first approximation is regularly cited when discussing theory and design of aperture array materials\[54\]. Here the waveguide has a finite height, $h$, and we assume that this distance sets the resonance condition, whence,

$$k_z = \frac{p\pi}{h}, \quad (3.2)$$

where $p$ is an integer.

Substituting this constrained value for the propagation constant into Eq.2.44 gives a set of discrete resonance frequencies,

$$\omega_{mn} = \frac{c}{\sqrt{\epsilon}} \left[ \left( \frac{p\pi}{h} \right)^2 + \gamma_{mn}^2 \right]^{1/2}. \quad (3.3)$$

Fig. 3.2 shows a graphical interpretation of this method. The dispersion curves are plotted, along with the restricted values for $k_z$ from Eq. 3.2 which
are vertical lines. The intersections between these curves correspond to resonance conditions for the effective cavity.

![Graphical interpretation of the resonance condition described by Eq. 3.3.](image)

Figure 3.2: A graphical interpretation of the resonance condition described by Eq. 3.3. Vertical lines correspond to the $k_z$ restricted by film thickness (Eq. 3.2), solid curves are the modal dispersion curves of the cylindrical cavities (Eq. 2.44). The intersections of the two curves (points for $p = 1$ line) correspond to resonance conditions. Here $h/a = 2.1$.

This FP model is insufficient for describing many of the effects of EOT [46, 51, 52, 55]. This solution does not depend on periodicity or the superstrate dielectric and ignores the contribution of the incident fields. Additionally, full field simulations (Fig. 3.3) of aperture arrays show that the fields at a transmission peak reach beyond the surface of the film, above and below, further challenging the notion of using $h$ as the FP cavity height.
3.1.3 A complete solution

We are still able to use the resonance condition 3.3 by simply extending the effective height of the cavity. That is, if the fields extend a distance $\delta_e$ above and below the metal surface, the aperture has an effective height

$$h_{\text{eff}} = h + 2\delta_e,$$  \hspace{1cm} (3.4)

which is the actual aperture height plus the total penetration depth into the superstrate and substrate, beyond which the cavity fields decay to zero. Note, that the approach of finding effective heights of cavities has been demonstrated in a circuit model for EOT in some grating structures[56]. Then, we
substitute this effective cavity height in Eq. 3.2, giving the new restriction

\[ k_z = p \pi / h_{\text{eff}}, \]  

(3.5)

where \( p \) is an integer. The distance the fields leak out of the cavity is determined by restrictions on the fields above and below the film, which depend explicitly on the periodicity of the apertures.

To find this distance, we must find the maximal spatial extent, in the \( z \)-direction, of localized fields in the superstrate. Here, we develop an approach which describes the role of evanescent, scattered diffracted fields in the superstrate in setting the spatial extent of the cavity. These localized fields, unlike incident plane waves, are able to couple to waveguide modes in the cavity.

We note that, due to continuity boundary conditions between an aperture and the superstrate, single-walled aperture structures are unable to support the normally-incident TEM waves which strike them. Specifically, TEM waves have no \( z \)-component to their fields, while the fields in the apertures require a non-zero \( E_z \) (TM modes) or \( H_z \) (TE mode)[57]. Likewise, light exiting an aperture can not directly excite a zero-order transmission plane wave. Nevertheless, normally-incident light scatters from periodic arrays of subwavelength holes in a manner which satisfies Bloch’s theorem, with a
CHAPTER 3. ECR AND SIMULATION METHODS

spatial dependence of

$$\exp \left[ i \left( k_{xm} x + k_{yn} y + k_{zmn}^f z \right) \right], \quad (3.6)$$

where

$$k_{xm} = mK \quad (3.7a)$$
$$k_{yn} = nK \quad (3.7b)$$
$$k_{zmn}^f = \sqrt{\epsilon_s \frac{\omega^2}{c^2} - (m^2 + n^2) K^2} \quad (3.7c)$$

where $m$ and $n$ are integers, and $K = 2\pi/\Lambda$ is the reciprocal lattice vector[24].

Note that this $k_{zmn}^f$ is not, in general, the propagating cavity $k_z$ used earlier.

These evanescent diffracted modes, where $(m^2 + n^2) K^2 > \epsilon_s \omega^2 / c^2$, introduce strong localized fields above and below the metal film. These fields decay exponentially away from the surface with a decay length

$$\delta_{mn} (\omega, \Lambda) = 1/\text{Im}[k_{zmn}^f (\omega, \Lambda)]. \quad (3.8)$$

In general, these scattered fields have non-zero $z$-components, which then interact with the fields inside the apertures. Thus, the strength, and scattered, although localized, nature of the evanescent modes is what drives the transmission through the film.

The maximal spatial extent of these localized fields then sets the penetration depth of the cavity fields into the superstrate and substrate. That
is,

$$\delta_e(\omega, \Lambda) = \max \left[ \delta_{mn}(\omega, \Lambda) \right].$$  \hspace{1cm} (3.9)

The inclusion of the max function picks the mode with the longest decay length which is, in general, the lowest-order non-propagating mode. Although the detailed behavior of the electromagnetic fields above and below the metal is due to a superposition of all evanescent and propagating diffracted modes, the extent of the localized fields is still limited by the lowest-order evanescent diffracted mode in the superstrate or substrate. This sets the maximal distance over which any evanescent diffracted modes can extend, and thereby the effective depth of the fields above and below the film. This predicted length is shown in Fig. 3.3 as the solid black line, oriented along the vertical direction above the film surface, and is seen to match the field simulation. Additionally, note the field strength at that point matches the field strength at cavity walls, and thus describes the edge of the effective cavity.

This length depends explicitly on the periodicity, which directly explains both the enhancement seen for periodic structures, and the variation in EOT with changes of periodicity. Furthermore, the dependence on superstrate dielectric is also explained in this approach, as it affects the diffracted modes. These effects are captured by Eq. 3.7c. Thus, we have a resonance condition
which depends on all relevant structural properties. We study this further in Section 3.1.4.

There is one notable limitation of this approach, which we now discuss. At a frequency where the radicand in Eq. 3.7c is zero, i.e. a propagating diffraction frequency,

\[
\omega_{\text{diff}} = \frac{c\pi}{p}\sqrt{\epsilon_s \sqrt{m^2 + n^2}},
\]

the field leakage depth asymptotically approaches infinity, with a discontinuity at the diffraction frequency. This can be seen in Fig. 3.4, which shows the leakage depth as a function of frequency. The tendency towards infinite evanescent decay lengths captures the smooth transition from a localized mode to a propagating diffracted mode. However, approaching this transition makes the lowest order evanescent fields less local, while the second order (shorter decay length) evanescent fields are still localized. The actual effective cavity addition $\delta_e$ must then depend on the relative weights of the first- and second-order evanescent modes, which we do not analyze. Thus, we expect this model to break down at frequencies just below the diffraction frequencies. It is likely that this analysis can be improved by considering the scattering efficiencies into different diffracted modes, however even without that addition, this model is still highly accurate for nearly all frequencies.

Until this point we have been analyzing open apertures in metal films. We
Figure 3.4: We plot the cavity field leakage length $\delta_e$ as a function of normalized frequency. Discontinuities at dashed vertical lines are the locations of the onset of propagating diffracted modes.

feel it is also worthwhile briefly noting that this approach can be generalized to closed cavities, with a different effective height,

$$h_{\text{eff}} = h + \delta_e + \delta_m,$$

(3.11)

where $\delta_m$ is the field penetration depth into the metal, and where we follow the assumption of our previous work, neglecting fields beyond a skin depth into metal[41].

Using these results, we can rewrite Eq. 3.3 using the effective height of Eq. 3.4,

$$\omega_{mnp} = \frac{c}{\sqrt{\epsilon_c}} \left[ \left( \frac{p \pi}{h + 2\delta_e(\omega_{mnp})} \right)^2 + \gamma_{mn}^2 \right]^{1/2}. \quad (3.12)$$

Since the effective height is itself a function of frequency, it is difficult to find
an exact solution for $\omega$ in all cases. Nevertheless, due to the analytic nature of this expression, we are still able to extract general trends in resonance changes due to cavity geometry. For ease of interpretation, we utilize the graphical approach discussed earlier.

### 3.1.4 ECR dependence on structure geometry

Figure 3.5 shows the dispersion curves overlaid with the restricted $k_z$ condition (Eq. 3.5) for different geometries. Note the discontinuity in the $k_z$ restriction at diffraction frequencies due to the limitations of the theory discussed earlier. The dependence of EOT peaks on cavity radius is found in Eq. 3.12; the radius only affects the waveguide mode dispersion. Thus, keeping the film thickness and periodicity fixed, and changing the radius, shifts only the modal dispersion curve up or down, see Fig. 3.5a. As the radius decreases, the allowed waveguide modes shift to higher frequencies, as expected. However, the rate of shifting is not uniform, in contrast to the FB model discussed in Section 3.1.2, and smaller shifts are found for the same change in radius as the resonance approaches a diffraction frequency.

Changing the period or film thickness leaves the waveguide modal dispersion curve untouched, shifting only the restriction on $k_z$ due to the effective cavity height. The relative size of $h$ and $\delta_e$ determine the dominant con-
tribution to the effective length. When $h$ is large relative to $\delta_e$, i.e. thick films, the resonance approaches the simpler model discussed earlier, where the dominant length is in the waveguide. When $\delta_e$ is large, i.e. extremely thin films or near diffraction, the effects of periodicity dominates the transmission spectrum.

Increasing the thickness of the film pushes the $k_z$ restriction curve closer to the straight vertical lines of Fig. 3.2. However, the lines never do reach $p\pi/h$ as there is always some field coupling depth, see Fig. 3.5c. The smooth transition from the enhanced transmission of a periodic structure, to propagation along regular, independent waveguides can be seen.
Figure 3.5: Graphical interpretation of the variation in the resonance condition due to changes in geometric parameters. For the case considered, there are four dimensional parameters $c/\omega, \Lambda, h,$ and $a,$ giving three independent dimensionless parameters defining the system namely $c/\omega/h,$ $\Lambda/h,$ and $a/h.$ Each of the plots shown above sweeps two of these parameters hence only two plots are needed to analyze the space. Nevertheless, all three plots are shown here to better illustrate the predicted characteristics in terms of the geometric parameters. (a) Effect of varying the radius. Arrow points along direction of decreasing radius with $2a/\Lambda$ of 0.7, 0.79, 0.87, and 0.96 plotted in green, yellow, red, and blue respectively. Here $h/\Lambda = 0.92,$ the black line is the $k_z$ restriction from film thickness, and the colored lines are the different waveguide modal dispersion curves. (b) Effect of varying the periodicity. Arrow points along direction of increasing periodicity with $p/h$ of 0.87, 0.96, 1.04, and 1.13 plotted in blue, red, yellow, and green respectively. Horizontal dashed lines are the diffraction frequencies for each period. Here $h/a = 2.63,$ the black line is the waveguide modal dispersion curve, and the colored lines are the $k_z$ restrictions from film thickness. (c) Effect of varying the film thickness. Arrow points along direction of increasing thickness with $h/a$ of 2.11, 2.63, 3.16, and 6.32 plotted in green, yellow, red, and blue respectively. Here $2a/\Lambda = 0.87,$ the black line is the waveguide modal dispersion curve, and the colored lines are the $k_z$ restrictions from film thickness.
Increasing the period shifts the first diffraction towards lower frequencies, drastically changing the curvature of this restriction curve, see Fig. 3.5b. This, in turn, shifts all resonances towards lower frequencies, with the most drastic changes occurring close to diffraction frequencies. As the period increases further, it pushes down the diffraction frequencies, and thereby increases the density of restricted $k_z$ lines crossing the dispersion curves. It should also be noted that expected transmission through a film drops above a diffraction frequency. If the lowest order scattered diffracted mode is a propagating mode, it leaves proportionally less electromagnetic energy to be scattered into the lowest order evanescent mode, thus decreasing the available localized light which can be coupled to the ECR.

This result further explains the differences in EOT between periodic and single apertures. As the period approaches infinity (i.e. single apertures), the discrete transverse diffracted wavevectors $\sqrt{(m^2 + n^2)K^2}$ can be made arbitrarily close together and can be considered a continuous variable which varies smoothly between 0 and $\epsilon_s \omega^2/c^2$. This leads to an infinite continuum of propagating reflected modes (i.e. a spherical scattered wave) and the number of evanescently decaying modes approaches zero. Thus, the number of modes which permit EOT approaches zero, leading to the expected weaker overall coupling and lower transmission.
3.1.5 Comparison to simulation

It is straightforward to numerically find the roots to Eq. 3.12 and calculate the dependence of peaks in EOT on geometrical properties over a large range of values. To verify the predictions, we simulated structures using HFSS, which is a commercially available full-wave finite element simulation tool. We simulate periodic cylindrical apertures embedded in idealized PEC metal film as well as cavities in a realistic gold film.

Figure 3.6 compares the simulated transmission through a PEC film with \( \epsilon_c = \epsilon_s = 1 \), overlayed with predicted peaks of EOT. There is extremely strong agreement between the predicted and simulated results. Any major differences between predicted and simulated values occur at frequencies very close to diffraction frequencies, which is a manifestation of the limitation of this theory discussed earlier.

Note, that the subwavelength condition \( 2a/\lambda < 1 \) is given in the normalized coordinates of Fig. 3.6a by

\[
\left( \frac{2a}{\Lambda} \right)^2 \leq 2 \left( \frac{h}{\Lambda} \right). \tag{3.13}
\]

Similarly, in the normalized coordinates of Fig. 3.6b by

\[
\left( \frac{\omega}{c \pi / h} \right) < \left( \frac{h}{a} \right). \tag{3.14}
\]
and in the normalized coordinates of Fig. 3.6c by

\[
\left( \frac{\omega}{c \pi / \Lambda} \right) < 2 \left( \frac{2a}{\Lambda} \right)^{-1},
\]

(3.15)

Then, the plotted range of values in Fig. 3.6 are entirely within the subwavelength regime. The existence of EOT through subwavelength PEC structures, where SP resonance is not a contributing factor, further highlights the minimal role of SPs in EOT. The ECR can be viewed as the dominant mechanism which enhances transmission for this class of structures.

As further verification of the validity of this approach, we compare the predictions of this model as it applies to cavities in metal, as per Eq. 3.11. Figure 3.7 compares the simulated specular reflection from a gold film with \( \epsilon_s = 2.1 \) and \( \epsilon_c = 2.1 + i \times 0.9 \), overlayed with predicted peaks of EOT. We introduced loss in the cavity dielectric to better identify the resonances; when there are strong fields built up in the cavity there is increased loss in the dielectric. There is reasonably close agreement between the predicted and simulated results. The weakest agreement is found upon varying the radius. Due to the fairly large skin depths of gold at optical frequencies, there is a small range of values where \( a/\delta_m \) is large, while \( 2a/\Lambda \) remains small. When these conditions are not satisfied, a large fraction of the fields are contained within the metal, and the ECR model and SDBC would not apply. Any other
differences between predicted and simulated values occur at frequencies very close to diffraction frequencies, which is a manifestation of the limitations of this theory discussed earlier in Section 3.1.3.
Figure 3.6: Simulated zero-order transmission through cylindrical apertures embedded in PEC, overlayed with predicted ECR peaks. The gray dashed lines are diffraction frequencies, and the black, blue and red (and green) colored lines are the lowest order TE$_{11p}$ curves for $p=1,2,3$ (and 4) respectively as a function of radius $a$, periodicity $b$ and film thickness $c$. 

(a) Effect of varying the radius. Here $h/\Lambda = 0.92$.

(b) Effect of varying the periodicity. Here $h/a = 2.63$.

(c) Effect of varying the film thickness. Here $2a/\Lambda = 0.87$. 
(a) Effect of varying the radius. Here \( h = 250 \text{nm} \) and \( \Lambda = 800 \text{nm} \).

(b) Effect of varying the periodicity. Here \( h = 250 \text{nm} \) and \( a = 190 \text{nm} \).

(c) Effect of varying the film thickness. Here \( a = 190 \text{nm} \) and \( \Lambda = 800 \text{nm} \).

Figure 3.7: Simulated specular reflection from an array of cylindrical holes embedded in gold, overlayed with predicted ECR peaks. The gray dashed lines are diffraction frequencies, the black and blue lines are the lowest order \( \text{TE}_{111} \) and \( \text{TM}_{011} \) curves, respectively as a function of radius \( a \), periodicity \( b \) and film thickness \( c \).
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3.1.6 Effective Cavity Resonance (ECR) Solutions for Square Aperture Array

Here we discuss a two-dimensional infinitely periodic array of square apertures of width $a$, filled with dielectric $\epsilon_c$ embedded in a perfectly conducting metal film of thickness $h$, periodicity $\Lambda$, see Fig. 3.8.

$$\omega_{mnp} = \frac{c}{\sqrt{\epsilon_c}} \left[ \left( \frac{p\pi}{h + 2\delta_e(\omega_{mnp})} \right)^2 + \left( \frac{m\pi}{a} \right)^2 + \left( \frac{n\pi}{a} \right)^2 \right]^{1/2}, \quad (3.16)$$

with $p = 1, 2, \ldots$, $m = 0, 1, \ldots$, and $n = 1, 2, \ldots$ giving the order of the cavity mode. This resonance constraint is derived using the dispersion of a square

Figure 3.8: (Color Online) A schematic of periodic square apertures in a thin film is shown from top down (a) and in cross section (b). The gray region represents the metal, the light blue regions are the dielectric-filled apertures, and the white is the superstrate and substrate.
waveguide while accounting for the finite cavity height, $h$, as well as the structural periodicity, $\Lambda$.

![Figure 3.9: (Color Online) Simulated and predicted dependence of the transmission on frequency and periodicity $\Lambda$ for an array of square apertures with $a = 400$ nm, $h = 500$ nm, and $\epsilon_c = 1$. The resonant peaks predicted using Eq. 3.16 for the first (blue-solid) and second (black-solid) order resonances are indicated by lines. They agree well with the simulated EOT peaks. The diffraction frequency dependence on periodicity is also indicated (blue-dashed).](image_url)
Figure 3.10: (Color Online) Simulated and predicted dependence of the transmission on frequency and waveguide width $a$ for an array of square apertures with $\Lambda = 600$ nm, $h = 500$ nm, and $\varepsilon_c = 1$. The resonant peaks predicted using Eq. 3.16 for the first (blue-solid) and second (black-solid) order resonances are indicated by lines. They agree well with the simulated EOT peaks. The diffraction frequency dependence on periodicity is also indicated (blue-dashed). The ECR approximation breaks down as the resonances approach the diffraction frequency.
Figure 3.11: (Color Online) Simulated and predicted dependence of the transmission on frequency and cavity height $h$ for an array of square apertures with $a = 400$ nm, $\Lambda = 600$ nm, and $\varepsilon_c = 1$. The resonant peaks predicted using Eq. 3.16 for the first (blue-solid) and second (black-solid) order resonances are indicated by lines. They agree well with the simulated EOT peaks. The diffraction frequency dependence on periodicity is also indicated (blue-dashed).

### 3.1.7 Comparison to simulation and discussion

As above, the roots of Eq. 3.16 can be determined numerically and the EOT resonance peaks obtained for various geometrical parameters. The predicted EOT peaks for square arrays are compared to the transmission peaks obtained via the finite element frequency domain domain solver. Figs. 3.9-3.11 display the simulated transmission for different periodicity $\Lambda$, square width $a$, and film height $h$ as well as the analytically predicted transmission reso-
nance peaks. The predicted resonances agree well with the simulated EOT peaks over a large range of geometric parameter values.

Figure 3.12: (Color Online) A cross-sectional slice of unit cell of a square cavity embedded in a PEC film is shown, with the magnitude of the electric field (in arbitrary units) plotted at the (a) first resonance and (b) second resonance with $\omega \Lambda / 2\pi c = 0.796$ and 0.876. For this structure $\Lambda / a = 1.5$, $a/h = 0.8$. The enhanced fields at resonance extend from the cavity to a distance on the order $\delta$ with $\delta / \Lambda = 0.26$ and 0.33 for the (a) first and (b) second order resonances, shown here in black lines.

However, when the EOT resonance frequency begins to approach the diffraction frequency (Fig. 3.10 and 3.11), the predicted resonance begins to significantly deviate from the simulated transmission resonance. As described above, this occurs because as the evanescent mode transitions to a propagating mode, the decay length $\delta_e$ becomes infinite. Therefore, as the first order diffraction mode transitions to a propagating mode, less electromagnetic energy is stored in that mode. In addition, the resonances predicted by
Eq. 3.16, when far from diffraction, are at slightly higher frequencies than the simulated resonances. This is most clearly seen in Fig. 3.11. This indicates that the effective height $h_{\text{eff}}$ used in Eq. 3.16 is too small to accommodate the spread of the localized resonant electromagnetic field. Indeed, the field profiles depicted in Figs 3.12a and 3.12b indicate that the enhanced fields drop to zero at a distance greater than $\delta_e$ from the aperture exit. A more accurate prediction may be attained by adding another weighting factor to $\delta_e$, which may need to be dependent on aperture geometry.

### 3.2 Rigorous Coupled Wave Analysis

Here we will discuss the semi-analytic method that can be used to efficiently solve cavity array metasurfaces, namely the rigorous coupled wave analysis (RCWA) method, for one-dimensional systems which can be generalized in a straightforward manner to two-dimensional systems. The primary idea of the RCWA method for periodic gratings is to use field expansions of maxwell’s equations with a basis that satisfy the periodic Floquet condition. This is done in each dielectric layer of the grating. In addition, within the metal grating regions, waveguide mode expansions are used, which consist of a basis set the satisfy maxwell’s equations in the waveguides. Maxwell’s Equations for linear dielectric media without free charges are given by Eq. 2.1-2.6. These
equations can be written as time harmonic by assuming all the fields have a time dependence that goes as: \( I \propto e^{i\omega t} \). In addition, for a grating, they can be decoupled into transverse magnetic (TM) and transverse electric (TE) modes which have only \( H_z \) and \( E_z \) components of the magnetic and electric fields respectively. The field equations can then be written for TM modes as follows:

\[
\begin{align*}
\frac{i\omega\epsilon}{c} \mathbf{E} &= \nabla \times \mathbf{H} \quad (3.17) \\
\mathbf{E} &= \frac{c}{i\omega\epsilon} \nabla \times \mathbf{H} \quad (3.18) \\
E_x &= \frac{c}{i\omega\epsilon\mu} \frac{\partial B_z}{\partial y} \quad (3.19) \\
E_y &= -\frac{c}{i\omega\epsilon\mu} \frac{\partial B_z}{\partial x} \quad (3.20)
\end{align*}
\]

and for TE modes:

\[
\begin{align*}
\frac{-i\omega\epsilon}{c} \mathbf{B} &= \nabla \times \mathbf{E} \quad (3.21) \\
\mathbf{B} &= \frac{-c}{i\omega\epsilon} \nabla \times \mathbf{E} \quad (3.22) \\
B_x &= \frac{-c}{i\omega\epsilon\mu} \frac{\partial E_z}{\partial y} \quad (3.23) \\
B_y &= \frac{c}{i\omega\epsilon\mu} \frac{\partial E_z}{\partial x} \quad (3.24)
\end{align*}
\]
3.2.1 Metallic Grating Expansion

In order to solve the metallic grating system using the RCWA, we must expand the fields into different basis set for each grating layer. In this description, we will adopt the bra-ket orthonormal basis notation for each layer. Every layer has a basis set for light waves traveling in opposite directions including the superstrate and substrate layers. The magnetic field for a dielectric layer in the TM case are given as:

![Figure 3.13: Example of grating to be solved](image-url)
\[ H_{z,l} = \sum_{i=\infty}^{\infty} I_{l,k_{x,i},i}^+ |\psi_{l,k_{x,i},i}^+\rangle + I_{l,k_{x,i},i}^- |\psi_{l,k_{x,i},i}^-\rangle \quad (3.25) \]

where \( |\psi_{l,k_{x,i},i}^+\rangle \) (\( |\psi_{l,k_{x,i},i}^-\rangle \)) is an upward (downward) plane wave with amplitude \( I_{l,k_{x,i},i}^+ \) \( (I_{l,k_{x,i},i}^-) \) for layer \( l \) and \( k \) vector \( k_{l,i}^\pm \) with x-component given by \( k_{x,i} \), which is given by the incident momentum and the diffraction momenta and y-component given by \( k_{l,y,i}^\pm \). The sum is over all possible plane waves satisfying the Floquet condition for a periodic grating. The \( k \) vector in dielectric layer \( l \) is given by:

\[ k_{l,i}^\pm = k_{x,i} \hat{x} + k_{l,y,i}^\pm \hat{y} \quad (3.26) \]
\[ |k_{l,i}| = \sqrt{\epsilon_l \omega / c} \quad (3.27) \]
\[ k_{x,i} = \alpha + ik_g \quad (3.28) \]
\[ k_{l,y,i}^\pm = \pm \sqrt{\epsilon_l k_0^2 - k_{x,i}^2} \quad (3.29) \]

with \( \alpha \) as the incident momentum and \( k_g \) as the grating momentum that is determined by the grating period \( \Delta \) as:

\[ k_g = \frac{2\pi}{\Delta} \quad (3.30) \]

The basis is orthogonal such that:
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\begin{equation}
\langle \psi_{l,k_x,i}^+ | \psi_{l,k_x,j}^+ \rangle = \delta_{i,j} \tag{3.31}
\end{equation}

for dielectric layers the orthogonal functions are given as:

\begin{equation}
|\psi_{l,k_x,i}^\pm\rangle = \frac{1}{\sqrt{\Delta}} e^{i(k_{x,i}x \pm k_{y,i}y)} \tag{3.32}
\end{equation}

and the orthogonal condition is given as:

\begin{equation}
\langle \psi_{l,k_x,i}^+ | \psi_{l,k_x,j}^+ \rangle = \int_0^\Delta \frac{1}{\Delta} e^{i(k_{x,i}x \pm k_{y,i}y')} e^{i(k_{x,j}x \pm k_{y,j}y')} \tag{3.33}
\end{equation}

which gives Eq. 3.31. The inner product defined in Eq. 3.33 gives the projection between the various basis functions and will be used at interfaces between layers to match boundary conditions of the expanded fields of each layer. In a metal grating region, there may be multiple apertures or slits, with multiple modes in each aperture. Grating layer expansions have the following form:

\begin{equation}
H_{z,l} = \sum_{m=1}^{M} \sum_{n=0}^{\infty} I_{l,m,n}^+ \phi_{l,m,n}^+ + I_{l,m,n}^- \phi_{l,m,n}^- \tag{3.34}
\end{equation}

where the double sum incorporates the $M$ different apertures in the grating layer $l$ and the second sum is for the $n$ modes in a given aperture $m$. The waveguide basis also has an orthonormal condition given by:
\[
\langle \phi_{l,m,n}^\pm | \phi_{l,m',n'}^\pm \rangle = \delta_{m,m'} \delta_{n,n'}
\] (3.35)

Some waveguide modes \( \phi_{l,m,n}^\pm \) were already described for rectangles and cylinders and can be expanded using the SDBC or SIBC methods to allow the modes to be applicable in different spectral ranges. These expansion basis functions allow us to describe the fields throughout each layer as just a vector. The method of calculating the fields for a given excitation is done using the scattering matrix method described below.

### 3.2.2 Scattering Matrix Method

The scattering matrix method has arisen to be one of the primary methods to solve grating problems in the computational electromagnetics community. The scattering matrix approach here is modeled primarily after the method described by Rumpf[58] as well as others. This method consists of forming scattering matrices for each layer in the device and then combining them via the Redheffer[59, 60] star product to obtain the device scattering matrix. An artificial layer of vacuum, defined here with layer index 0, is inserted at each interface of the device in order to make the process computationally simpler. This enables each layer to be treated as identical cases. This layer is then reduced to zero thickness when the full device scattering matrix is computed,
which is mathematically equivalent to having no additional layer at all.

The scattering matrix of each layer is determined by matching the boundary conditions on each side:

\[
\begin{align*}
H_{z,0}|_{z=0^+} &= H_{z,l}|_{z=0^-} \\
\frac{\partial H_{z,0}}{\partial y}|_{z=0^+} &= \frac{\partial H_{z,l}}{\partial y}|_{z=0^-} \\
H_{z,0}|_{z=(-t_l)^-} &= H_{z,l}|_{z=(-t_l)^+} \\
\frac{\partial H_{z,0}}{\partial y}|_{z=(-t_l)^-} &= \frac{\partial H_{z,l}}{\partial y}|_{z=(-t_l)^+}
\end{align*}
\] (3.36)

where \(z = 0^\pm\) refers to the top interface approaching from the top (+) and bottom (−) of the interface and \(z = (-t_l)^\pm\) applies to the bottom interface for a layer of thickness \(t_l\). For a uniform dielectric layer matching these conditions at both the entrance and exit interface is trivial since both are expanded in a Floquet plane wave basis with the same number of modes and unknowns. The result is simply the Fresnel equations for reflection and transmission relating the plane waves of the same wavenumber on each side. Explicitly this is given as:
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\[
\sum_{i=-N}^{N} I_{0,k_{x},i}^{+} |\psi_{0,k_{x},i}^{+}\rangle + I_{0,k_{x},i}^{-} |\psi_{0,k_{x},i}^{-}\rangle = \sum_{i=-N}^{N} I_{l,k_{x},i}^{+} |\psi_{l,k_{x},i}^{+}\rangle + I_{l,k_{x},i}^{-} |\psi_{l,k_{x},i}^{-}\rangle \tag{3.37}
\]

\[
\frac{\partial}{\partial y} \sum_{i=-N}^{N} I_{0,k_{x},i}^{+} |\psi_{0,k_{x},i}^{+}\rangle + I_{0,k_{x},i}^{-} |\psi_{0,k_{x},i}^{-}\rangle = \frac{\partial}{\partial y} \sum_{i=-N}^{N} I_{l,k_{x},i}^{+} |\psi_{l,k_{x},i}^{+}\rangle + I_{l,k_{x},i}^{-} |\psi_{l,k_{x},i}^{-}\rangle \tag{3.38}
\]

\[
\Rightarrow k_{0,y,i} I_{0,k_{x},i}^{+} + k_{0,y,i} I_{0,k_{x},i}^{-} = I_{l,k_{x},i}^{+} + I_{l,k_{x},i}^{-}
\]

\[
k_{0,y,i} I_{0,k_{x},i}^{+} - k_{0,y,i} I_{0,k_{x},i}^{-} = k_{l,y,i} I_{l,k_{x},i}^{+} - k_{l,y,i} I_{l,k_{x},i}^{-} \tag{3.39}
\]

This is applied at the exit interface as well, however we must also take into account the unitary phase factor (exponential for evanescent modes) accrued due to propagation in the material of length \(-t_{l}\) which for each floquet mode is given by:

\[
I_{l,k_{x},i}^{\pm} |_{sup} = e^{-ik_{l,y,i}^{\pm}t_{l}} I_{l,k_{x},i}^{\pm} |_{sub} \tag{3.40}
\]

where the \(sup\) and \(sub\) mark the superstrate and substrate interface respectively. It is evident that the downward propagating modes accrue positive phase whereas the upward propagating modes accrue negative or retarded phase. For evanescent modes, these become exponentially decaying (downward) or exponentially growing (upward) terms. This can be written as a propagation diagonal matrix \(P\). We obtain the scattering matrix of the layer.
in the following manner:

\[
\begin{pmatrix}
1 & 1 \\
K_0 & -K_0
\end{pmatrix}
\begin{pmatrix}
I_0^+ \\
I_0^-
\end{pmatrix}_{sup} =
\begin{pmatrix}
1 & 1 \\
K_1 & -K_1
\end{pmatrix}
\begin{pmatrix}
I_1^+ \\
I_1^-
\end{pmatrix}_{sup}
\]

\[
\begin{pmatrix}
1 & 1 \\
K_l & -K_l
\end{pmatrix}
\begin{pmatrix}
P_1 & 0 \\
0 & P_1
\end{pmatrix}
\begin{pmatrix}
I_l^+ \\
I_l^-
\end{pmatrix}_{sup} =
\begin{pmatrix}
1 & 1 \\
K_0 & -K_0
\end{pmatrix}
\begin{pmatrix}
I_0^+ \\
I_0^-
\end{pmatrix}_{sub}
\]

\[
\begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
I_0^+ \\
I_0^-
\end{pmatrix}_{sup} =
\begin{pmatrix}
I_0^+ \\
I_0^-
\end{pmatrix}_{sub}
\]

(3.41)

where the scattering matrix S can be obtained by rearranging Eq.3.41:

\[
\begin{pmatrix}
C_{11} & C_{12} \\
C_{21} & C_{22}
\end{pmatrix} = 
\begin{pmatrix}
1 & 1 \\
K_0 & -K_0
\end{pmatrix}^{-1}
\begin{pmatrix}
1 & 1 \\
K_1 & -K_1
\end{pmatrix}
\begin{pmatrix}
P_1 & 0 \\
0 & P_1
\end{pmatrix}
\]

\[
\begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix} = 
\begin{pmatrix}
-C_{11} & 0 \\
-C_{21} & 1
\end{pmatrix}^{-1}
\begin{pmatrix}
C_{12} & -1 \\
C_{22} & 0
\end{pmatrix}
\]

(3.42)

For a waveguide metasurface grating, there are spatially discreet waveguide modes instead of floquet modes. The matched boundary condition is therefore given as:
\[
\sum_{i=-\infty}^{\infty} I_{0,kx,i}^+ |\psi_{0,kx,i}^+\rangle + I_{0,kx,i}^- |\psi_{0,kx,i}^-\rangle = \sum_{m=1}^{M} \sum_{n=0}^{\infty} I_{l,m,n}^+ |\phi_{l,m,n}^+\rangle + I_{l,m,n}^- |\phi_{l,m,n}^-\rangle \quad (3.43)
\]

\[
\frac{\partial}{\partial y} \sum_{i=-\infty}^{\infty} I_{0,kx,i}^+ |\psi_{0,kx,i}^+\rangle + I_{0,kx,i}^- |\psi_{0,kx,i}^-\rangle = \frac{\partial}{\partial y} \sum_{m=1}^{M} \sum_{n=0}^{\infty} I_{l,m,n}^+ |\phi_{l,m,n}^+\rangle + I_{l,m,n}^- |\phi_{l,m,n}^-\rangle \quad (3.44)
\]

When truncated, this can be rewritten as a set of linear equations by taking the inner product of Eq.3.37-3.38 with the orthogonal superstrate floquet modes \( \psi_{0,kx,i} \) and the waveguide orthonormal modes \( \phi_{l,m,n} \) obtain:

\[
\begin{pmatrix}
K_{1,1} & K_{1,2} \\
K_{2,1} & K_{2,2}
\end{pmatrix}
\begin{pmatrix}
I_{1,kx,i}^+ \\
I_{1,kx,i}^-
\end{pmatrix} = \begin{pmatrix}
m_{11} & m_{12} \\
m_{21} & m_{22}
\end{pmatrix}
\begin{pmatrix}
I_{l,m,n}^+ \\
I_{l,m,n}^-
\end{pmatrix} \quad (3.45)
\]

the \( K \) matrix has dimension \((2n \times M \times (2(2N+1)))\) and the \( m \) matrix has dimensions \((2(2N+1)) \times 2n \times M\). There is an identical equation relating the components at the exit of the waveguide grating except with a propagating matrix acting on the waveguide modes to account for the phase accrued while propagating through the layer.

\[
\begin{pmatrix}
K_{1,1} & K_{1,2} \\
K_{2,1} & K_{2,2}
\end{pmatrix}
\begin{pmatrix}
I_{1,kx,i}^+ \\
I_{1,kx,i}^-
\end{pmatrix} = \begin{pmatrix}
m_{11} & m_{12} \\
m_{21} & m_{22}
\end{pmatrix}
\begin{pmatrix}
P_{11} & P_{12} \\
P_{21} & P_{22}
\end{pmatrix}
\begin{pmatrix}
I_{l,m,n}^+ \\
I_{l,m,n}^-
\end{pmatrix}
\]
we use these two sets to relate the superstrate and substrate plane waves as follows:

\[
\bar{K} I_{\text{sup}} = \bar{m} I_{\text{cav}} \quad (3.46)
\]

\[
\bar{m} \bar{P} I_{\text{cav}} = \bar{K} I_{\text{sub}} \quad (3.47)
\]

\[
\bar{K} I_{\text{sup}} = \bar{C} I_{\text{sub}} \quad (3.48)
\]

\[
\bar{C} = \bar{m} \left( (\bar{m} \bar{P})^T \right)^{-1} (\bar{m} \bar{P})^T \bar{K} \quad (3.49)
\]

By rearranging the result we obtain the scattering matrix relating the input to the output:

\[
\begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
I_{\text{sup}} \\
I_{\text{sub}}^+
\end{pmatrix} = 
\begin{pmatrix}
I_{\text{sup}}^+ \\
I_{\text{sub}}^+
\end{pmatrix}
\quad (3.50)
\]

\[
\begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix} = 
\begin{pmatrix}
-K_{11} & C_{12} \\
-K_{21} & C_{22}
\end{pmatrix}^{-1}
\begin{pmatrix}
K_{12} & -C_{11} \\
K_{22} & -C_{21}
\end{pmatrix}
\]

With the scattering matrix of each grating layer and dielectric layer known, we can use the Redhoffer product to obtain the overall system matrix and solve for the reflection and transmission for a known excitation. The Redhoffer product for two scattering matrices given by \( S^{AB} \) depend on the separate scattering matrices \( S^A \) and \( S^B \) as follows:
\[ \begin{align*}
S_{11}^{AB} &= S_{11}^A + S_{12}^A \left[ I - S_{11}^B S_{22}^A \right]^{-1} S_{11}^B S_{21}^A \\
S_{12}^{AB} &= S_{12}^A \left[ I - S_{11}^B S_{22}^A \right]^{-1} S_{12}^B \\
S_{21}^{AB} &= S_{21}^B \left[ I - S_{22}^B S_{11}^A \right]^{-1} S_{21}^A \\
S_{22}^{AB} &= S_{22}^B + S_{21}^B \left[ I - S_{22}^A S_{11}^B \right]^{-1} S_{22}^A S_{11}^B
\end{align*} \] (3.51)

In the general case, \( S^{AB} \neq S^{BA} \). Solving the resulting system is a straightforward matrix solve that can be achieved with standard numerical libraries.

### 3.3 Finite Element Method

Another versatile method for simulating the behavior of electromagnetic and other physical systems is the finite element method. There has been significant research into this method and a full derivation will not be done here. The essence of the method is to break the system volume into subregion elements or mesh and expand the unknown electromagnetic fields as a finite sum of known basis function with unknown coefficients in each mesh element thereby linearizing the system. Maxwell’s equations can then be used to relate the expanded fields between neighboring elements which constructs a system interaction matrix which can in turn be related to the fields at the boundary of the system. By defining the boundary conditions of the system as electromagnetic sources, sinks, periodic conditions and other boundary conditions, the unknown field expansion coefficients can be solved. This
method allows for simulating complex geometries with virtually any material dielectric and can be used to model devices ranging from the microwave to visible electromagnetic spectrum.

The primary FEM modelling software used in this work is Ansoft’s HFSS package. This tool allows for virtually any CAD geometry and provides built in material properties or user defined material properties. The metasurface designs modelled in this work are periodic in either one or two dimensions and the unit cells were therefore simulated by bounding the unit cell in a box with the appropriate substrate and superstrate properties. The boundary conditions on the periodic box faces were then defined using continuity boundary conditions (PEC and PMC) for normal incidence excitations and Floquet boundary conditions for off-normal incident excitations. Wave ports were defined at the entrance (top) and exit (bottom) boundary faces to supply the excitation and enable the S-parameters, and therefore the reflection and transmission, to be obtained.

3.4 Summary and conclusion

We have presented a new analytical theory for the mechanism of EOT through arrays of subwavelength apertures. This theory demonstrates that an effective cavity is described by the cavity dimensions in conjunction with the
decay length of strong, localized evanescent diffracted modes in the regions above and below the metal film. These localized fields are the primary cause for coupling light between the apertures and the other regions. Thus, this model is a fundamental theory for the mechanism of EOT.

Furthermore, we have shown how to predict the frequencies where peaks in enhanced transmission occur and how these frequencies depend on the cavity dimensions, metal choice, as well as periodicity of the structure. This model is valid over an extremely broad range of geometries, limited only at frequencies close to diffraction. We have shown strong agreement between our theory and simulations for both apertures through PEC and cavities embedded in real gold.

Although the model was applied to cylindrical apertures, this approach can be generalized to apertures of arbitrary shape. Other apertures change the value of the transverse wavevector $\gamma_{mm}$ in dispersion relation of Eq.2.44, leaving everything else unchanged. Similarly, this can be generalized to rectangular, and perhaps arbitrary, periods, changing only the reciprocal lattice vectors in Eq. 3.7. Likewise, the dependence of EOT on incident angle can likely be deduced from the changes this makes to the propagation vectors in the superstrate.

In addition, we have described a semi-analytical rigorous coupled wave
analysis method, which can be implemented to solve cavity array metasurfaces to a desired accuracy. This method is versatile and can be adopted for multiple layers, multiple cavity types, multiple dimensions, cavity shapes, and incident beam profiles. Given that it uses solutions to Maxwell’s equations as basis functions it is able to solve complex systems in a fraction of the time it would take for a finite element solver.
Chapter 4

Polarization Photon Sorting Using Cavity Array Metasurfaces in the Visible

In the previous chapters we discussed general properties of waveguide cavity mode meta-atoms and metasurfaces composed of a single meta-atom type. We investigated theoretical and semi-analytical methods for predicting their behavior, namely the effective cavity mode approximation and the rigorous coupled wave methods. In this we will implement multiple meta-atoms in a metasurface to design novel photon sorting properties. We will present a polarization sorting metasurface for use as a compact polarization sensor.

4.1 Introduction

Since the discovery of optical polarization, the expanding field of polarimetry has contributed to multiple applications. One such application, polarization
imaging, can extract additional information that is not possible with con-
ventional imaging. Measurement of the polarization state, commonly in the
form of Stokes parameters, enables more information to be obtained from
an image such as the determination of surface orientation of an object[61],
image stress mappings of a material via the effect of photoelasticity, charac-
terization of material dielectric properties via ellipsometry, or can be used to
produce enhanced contrast images in low intensity contrast conditions[62].
There has been increasing interest over the past few years in the develop-
ment of compact imaging sensors operating in the visible regime that can
measure polarization information with high spatial and temporal resolution.
Past polarization sensors made use of a linear polarizer placed within the
optical path leading to a light intensity measuring array. These polarimeters
make use of a division of aperture method[63], and of a division of ampli-
tude method[64] to simultaneously measure the Stokes parameters, which
requires splitting the incident beam to multiple sensors. Division of focal
plane polarimeters[65] provide another method for attaining high resolution
polarization sensors. This method relies on a micropolarizer array layered
directly above the imaging sensor array, and may be best suited for purposes
of miniaturizing image polarization sensors. Research has been performed
on approaches to develop monolithic micropolarization sensors for high reso-
lution polarization imaging using liquid crystals\cite{66}, polymers\cite{67}, and wire grid polarizers\cite{68} to name a few.

A standard approach is the use of wire grid polarizers that can be fabricated using CMOS fabrication techniques (Fig. 4.1). Wire grid polarizers (WGPs) have been shown to have extinction ratios on the order of 1000\cite{69} or more over particular wavelength bands and are effective for large incident angles\cite{70}. The high extinction ratios provided by WGPs are due to the high reflection of the TE polarized component of the incident beam while the transmission of the TM component can approach unity. Polarimetric sensors using WGPs, fabricated in a 2-polarizer or 4-polarizer superpixel array, have been integrated atop CCD and CMOS arrays using established fabrication techniques\cite{71–73} allowing for the measurement of the Stokes parameters of incident light by measuring subpixel intensity using standard technologies. Sensors implementing WGPs in arrays have been designed to measure TE polarized light\cite{72}. Working from these previous designs, we further improve the functionality of the wire grid polarizing layer by replacing it with a 1-dimensional metasurface grating using two distinct meta-atoms, allowing for further miniaturization of about a factor of 2.
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4.2 Subpixel Design

The metasurface described in this work consists of a compound transmission grating (CTG) with four rectangular sub-wavelength metallic grooves per unit cell (Fig. 4.2). The first function of the metasurface is to split and selectively channel light incident upon the grating according to the polarization state. This is accomplished by using two meta-atoms which selectively transmits a single polarization.

The second function of the metasurface grating is to transmit the light
into the semiconductor substrate where it will be absorbed. The spatially
separated polarization components of the light generate electron/hole pairs in
the semiconductor substrate directly underneath the two grooves from which
the polarization components of the light were transmitted (Fig. 4.3-4.4). In
this design, GaAs was used as the semiconductor for its high absorption
properties in the visible spectral range as discussed in depth below. The
third function of the metasurface grating is to serve as the contact array
used for current collection. The generated photocurrent distributions pro-
duced by the TE and TM components of the incident beam are collected by
separate electrically biased contacts producing two currents, $I_o$ and $I_i$. By
analyzing the resulting currents, the polarization state, and therefore two
of the Stokes parameters can be determined in a single pixel. This design
can improve the resolution of division of focal plane polarization sensors and
reduce instantaneous field of view errors that arise from using superpixel
structures. Currently, methods of interpolation of the subpixels are used to
reduce these errors[74,75]. This polarimetric photodetector can be pixelated
and used to make polarimetric focal plane array sensors and imaging systems
that perform polarization discrimination and photodetection, all integrated
within one monolithic, compact, lightweight and robust device—making it
potentially useful for space-based imaging systems.
Figure 4.2: A cross-section of the optical and electrical unit cell of the structure. It consists of a GaAs substrate with a metallic grating layer. The unit cell of the device has a period $\Lambda = 630$ nm. The grating consists of two different resonant cavities with widths $a = 83$ nm and $b = 168$ nm, with five silver wires of width 32 nm, and a height $h$ of 180 nm, and a dielectric, $Si_3N_4$ between the wires. The outer cavities inhibit transmission of the TE mode causing channeling of the TE mode only through the center grooves.
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Figure 4.3: Illustration of a cross-section of the unit cell operating under TE polarized light. Incident light (solid arrows) is channeled by the metasurface layer through the center cavities into the GaAs substrate. Photogenerated electrons (circles) are generated beneath the central wire. The electron current (dashed arrows) is collected by the grating’s center contact, and is driven by the bias applied to the contacts. An illustration of the electric field lines generated by the contact bias are shown (blue arrows).
Figure 4.4: Illustration of a cross-section of the unit cell operating under TM polarized light. Incident light (solid arrows) is channeled by the metasurface layer through all the cavities into the GaAs substrate. Photogenerated electrons (circles) are generated throughout the GaAs substrate. The electron current (dashed arrows) is collected by the center and outer contacts. An illustration of the electric field lines generated by the contact bias are shown (blue arrows).

The proposed sensor structure consists of an array of pixels. Each pixel can be composed of one or two subpixels (depending on whether the sensor is designed to determine the first two or first three Stokes parameters), with each subpixel composed of a large number of periods of the unit cell shown in (Fig. 4.2, Fig. 4.5). Every subpixel is capable of measuring the linear polarization state of an incident beam and it is the functionality of the subpixel
that is of interest and the focus of this chapter. The subpixel structure is composed of a 3 μm thick GaAs substrate coated with a metallic compound transmission grating layer.

In order for the device to simultaneously measure both polarizations, the current generated by each polarization must be separately collected. The separation and collection of the TE and TM generated current is done by alternately changing the bias voltage on adjacent contacts. This generates an electric field close to the grating interface that collects the carriers (see Fig. 4.3-4.4). GaAs is well suited as a substrate versus other photodetecting materials such as silicon. Compared to silicon, GaAs has a significantly shorter absorption length thereby generating most of the carriers closer to the grating interface, which is essential to the functioning of the device. Silicon would absorb the transmitted light, and generate carriers, further from the grating where they are less likely to be swept to the desired electrode due to reduced magnitude of the biasing field.

Figure 4.2 shows the unit cell of the grating, which has a period of Λ = 630 nm, and possess two pairs of two different grooves. The resonant cavities of the grating contain Si₃N₄ with a dielectric constant of 4.0. The widths \( a \) and \( b \) of the two types of cavities are 83 nm and 168 nm respectively, and are bounded on their left and right hand sides by rectangular metal wires of
height \( h = 180 \text{ nm} \) and width \( w = 32 \text{ nm} \).

Figure 4.5: The polarimeter pixel structure composed of multiple unit cells per pixel. The three current components in the three separate leads are shown in the inset. The structure measures both TE and TM polarizations in one pixel.
4.3 Optical Properties of the Metasurface

The metasurface is designed to selectively channel TE and TM polarized light using cavity meta-atom grooves with different resonances for TE and TM polarizations. These are used in order to spatially separate the different polarizations before being transmitted into the semiconductor substrate. The channeling of the TE mode to the center grooves is accomplished by choosing the dimensions of the grooves to allow for TE mode propagation in the center grooves while the outer grooves waveguide modes remain below cutoff in the operating spectral range. For rectangular grooves of thickness $t$, width $a$, dielectric material within the groove with index of refraction $n$ such that $n_{\text{substrate}} > n > n_{\text{superstrate}}$, the wavelengths, $\lambda_{s,p}$, of these WCMs, and the wavelengths of incident light that can excite them, are approximately given by the ECR:

$$\lambda_{s,p} = \frac{1}{2n} \sqrt{\left( \frac{s}{a} \right)^2 + \left( \frac{p + \frac{1}{2}}{t + n_{\text{eff}}} \right)^2}.$$  \hspace{1cm} (4.1)

where $s$ and $p$ are integers with possible values of $p = 0, 1 \cdots$ for both TM and TE polarized WCMs and $s = 0, 1 \cdots$ for TM polarized WCMs, but with the $s = 0$ mode excluded for TE polarized WCMs. Eq. 4.1 would predict a degeneracy in energy for the same order TE and TM WCMs, yet the different boundary conditions at the entrance and exit of the grooves lifts
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this degeneracy and shifts $\lambda_{s,p}$ relative to the values predicted by Eq. 4.1. These approximate feature sizes for the individual grooves are then used as a starting point for the final 4-groove/period metasurface grating (Fig. 4.2). The final optical design of the grating is modeled and optimized, first using a rigorous coupled wave (RCWA) algorithm, and then a full-wave finite element method approach (HFSS). The optical parameters for the silver metal was obtained from Palik [76]. This design is optimized to have the placement of the four grooves within the unit cell that maximizes light channeling and minimizes crosstalk. Fig. 4.6a-4.8b show reflection and absorption vs. wavelength of incident light in the wavelength range the device is designed to operate and the resonant field profiles of the structure for the TM and TE polarized WCM at $\lambda = 700$ nm.

The metasurface grating has a maximum of transmission for TE polarization due to a WCM resonance that occurs at a wavelength of about $\lambda = 700$ nm. The TM transmission resonance occurs at a lower wavelength, yet is still large enough at $\lambda = 700$ nm for the device to readily resolve the polarization state of an incoming light beam. Simulations show that there is considerable absorption and optical loss within the metal because real metal parameters are used, reducing the transmitted light into the GaAs substrate. A crucial aspect of the device is the channeling of the TE polarized light to and through
the center apertures. This localization of the TE light is shown in Fig. 4.8a. The first order TE polarized WCM resonance is readily apparent in the two center cavities adjacent to the center contact. The extinction ratio for the device is shown in Fig. 4.7 and is close to unity over the wavelength range of interest which is in stark contrast to conventional wire grid polarizers, which favor one polarization. The need for this characteristic is discussed in Sec. 4.4. The volume loss densities for TE and TM polarized incident light are shown in Fig. 4.9a-4.9b. The grating concentrates the TE light underneath the center contact.

The simulated optical behavior of the device shows stability with respect to deviations of parameters from the optimized design. This is shown in Figs. 4.10a-4.10c by varying the width $b$ of the center aperture. Since the center apertures cause the TE polarized light to be spatially localized, this parameter is most crucial for the device. The only significant change occurs in the transmission for the TE polarized light, which shifts to higher (lower) energies for increasing (decreasing) values of $b$. The device remains functional for deviations in $b$ of up to 10%.
Figure 4.6: The normalized optical losses for a unit cell of the device. The three loss mechanisms are the loss in the GaAs (light gray), loss in the silver grating (dark gray), and reflection (black) for a range of wavelengths about the resonance for: (a) TE polarized incident light, and (b) TM polarized incident light. As expected, the sum of all three losses add to unity at each wavelength.
Figure 4.7: The extinction ratio for the normalized transmission of the TM to TE polarized light is shown for the wavelength spectrum of interest for the proposed device. The extinction ratio is close to unity for all wavelengths, indicating that the designed metasurface grating does not favor the transmission of a particular polarization unlike conventional wire grid polarizers which tend to favor one polarization.
Figure 4.8: Simulated magnitude of the electric field plotted on a cross-section of a unit cell of the structure for (a) TE polarized incident light of wavelength $\lambda = 700$ nm, and (b) TM polarized incident light of the same wavelength. The TE fields are localized to the center apertures and the resonant mode behaves like an effective cavity. (b) For the TM mode light large spatial separation does not occur and the fields are channeled through all the apertures.
Figure 4.9: The volume optical loss density distribution (which is directly proportional to the electron-hole pair generation rate) in the GaAs substrate for (a) TE polarized incident light of wavelength $\lambda=700$ nm, and (b) TM polarized incident light of the same wavelength. The TE volume optical loss density is localized beneath the center grooves close to the center contact. The TM mode volume optical loss is more uniformly spread across the structure.
Figure 4.10: The dependence of the transmission for TM (a) and TE (b) as well as the extinction ratio (c) on wavelength is shown for deviations of the optimal value for center aperture width $b$. The transmission peak for the TE polarization shifts to higher energies for larger widths, however, the functionality of the device remains for deviations of within 10%. The transmission for the TM mode remains almost unchanged with the varying of the width. The extinction ratio remains close to unity for deviations of within 10%.

### 4.4 Electrical Properties of Polarization Sensing Pixel

With the TE polarized light being transmitted almost exclusively through the two center grooves, the resultant TE photogenerated current will be collected mainly by the center contact. The current due to TE polarized incident light is thereby distinguishable from the TM photogenerated current, which is
fairly uniformly transmitted throughout the grating. By measuring the ratio of currents $I_i/I_t$ and $I_o/I_t$, the polarization state of the incident light can be determined. Again, the values of $I_o$, $I_i$, and $I_t$ are the measured outer contact current, inner contact current, and total current, $I_o+I_i$, respectively.

In the linear response regime, the general relation between the polarization state of an incident beam and the output currents for this subpixel can be written as:

\[
\begin{align*}
\alpha_{TE} I_{TE} + \alpha_{TM} I_{TM} &= I_o \\
\beta_{TE} I_{TE} + \beta_{TM} I_{TM} &= I_i
\end{align*}
\]

$I_{TE}$ and $I_{TM}$ are the values to be determined and are the optical powers of the TE and TM polarized components of the incident beam respectively. The $\alpha$ and $\beta$ parameters are associated with the light-splitting and can be determined by calibrating the device by measuring $I_o$ and $I_i$; $\alpha_{TE}$ and $\beta_{TE}$ can be determined by illuminating the device with only a TE polarized light (i.e., $I_{TE} \neq 0$ and $I_{TM} = 0$) and similarly for $\alpha_{TM}$ and $\beta_{TM}$. In the ideal sensor of the type discussed here, there would be perfect current separation for the TE and TM modes to the inner and outer contacts, with $\alpha_{TE}$ and
\( \beta_{TM} \) both zero, and Eq. 4.2 and Eq. 4.3 would simply reduce to:

\[
\alpha_{TM} I_{TM} = I_o \quad (4.4)
\]
\[
\beta_{TE} I_{TE} = I_i \quad (4.5)
\]

Such a sensor would give a direct measurement for the polarization state of the incoming beam. As previously mentioned, the device studied here is not ideal, thus the polarization state is determined from solving Eq. 4.2 and Eq. 4.3. When written in matrix form and solved for \( I_{TE} \) and \( I_{TM} \), these equations become:

\[
\begin{pmatrix}
  I_{TE} \\
  I_{TM}
\end{pmatrix}
= M^{-1}
\begin{pmatrix}
  I_o \\
  I_i
\end{pmatrix},
\]

where,

\[
M = \begin{pmatrix}
  \alpha_{TE} & \alpha_{TM} \\
  \beta_{TE} & \beta_{TM}
\end{pmatrix}.
\]

(4.7)

The Stokes parameters for a subpixel can then be computed as:

\[
S_0 = I_{TE} + I_{TM}
\]

(4.8)

\[
S_1 = I_{TE} - I_{TM}
\]

(4.9)

The uncertainty in the Stokes parameters can be analytically approximated using error propagation techniques assuming a variance in the currents \( I_i \) and \( I_o \) of \( \sigma_i \) and \( \sigma_o \). It has been shown in [77] that the uncertainty
in the current can be approximated from the signal shot noise and thermal noise. The uncertainties for $I_i$ and $I_o$, expressed as $\sigma_i$ and $\sigma_o$ respectively, can be written as:

\[
\sigma_i = \sqrt{I_i + R_i^2} 
\]

\[
\sigma_o = \sqrt{I_o + R_o^2} 
\]

with $R_i$ and $R_o$ being related to thermal noise and not dependant on the signal strength. The coefficient of variation ($\Delta_{TE}$) for the measured polarization is estimated as:

\[
\Delta_{TE} = \frac{\sigma_{TE}}{I_{TE}} = \frac{\sqrt{\beta_{TM}^2 \sigma_o^2 + \alpha_{TM}^2 \sigma_i^2}}{|\alpha_{TM} I_o - \beta_{TM} I_i|} 
\]

$\Delta_{TE}$ is minimized when either $\alpha_{TM}$ or $\beta_{TM}$ goes to zero; in the device described in this chapter the high amount of light-splitting results in small values for $\alpha_{TE}$, and $\Delta_{TM}$ approaches the minimum of $\sigma_i/I_o$. There are complementary expressions for $\Delta_{TM}$.

### 4.5 Modeling of Electrical Performance

The device’s current and voltage characteristics were simulated by inputting the photogenerated current for both TE and TM-polarized light into a finite element semiconductor equation solver (ATLAS). To reduce dark current, the device was modeled at a temperature of 77K. The electric field in the GaAs
substrate produced by the applied electrical bias remains close to the surface and drives the charge separation and collection. The device is simulated at an operating voltage of 2 V, allowing rapid current collection without exceeding the breakdown field, which occurs at around 3 V.

The $\alpha$ and $\beta$ parameters are determined from simulations by illuminating the device with only TM-polarized incident light (with intensity $I_{\text{TM}}$) and noting the currents $I_{o,\text{TM}}$ and $I_{i,\text{TM}}$, and then switching to only TE-polarized incident light (with intensity $I_{\text{TE}}$) and recording the new values for $I_{o,\text{TE}}$ and $I_{i,\text{TE}}$. With these four current values, the $\alpha$ and $\beta$ values are:

\[
\begin{align*}
\alpha_{\text{TM}} &= \frac{I_{o,\text{TM}}}{I_{\text{TM}}} \quad (4.13) \\
\beta_{\text{TM}} &= \frac{I_{i,\text{TM}}}{I_{\text{TM}}} \quad (4.14) \\
\alpha_{\text{TE}} &= \frac{I_{o,\text{TE}}}{I_{\text{TE}}} \quad (4.15) \\
\beta_{\text{TE}} &= \frac{I_{i,\text{TE}}}{I_{\text{TE}}} \quad (4.16)
\end{align*}
\]

The magnitude of the ratios $\beta_{\text{TE}}/\alpha_{\text{TE}}$ and $\beta_{\text{TM}}/\alpha_{\text{TM}}$ provide an indication of the extent of light splitting of TE polarized incident light and TM polarized incident light respectively. These two ratios are plotted as a function of wavelength in (Fig. 4.11) for a device structure that has a GaAs thickness of 2 $\mu$m. Fig. 4.11 shows that $\beta_{\text{TE}}/\alpha_{\text{TE}}$ is consistently high over the broad wavelength range of 650 nm to 850 nm, indicating that the TE mode indeed
produces far more current in the center contact than the outer contact. With \( \beta_{\text{TE}}/\alpha_{\text{TE}} >> 1 \), Eq. 4.12 predicts that the device provides a highly accurate measurement of the TM mode, whereas the TE mode has more uncertainty because \( \beta_{\text{TM}}/\alpha_{\text{TM}} \simeq 1 \).

Besides the ability of the device to determine the polarization of the incident beam, the device must also have a high overall responsivity. The responsivity of the device, normalized by the maximum responsivity at each wavelength (\( R_{\text{max}} = q\lambda/hc \)) is the sum of the \( \alpha \) and \( \beta \) parameters for each polarization, namely, \( R_{\text{TM}} = \alpha_{\text{TM}} + \beta_{\text{TM}} \) for TM polarized light, and \( R_{\text{TE}} = \alpha_{\text{TE}} + \beta_{\text{TE}} \) for TE polarized light. These normalized responsivity values are shown in Fig.4.12 for a GaAs substrate thickness of 2 \( \mu \text{m} \). Both the normalized responsivities and \( \beta_{\text{TE}}/\alpha_{\text{TE}} \) and \( \alpha_{\text{TM}}/\beta_{\text{TM}} \) ratios are dependent on the thickness of the active GaAs substrate; if thicker active layers are used, responsivity increases at the expense of polarization determination (Fig.4.12).
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Figure 4.11: Simulated value of $\beta/\alpha$ as a function of wavelength for both TE (solid) and TM (dashed) polarizations.

Figure 4.12: Normalized responsivity dependence on GaAs substrate thickness for both TE (solid) and TM (dashed) polarizations.
The wavelength dependent $\alpha$ and $\beta$ parameters under separate TE and TM polarized illumination were simulated. The normalized wavelength dependent responsivity is presented in Fig. 4.13 for both polarizations.

The ability of the polarimeter to determine the polarization state of an incoming beam using the known $\alpha$ and $\beta$ parameters is simulated. The structure was illuminated with a beam of known polarization ratio, $x = \frac{I_{TE}}{I_{TE} + I_{TM}}$, varying from 0 to 1. The simulated currents, $I_{o, TM}$ and $I_{i, TM}$, produced by the sensor were then input into Eq. 4.6, and the measured ratio $x_{measured}$ computed. The ratio of $x_{measured}$ to $x_{incident}$ thus obtained agreed to within 1%, showing that the device can accurately measure the polarization state.
Conclusion

A novel monolithic polarimeter was described that uses a 1-dimensional meta-
surface grating with two meta-atom types to spatially split incident light ac-
cording to polarization state and then channel the two different polarization
states to different portions of a GaAs substrate where the resulting photo-
generated electron/hole pairs are collected by different electrical contacts.
In this device, the metallic wires defining the 4 grooves within the unit cell
of the metasurface grating are the electrical contacts. We demonstrated the
proposed subpixel structure’s ability to detect the incident beam polarization
state. The multi-functional, monolithic aspects of this device, along with the
good optical performance (i.e., polarization determination and responsivity)
make it compelling for polarimetric imagery applications that require the
measurement of either two or three Stokes parameters. The subpixel design
may be further improved by enhancing the groove light channeling and selec-
tivity to lower the electrical crosstalk. The proposed design could be coupled
with spectral filters to develop sensors capable of capturing both spectral
and polarization information simultaneously.
Chapter 5

Full Polarization Selective Absorption Using Coupled Cavity Metasurfaces

In this chapter, we advance on the previous design and present a cavity meta-atom array metasurface with the ability to obtain all four Stokes parameters in a single pixel. This is accomplished by using multiple linear and phase dependent meta-atom elements in the metasurface, enabling the exact incident elliptical state of the incident radiation to be determined.

5.1 Introduction

In recent years there has been increasing interest in developing a sensor that is able to measure all the Stokes parameters of an incident beam without a reduction in image resolution and there have been rapid developments in new approaches to measure and filter light using metamaterials. As presented
in Chapter 4, metasurfaces show particular promise for engineering a new generation of polarimetry devices. Here we will present a cavity array metasurface applicable to polarization sensing which is capable of determining the complete elliptical polarization state of an incident beam. The metasurface allows for the Stokes parameters to be calculated within a single pixel. The metasurface consists of a metal film with periodically patterned cavities filled with an absorbing dielectric. Each unit cell of the periodic array contains three different cavity meta-atoms with each individual cavity interacting in a distinctive manner with the incident beam while the cavities are also coupled to each other. The absorption in each of the three cavities depends on the incident polarization state and phase of the incident beam and hence will differ for various incident elliptical polarizations. An isolated measurement of the absorption in each cavity within the unit cell is possible with separate collection of photogenerated carriers. This will enable the elliptical polarization state of an incident beam to be measured up to an overall phase.

The Stokes parameters are obtained from an incident plane wave by measuring the amplitudes of different basis projections of the beam. A general description of an incident plane wave traveling in the z-direction can be given as:

$$\vec{E} = \text{Re} \left( A e^{i\psi} (\hat{e}_x + \beta e^{i\delta} \hat{e}_y) e^{i(kz-\omega t)} \right)$$

(5.1)
where $A$ is a real scalar amplitude, $\psi$ is the overall phase relative to the coordinate basis set, $\beta$ is the real ratio between the $x$ and $y$ polarization components, $\delta$ is the phase delay between the $x$ and $y$ polarizations, $k_z$ is the wavenumber, and $\omega$ is the frequency (See Fig. 5.1). The Stokes parameters are a metric for determining different basis elements for the incident plane wave. In the $\hat{e}_x - \hat{e}_y$ basis, the Stokes parameters can be written as:

$$\bar{F}(t) = \text{Re}[A e^{i\phi} (\hat{e}_x + \hat{e}_y \beta e^{i\delta}) e^{i\omega t}]$$

Figure 5.1: Illustration of a plane wave elliptical state. $A$ is the real scalar amplitude, $\psi$ is the overall phase relative to the coordinate basis set X and Y, $\beta$ is the real ratio between the $x$ and $y$ polarization components.
\[ I = |E_x|^2 + |E_y|^2 \]  
\[ Q = |E_x|^2 - |E_y|^2 \]  
\[ U = 2\text{Re}(E_x E_y^*) \]  
\[ V = 2\text{Im}(E_x E_y^*) \] 

Using Eq. 5.1, Eq. 5.2-5.5 can be written as:

\[ I = A^2(1 + \beta^2) \]  
\[ Q = A^2(1 - \beta^2) \]  
\[ U = 2A^2\beta\cos(\delta) \]  
\[ V = -2A^2\beta\sin(\delta) \] 

Measuring the Stokes parameters therefore give information into the elliptical state of the light, and vise versa. As mentioned in Chapter 4, wire grid polarizers have been used extensively in the past to design sensors capable of measuring 2 or 3 Stokes parameters by arranging grating filters of different directions in a pixelated array[69]. Recently, more compact devices have been proposed using metasurface gratings with local photon sorting properties[12,20] allowing for higher resolution integrated Stokes sensors. These
2D metasurface gratings can be used to determine the Stokes parameters associated with linear polarization basis, enabling up to 3 such parameters to be measured. These devices are only able to measure the amplitudes of each linear polarization i.e. $|A|$ and $|A\beta|$ while the relative phase information $\delta$ is lost. To measure the fourth Stokes parameter, which measures the circularity of the incident beam, other methods need to be employed which allow the metasurface to possess circularly selective responses. Metasurfaces showing such optical activity have been demonstrated with L-cavities\cite{78,79}, directed slit apertures\cite{80,81}, and antennas\cite{82}. The metasurface described by Lin et al. sorts right and left-circularly polarized light allowing for the fourth Stokes parameter to be determined. The metasurface of this chapter combines these elements into a single unit cell.

5.2 Principle of Design

The metasurface discussed here is composed of a metallic film with a periodically repeating array of apertures. The periodic array is formed of identical unit cells. Figure 5.2 shows the top view of the metasurface unit cell, which are in a square lattice array with period $\Lambda$. Each unit cell contains three apertures, two slit apertures and one L-shaped aperture, filled with an absorbing dielectric with permittivity of $\epsilon_{abs}$. The slit apertures have width $W_1$ and
length $L_1$ with both slits oriented perpendicular to each other. The L-shaped aperture has leg widths of $W_2$ and leg lengths of $L_3$, with $L_2 = L_3 - W_2$. The metasurface has a finite thickness $t$ with a metallic substrate beneath each aperture forming a cavity array. The purpose of each cavity is to enable coupling to separate basis elements of the incident beam. The x and y slit cavities couple directly to the x and y polarization basis respectively, and the L-shaped cavity, which has been shown to posses optical activity, couples directly to the mixed diagonal basis.

![Figure 5.2: Top view of the metasurface unit cell. The unit cells form a square lattice with period $\Lambda$ and contains three apertures in a metal film, two slits of length $L_1$ and width $W_1$, and an L-shaped aperture with leg length $L_2$ and width $W_2$. The apertures are filled with an absorbing dielectric $\epsilon_{\text{abs}}$, for sensing purposes the dielectric would be a semiconductor capable of producing electron-hole pairs from the absorbed radiation.](image)

The L-shaped cavity has a first order symmetric waveguide eigenmode
and a second order asymmetric mode. With the configuration selected here, the first order mode couples directly to the $\hat{e}_{135^\circ} = \frac{\hat{e}_x + \hat{e}_y}{\sqrt{2}}$ polarization state whereas the second order mode is still below the cutoff frequency. The three selective cavities will couple to each other through near field electromagnetic surface modes. Thus each cavity is driven by the external incident field as well as the neighboring cavities causing the absorption in each cavity to be dependent on the amplitude of the the x and y polarization states as well as the phase difference between them as the drive the individual meta-atoms.

The meta-atom cavity dimensions, namely the lengths, widths, and thicknesses, are chosen to produce a waveguide cavity mode\cite{10} (WCM) that have the same resonance frequency. Figure 5.3 shows the simulated absorption profile for periodic arrays of each type of cavity meta-atom; both types are designed to have a resonance around 27.2 THz. The simulations were done using a finite element frequency domain electromagnetic solver where the metal is assumed to be a perfect electric conductor and the material in the cavities have a dielectric of $\epsilon_{abs} = 9 - 0.09i$ with the dimensions $L_1 = 2.2 \mu m$, $W_1 = 0.2 \mu m$, $L_3 = 1.475 \mu m$, $W_2 = 0.5 \mu m$, $t = 2 \mu m$, and $\Lambda = 4 \mu m$ for each respective cavity. For a physically realizable device, real metal properties with loss would have to be included, the dielectric material would have to be a semiconductor with a bandgap below the desired frequency energy
and the dimensions would have to be altered to incorporate these changes, however, the same physical behavior as discussed in this work would apply. Separate contacts connected to each cavity would collect the generated carriers, allowing for the absorption of each cavity to be individually measured, which may be used to determine the incident beam’s elliptical state.

Figure 5.3: Simulated absorption for the periodic arrays of the only the slit and L-shaped cavities. The dimensions of the cavities were selected to produce an absorption resonance frequency that are identical for both the slits and the L-shaped cavity.

5.3 Simulation Results

In order to see the response of the proposed device, simulations with incident beam excitations of known elliptical state were performed. The absorption in each cavity was then computed by integrating the real part of the Poynting vector on the respective cavity entrance. Figure 5.4 shows the normalized absorption of each cavity of Fig. 5.2 as well as the total absorption for
various values of $\beta$ and phase $\delta$ of the incident beam as expressed in 5.1. The absorption profile changes with both parameters. The dependance on phase is most evident when $\beta = 1$. In this case, the amplitudes of each polarization is the same and sweeping the phase changes the incident beam from linear polarizations to right-handed and left-handed polarizations. At $\delta = 0$, the incident beam is linearly polarized parallel to the line of symmetry of the L-shaped cavity resulting in the strongest coupling to that cavity. At $\delta = 180^\circ$, the incident beam is linearly polarized perpendicular to the line of symmetry of the L-shaped cavity and the absorption in that cavity drops to nearly zero. The total absorption and the absorption in the L-shaped cavity is symmetric about $\delta = 180^\circ$, however the slit absorption is not symmetric, and they have distinct responses for the various phases. Thus, the different absorption ratios allow the exact phase to be determined.

For the other values of $\beta$ the same effect occurs. As indicated by Eq. 5.9, the power of the amplitude depends on $\beta^2$, thus for $\beta = 0.1$, the power between both polarizations differ by two orders of magnitude. Hence for smaller values of $\beta$, we expect there to be a significantly less pronounced dependence on the phase. Nevertheless, since the cavity coupling and absorption depends directly on the fields and not the amplitude, even when $\beta = 0.1$, there is a significant effect on the absorption profiles by sweeping the phase across the
360$^{\circ}deg$ range suggesting the device has a sensitive to incident beam states with extinction ratios around 100.
Figure 5.4: Simulated absorption for each cavity as well as the total absorption for various values of $\beta$ and for swept phase $\delta$. The absorption in each cavity shows dependence on both parameters allowing for the total power, the ratio of both polarization amplitudes, and the phase delay of the incident beam to be determined.
In order to determine the stokes parameters from the absorption profile, each cavity must be individually measured. One possible contact scheme that would allow this is shown in Fig. 5.5. Three separate contacts are run beneath the unit cell, where multiple units cells together would composing a single imaging pixel. The separate contacts serve two functions, to collect photogenerated carriers and an electromagnetic mirror that forms the cavity absorption resonance. The metasurface metal also serves a dual function, as a photon sorter and as the common ground contact for all three cavities.

Figure 5.5: Proposed contact array for measuring the absorption of each individual contact. The metasurface metal film serves as the common ground contact, and separate contacts run beneath each cavity serving for both carrier collection and as an electromagnetic mirror.
Conclusion

An integrated metasurface device consisting of a cavity array in a metallic film that can determine the elliptical state of an incident beam has been proposed. Simulations illustrating the ability of the three cavities in each unit cell to have polarization and phase dependent absorption have been presented. By collecting carriers from semiconductor dielectric placed within the cavities, the three cavities’ absorption can be individually measured and used to determine the Stokes parameters of the incident beam. For the development of a functioning device, real material parameters will be used, fabrication limitations will incorporated into the dimensions and design and an analytical calibration curve predicting the absorption behavior is currently being investigated.
Chapter 6

Frequency Photon Sorting using Cavity Array Metasurfaces in the Microwave

The previous cavity array metasurfaces implemented two and three meta-atom types in order to sort an incident beam by polarization. In this chapter we will discuss and demonstrate a cavity array metasurfaces using two types of polarization independent meta-atoms in order to sort photons by frequency.

6.1 Introduction

Photon sorting of light of different frequencies has long been an area of heightened research due to its endless applications ranging from physical processes such as imaging, photovoltaics, telecommunications, signal processing, and chemistry, to the realm of aesthetics such as painted glass and art. Many of
the devices designed to sort and select different frequencies are electrically large and hinder miniaturization. It is desirable to be capable of achieving such frequency selective photon sorting on subwavelength scales. Such properties can be achieved by using metasurfaces which utilize subwavelength meta-atoms.

Cavity array metasurfaces have been shown to combine the functionalities of photon sorting, localization, and enhanced dual band absorption[21] on subwavelength scales. Cavity array metasurfaces may be of particular interest for use in sensing since the continuous metal of the metasurface may also serve as an electrical contact as shown in Chapter 4 and 5 unlike other multiband absorbers which use split ring resonators[83] or local plasmon resonances[84,85]. The photon sorting capabilities of a dual band cavity array metasurface absorber have been demonstrated in numerical calculations[21]. Here the experimental verification of the photon sorting process is performed in a dual band cavity array metasurface by probing the strength of the electric field above the resonating cavities.

6.2 Metametasurface Design

In this chapter, the structure under investigation is a two-dimensional square array of subwavelength cylindrical cavities embedded in a 40cm x 40cm sam-
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Figure 6.1: The photon sorting metasurface. Each unit cell has two cavities of different radii which resonate at different frequencies.

each cavity is filled with an absorbing silicone elastomer dielectric (Sylgard 184), doped with graphite powder (8.36%), which was selected to maximize the absorption. An Anritsu M4640A vector network analyzer (VNA) was used to record the measured complex S-parameters of the graphite loaded elastomers in an 8-12 GHz waveguide. The dielectric properties of the elastomer composites were subsequently extracted using the Nicholson-Ross-Weir algorithm, giving a complex dielectric permittivity of $\epsilon_r = 4.33 + 0.22i$. Each unit cell contains two cavities of different radii and identical heights, arranged in a square lattice, see Fig. 6.1. The structure’s electromagnetic response is due to cavity mode resonances, which are tuned by adjusting the radii and heights of the cavities, as well as the periodicity of the array, see [21] for further discussion. Here the periodicity is $\Lambda = 26$ mm, cavity radii are $a_1 = 8.03$ mm and $a_2 = 5.74$ mm, and cavity height
Figure 6.2: Experimental and simulated specular reflection intensities from the material surface for s-polarized radiation at a $\theta = 17^\circ$ angle of incidence. The two dips in the reflected intensity correspond to the two cavity resonances[21].

is $h = 7$ mm. The simulated and experimentally measured reflection of the metasurface is shown in Fig. 6.2; the response of the metasurface has peaks in absorption at 8.10 GHz and 9.25 GHz[21] and is polarization independent due to the $90^\circ$ rotational symmetry. The experimental setup for obtaining reflection is described below. The electromagnetic response of the metasurface was simulated with periodic boundary conditions on a single unit cell using HFSS a finite element frequency domain solver. In the simulation, the metals were modeled as perfect electric conductors and the measured dielectric permittivity of the graphite doped elastomer was used for the material parameters in the cavities.
Figure 6.3: Experimental setup for measuring the spatial dependence of the electric field strength. The translation stage allows the measuring probe, shown in the inset, to be swept across the top of the metasurface.

### 6.3 Results

To verify that this device spatially sorts the incident light, we measured the reflection of the sample to determine the resonances and then measured the component of the electric field parallel to the polarization of the incident beam 1 mm above the structure’s surface at the resonant frequencies. To obtain the reflection, two broadband (8-40GHz) horns from Flann Microwave were placed adjacent to each other approximately 2m from the sample such that the angle of incidence was 17°. The horns were attached to an Anritsu M4640A vector network analyser (VNA) which swept a frequency range of 7.5-15GHz in 2001 points, at a power of +5dBm, and with no averaging.
was measured and was normalised to the reflection of a flat aluminium plate in order to determine the absolute reflectivity of the sample, the results of which is shown in Fig 6.2. The field profiles were then obtained using the setup shown in Fig. 6.3. One of the same broadband horns was placed vertically approximately 1.5m above the sample. A small probe formed of a 2mm long piece of stripped coaxial cable was attached to a computer controlled translation stage in order to spatially probe the fields 1mm above the sample. The horn and probe were connected to the Anritsu M46040A VNA, with a frequency sweep of 7.5-15GHz (2001 points). The power was +5dBm, and there was no averaging. S21 was measured as the probe was moved in a plane 1mm above the sample, giving a direct measure of the spatial field profile. Figure 6.4 shows a direct plot of the magnitude of this quantity, where the red color corresponds to the field strength at the 8.1 GHz resonance and the blue corresponds to the field strength at the 9.25 GHz resonance. The dashed circles mark the approximate edges of the cavities within the metasurface; the enhanced field intensities are localized within the circles. This localization demonstrates the photon sorting property of the metasurface. The vertically-oriented “stripes” of blue between the larger apertures are artifacts of the measurement. Rotating the sample or the source does not change the orientation of the stripes. The likely cause of this effect is the
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Figure 6.4: Pseudo-color plot of the electric field component along the polarized y-direction measured 1 mm above the metamaterial. The red (blue) color corresponds to the 8.1 GHz (9.25 GHz) resonances, which are overlayed to see the photon sorting. The dashed circles are the approximate edges of the cavities below.

probe wire, which scatters and interferes with the incident radiation. The field maps indicate that the incident light is sorted into different cavities for different spectral bands.

Characterization of the spatially selective absorption of the metasurface cannot be distinguished since the absorption in each individual cavity cannot be directly measured, i.e. the total absorption is inferred from the reflection
of the metasurface. However, the absorption in each cavity is dependent on
the excitation of a cavity resonance, which results in enhanced field strength
in addition to the absorption. Since the tangential component of the electric
field is continuous across the interface of the metasurface and the free space
above it, a map of the electric field above the metasurface would correspond
to a mapping of the fields, and therefore absorption, within the metasurface,
i.e. within each cavity. We can therefore use the measured field strength
$F$ just above the surface of the metamaterial to calculate an approximate
photon sorting efficiency, i.e. the fraction of energy absorbed in the desired
cavity [21]. We can estimate the sorting efficiency (SE) by

$$SE_n \approx \frac{F_n}{F_T},$$

where $F_n$ is the field strength above a cavity and $F_T = F_1 + F_2$ is the total
field strength. Figures 6.5 and 6.6 shows the average field strength from
experiment along lines crossing the large and small cavities. The range of
values are shown in the shaded region. Using this approach, and averaging
over a few peaks, gives an estimated sorting efficiency of 98% at 8.1 GHz and
92% at 9.25 GHz. These values compare favorably with the calculated values
for the absorption in each cavity obtained from simulation, see Table 6.1. The
estimated SE is higher at 9.25 GHz, as this is a measure of field strength, not
Figure 6.5: Experimental measurement of light splitting using field strength above the cavities at 8.1 GHz. The solid lines are the spatial field strength averaged over multiple lines passing through the center of the cavities. Shaded regions show the variation of the average.

Table 6.1: Splitting efficiency from simulated absorption compared to approximate splitting efficiency calculated from measurements.

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>Simulated SE</th>
<th>Measured approximate SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.1</td>
<td>96</td>
<td>98</td>
</tr>
<tr>
<td>9.25</td>
<td>93</td>
<td>92</td>
</tr>
</tbody>
</table>

directly of the absorption; although the fields are higher above the smaller cavity, the absorption may be lower depending on edge effects. Additionally, the value of the SE at this frequency is less precise due to the experimental artifact (i.e., scattering of the probe wire).

In conclusion, we have demonstrated photon sorting for a metasurface that uses cavity resonances as its absorption mechanism. By measuring the
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Figure 6.6: Experimental measurement of light splitting using field strength above the cavities at 9.25 GHz. The solid lines are the spatial field strength averaged over multiple lines passing through the center of the cavities. Shaded regions show the variation of the average.

electric field above the metasurface while under illumination, electric field maps were obtained that displayed the spatial and spectral selectivity of the metasurface absorber showing good agreement with simulated results. Multi-band photon sorters of this type may be limited by the amount of cavity meta-atoms that can be placed within a unit cell. In addition, higher order cavity modes may share resonances with other cavities, reducing photon sorting. These issues may be resolved in the future by implementing cavities of different geometries and dielectrics in each unit cell.
Chapter 7

Frequency Photon Sorting using Cavity Array Metasurfaces in the Near-IR

In this chapter a photon sorting frequency selective metasurface operating through a mechanism analogous to the metasurface in Chapter 5 but capable of sorting and transmitting photons in the near-infrared spectral range is designed, fabricated, and characterized. Similar in design to the metasurface in the previous chapter, the metasurface designed here is a periodic array of dielectric cylindrical cavities in a gold film. It localizes and transmits light of two spectral frequency bands into spatially separated cavity meta-atoms, resulting in near-field light splitting. The additional challenges in fabrication and optical material properties in developing a photon sorting metasurface in the infrared range are discussed. The transmittance and
photon sorting properties of the designed structure is simulated numerically and the measured transmission is presented.

7.1 Introduction

Research in photon sorting in the near-IR and visible spectrum is, in part, driven by the practical use of spatially sorting light of different frequencies for applications in photovoltaics, sensing, and telecommunication. Photon sorting devices operating in transmission mode have been demonstrated by using surface plasmons[86], and photonic crystals[87], however the relatively large size of these structures limits their applicability for certain practical uses. Subwavelength sorters operating as absorbers for a single polarization have been demonstrated using localized plasmons[84], and compound gratings[20,88] however these do not transmit the light, which is a property that is required for certain devices. In this chapter we present a polarization-independent transmissive subwavelength photon sorter operating in the near-IR composed of a metasurface, which does not share the limitation of a large footprint as in the surface plasmon or photonic crystal devices, making it applicable for sensor and photovoltaic technologies.
Figure 7.1: A schematic of periodic cylindrical cavities in a metal is shown from top down (a), and a cross section through one set of cavities (b). The dashed square in (a) indicates the infinitely repeating unit cell and the dashed line indicates the cross section shown in (b). Here $\Lambda = 500$ nm, $a_1 = 80$ nm, $a_2 = 125$ nm, $h = 35$ nm, and amorphous silicon is the dielectric $\epsilon$ used in this work.

7.2 Metasurface Design

The goal of the design is to have a device that has two transmission peaks that are well-separated with respect to each other, while maintaining as large of a bandwidth as possible for each peak, allowing it to function as a photon sorter. The target frequencies of the transmission peaks were chosen to be below the onset of far-field diffraction, as these diffraction modes carry energy away from the material surface, and thus compete with the cavity modes for the energy of the incident beam. This competition between back-scattered
far-field diffracted modes and transmissive cavity modes impose an important constraint on the design that ultimately limits the number of different cavities that can fit within one unit cell, and, therefore, the number of photon sorting bands in the device.

The structure described in this work consists of a gold film embedded with a periodic array of subwavelength-sized cylindrical cavities filled with dielectric: Two cavities of different radii are present in each unit cell of the periodic array, arranged in a square lattice with amorphous silicon filling each cavity, Fig. 7.1. The individual cavities within the unit cell are designed to support an effective cavity mode (CM) of different spectral bands such that incident light within a particular band will be localized and channeled through the designated cavity within each unit cell. Thus, the incident light is spatially sorted according to wavelength as seen in Fig. 7.6 and discussed in greater depth below. The frequency of the lowest order CM is approximately given by Eq. 3.12 as described in Sec. 3.1.3 which incorporates the skin depth, the height of the metal film, and the additional extension of the localized fields beyond the film surface due to the excited evanescent fields which depend implicitly on the periodicity. The radii of the cavities were tuned to resonate within a specific spectral band, with additional considerations for reducing coupling between the different cavities in the unit cell while
maximizing the photon sorting and transmittance of the structure. The use of cylindrical cavities, as well as the cavity configuration within the unit cell, is chosen to promote a polarization independent response for normal incident light. Taking these considerations into account, the device has a periodicity of \( \Lambda = 500 \text{ nm} \), and two cavities with identical heights of \( h = 35 \text{ nm} \), but different radii of \( a_1 = 80 \text{ nm} \) and \( a_2 = 125 \text{ nm} \).

Once the preliminary design was obtained by using Eq. 3.3, the device was further optimized and analyzed using HFSS, which is a full-wave, finite element, electromagnetic simulation software. The structures were simulated using periodic boundary conditions in the transverse directions and a Floquet port for the incident beam. Gold structures were simulated using the optical properties of gold presented by Palik\(^{[76]}\) and experimentally determined dielectric properties were used for the a-Si. It is important to note that there is some degree of variation and uncertainty in the measurements of dielectric constants, which can cause a substantial deviation from the results of simulations.

The spectral and spatial resonant properties of the cavity modes can be analyzed using direct and indirect methods. In the direct method, the spatial characteristics of the resonances are determined from the electromagnetic fields. In simulation, the Poynting vector derived from the solved electromag-
netic fields can be directly integrated over the exit of each cavity to obtain the light transmitted through the individual cavity. Off resonance, the fields in the cavities are not excited and the total power flow will be minimized. This metric is useful for determining where in a structure the fields are localized, however this is difficult to measure experimentally. In addition, the energy density around the cavities also provides a metric for the ability of the meta-surface to spatially separate the fields. In this work, the spectral properties of the cavity resonances are indirectly verified through use of the transmission intensity. We utilize the $S$-parameters from simulation to determine the predicted transmission and experimentally measure the transmitted light. This metric is useful for a simple comparison to experimental measurements, however it does not, by itself, experimentally determine where, spatially, in a structure the fields are localized.

7.3 Fabrication

The device sample was fabricated on a fused silica wafer. The wafers were cleaned and a 5 nm thick titanium adhesion layer was evaporated using e-beam deposition. The deposition of a-Si was done using PECVD. Hydrogen gas was added into the chamber in order to help reduce stress in the resulting film and repair any crystalline damage. Electron-beam lithography was used
to create a dual pillar pattern in 300 nm thick NEB resist, see Fig. 7.2 (a).

Figure 7.2: SEM images of the experimental device during different stages in the fabrication process.

The surface was de-scummed in oxygen plasma for 5 seconds. The features were then transferred into the a-Si using an SF6 based reactive ion etch. A metal layer consisting of 3 nm of chrome and 35 nm of gold was deposited
using directional e-beam evaporation. The resist that remained after the dry etch was used to lift off the metal on top of the a-Si pillars. Figure 7.2 (b) shows the metasurface after lift off. A contact lithography step was used to pattern a photoresist feature on top of 500 μm square active area. An additional 150 nm thick opaque gold layer was evaporated and lifted off from the metamaterial surface, leaving a shield everywhere outside of the active area in order to prevent any light from transmitting through non-metasurface portions of the wafer.

7.4 Results

The absolute transmission of the fabricated device was measured with a collimated monochromator beam at normal incidence. The simulated and measured absolute transmission of the structure is shown in Fig. 7.3a. There are two distinct resonances apparent in both transmission spectra, however, there is a significant blueshift observed in the fabricated structure when compared to the simulated transmission. The simulated structure possesses two spectrally separated transmission peaks, one centered at a wavelength of 1094 nm and the other centered at 1304 nm, whereas the fabricated transmittance peaks at 910 nm and 1170 nm respectively. The measured peaks in transmission also show a reduction in magnitude from the simulated peaks.
These discrepancies are due to uncontrollable factors that arise during fabrication. The need for adhesion layers between the gold metasurface and the substrate, the porosity of the amorphous silicon, and gold diffusion into the amorphous silicon are some of the factors contributing to the blue-shifted response. Nevertheless, the overall qualitative behavior of the transmission for the fabricated device agrees with the simulated structure, and the physical behavior of the fields is also expected to demonstrate similar behavior. The polarization independence of the experimental transmission is shown in Fig. 7.3b. The dependence of the simulated reflection for an off-normal angle of incidence is shown for both polarizations in Fig. 7.4. As expected of cavity modes, which are localized in three dimensions, the resonances are independent of the incident angles for shallow angles.
Figure 7.3: (a) Absolute transmission for the designed structure obtained from simulation (solid) and experimental measurement (dashed). There are two measured transmission peaks, one centered at a wavelength of 910 nm and the other centered at 1170 nm. (b) Experimentally measured absolute transmission for the designed structure obtained for TE (solid) and TM (dashed) polarized incident light for wavelengths around the second resonance.

Figure 7.4: Plots for the simulated reflection for x-polarized (left) and y-polarized (right) for various degrees off normal incidence. The cavity mode resonant frequencies do not shift for shallow angles for either polarization. For large angles $\psi > 25$ the frequencies and quality factor of the resonances begin to depend on the incident angles.
The photon sorting characteristics of the structure can be measured in terms of power flow through the respective apertures and through the local fields at the respective cavities, which are shown in Fig. 7.5a and Fig. 7.5b. The simulated power flow dependence presented in Fig. 7.5a shows that light preferentially flows into the larger (smaller) cavity around the longer (shorter) wavelength resonance. This preference is less pronounced at the shorter wavelength resonance and the power flowing through the cavities becomes negative in certain wavelength intervals. This is due to coupled cavity effects, which are promoted by fields coupling between the two interfaces through the two cavities and through plasmon modes propagating on the surface; this leads to light circulation and hence a negative transmission through the exit aperture of the cavities[12,89,90]. An interesting result of this effect is that perfect sorting of power flow occurs when the transmission of one cavity goes to zero, which does not occur at the peaks in total transmission.

Photon sorting of the electric field is determined from the time averaged electromagnetic energy stored and localized around the cavities, shown in Fig. 7.5b. The stored electromagnetic energy shows strong localization around each cavity for their respective resonances. The magnitude of the electric field for both resonances is shown in Fig. 7.6. The electric field is enhanced and localized near the respective resonance cavity indicating that
this structure serves as an electric field and photon sorter.
Figure 7.6: Plot of the simulated complex magnitude of the electric field for a vertical plane crossing both apertures in the unit cell at the low energy (frequency) resonance (left) and the high energy (frequency) resonance (right). The electric field is highly localized in and above the cavity associated with the resonance.

7.5 Conclusions

We have demonstrated the capability of a metasurface composed of a compound subwavelength cavity array to spatially split, concentrate, and transmit infrared radiation. This response is polarization independent for shallow angles. Other structures with narrower bandwidth transmission peaks and with more spectral sorting bands may be possible and would be useful in developing multi-wavelength bolometers, photodetectors, and thermal emitters.
In the previous chapters metasurface structures that enable discreet frequency selectivity were presented and discussed. However there is also interest in continuously tunable frequency selective metamaterials for use as absorbers or sensors. These would have application in multiple technological fields particularly that of hyperspectral imaging. Hyperspectral imaging is a method that takes multiple images of a single scene with a continuum of electromagnetic bands in the mid-IR, near-IR, visible and other frequency ranges. Hyperspectral imaging thus allows a high level of analysis of a scene due to the unique characteristics of different materials and processes within these varying bands of interest. These imaging systems have application in astronomy, medical imaging, chemistry, environmental sensing, industrial processing, and many other fields. There has been growing interest in adapt-
ing the novel properties of metamaterials to improve on current sensor technologies by enhancing absorption and reducing bandwidth relative to current sensors.

One such type of sensor where metasurfaces show promise is the microbolometer. Microbolometer sensors measure light intensity by absorbing the incident electromagnetic radiation which in turn heats up a temperature dependent resistive element. The change of resistance of this element is subsequently measured with a readout circuit and used to determine the incident electromagnetic intensity. In this chapter we present the design and simulated characteristics of a continuously tunable metasurface absorber that can be used as the basis of a hyperspectral microbolometer pixel with near unity absorption in the $8 - 10\mu m$ and a full width half maximum (FWHM) less than 5% while minimizing the overall thermal mass.

8.1 Design

In order to achieve the desired continuous tunability required for a hyperspectral sensor the metasurface design must have a continuously tunable parameter that will change its absorption characteristics. To achieve the narrow bandwidth, the absorption must be a resonant phenomena. Thus we require a tunable resonator, however the distinctive resonant properties of
most metamaterials in the mid-IR can not be tuned after fabrication due to the meta-atom geometry being fixed. Some tunability can be achieved with the use of tunable refractive index materials yet even these materials do not have the range needed to tune the resonance for the whole $8 - 10 \mu m$ spectrum.

Although the geometry of a fabricated meta-atom element cannot be altered post fabrication, the separation between elements can be changed using MEMs actuators. This method would allow for a continuously tunable resonator if the resonance depends on this design spacing and would be polarization independent. Due to these considerations, the structure was chosen to consist of a Fabry-Perot resonator where the two reflecting interfaces are metasurfaces with polarization independent responses. The resonant frequency can then be tuned by the separation of the metasurfaces and the absorption and the FWHM can be controlled by the metasurface layers.

### 8.1.1 Metasurface Aperture Array

Fabry-Perot Resonators consist of two interfaces or layers. To obtain the tunability with the desired resonance properties, namely, a sharp absorption resonance that behaves identically as the resonance frequency is tuned, each of the two layers must show frequency independent responses so that only the
tunable coupled system has a sharp variable resonance. In order for a Fabry-Perot resonator to have a sharp or high-Q resonance, the two interfaces must have reflection coefficients close to unity. However, the top layer must be able to transmit light to the bottom layer, which would in turn reflect that light back to the top thereby resulting in a resonance cavity. In order to control the reflection and absorption at these interfaces, we will be implementing thin patterned metamaterials that have the effective characteristics of single layer interfaces. The top layer of the device is a metasurface composed of a metal film with a periodic array of holes. The unit cell is illustrated in Fig.8.1. It consists of a thin film of gold with thickness $t_1$ with cylindrical apertures that have a radius $r_a$ and are spaced with period $\Delta$ in both directions. The equal spacing results in a polarization independent response for normal incidence light.
Figure 8.1: Top aperture array metasurface used in the device. It consists of a thin film of gold with thickness $t_1$ with a periodic array of apertures. The apertures have a radius of $r_a$ and are spaced with period $\Delta$ in both directions. The equal spacing results in a polarization independent response for normal incidence light.

This metasurface may be said to operate in the frequency selective surface (FSS) regime since it does not possess novel resonant characteristics, however it has an engineered bulk response which still classifies it under the larger class metamaterials. The primary variable parameters for the top layer are the period and radius of the apertures in the film. The thickness must remain strongly subwavelength in order for the metasurfaces’ meta-atoms not to begin exhibiting independent resonant behaviour, in addition, the thermal mass must be kept as low as possible to maintain sensitivity in the resulting device. In Fig.8.2 we see a plot of the reflection and phase as a function of
the aperture radius. As can be seen, as the radius increases, the reflection decreases monotonically for all wavelengths until the radius reaches its largest possible value of $\Delta/2$. The periodicity must be kept subwavelength in order to inhibit diffraction effects which would open channels for incident energy to escape. Thus to inhibit diffraction for the entire interval the period must be at least less than $\Delta < \lambda_{\text{min}} < 8\mu m$.

Figure 8.2: Simulated normalized reflection for the top aperture array meta-surface used in the device. The plot shows the dependance of the reflection on wavelength and aperture radius. As the radius approaches the periodicity of $4.24[\mu m]$ the reflection decreases as would be expected as the fill factor of metal is less than unity. For a radius of $1.2\mu m$, the reflection remains above $98\%$ for the entire wavelength range yet retains a nonzero transmission coefficient.
8.1.2 Plasmonic Disk Metasurface

To promote higher absorption and therefore a higher increase in temperature in the bottom layer, which would serve as the temperature dependant resistive element, a metasurface with field localization and concentration properties was designed. The bottom metasurface layer consists of a thin film of gold with thickness, $t_{sub}$, which will be enough to act as an optically opaque mirror yet thin enough to have a low thermal mass. On top of the metal film is a periodic array of germanium dielectric disks covered with gold disks.
of the same thickness as illustrated in Fig. 8.4 which displays the unit cell. Gold and germanium were selected for ease of processing in a fabrication facility via thermal vapor deposition. In addition germanium is required as a dielectric as it is transparent in the desired wavelength range and possesses a relatively high dielectric permittivity, allowing the meta-atom to be made spatially small.

Figure 8.4: Bottom plasmonic disk metasurface array used in the device. It consists of a thin film of gold with thickness \( t_{\text{sub}} \), just enough to be opaque with a periodic array of germanium dielectric disks covered with gold disks of the same thickness.

This metal-insulator-metal (MIM) structure supports local plasmonic cavity modes that increase the field concentration and therefore absorption. However this device must possess properties that are not strongly frequency dependant otherwise the coupled resonant system containing both layers will not function as needed. The solution adopted in this design aims to construct
the metasurface to be off its inherent resonance in the frequency of interest, namely $8 - 10 \mu m$, thus we can still achieve a broadband enhancement in field concentration and absorption. The geometric parameter controlling the resonant frequency is the radius of the disks. The reflection, and therefore absorption, dependance on radius and frequency is shown in Fig.8.5 for the design parameters $\Delta = 4.24 \mu m$ $t_{Ge} = 0.2 \mu m$ $t_{Au} = 0.15 \mu m$. There is a first order plasmonic absorption resonance with a wider bandwidth than desired by the device seen for $0.5 \mu m < r < 0.8 \mu m$. The next order plasmonic resonance begins to appear at $r > 1.4 \mu m$. The radius selected lies in between these two resonances to allow an evanescent resonant mode to enhance the absorption, namely $r = 1.2 \mu m$. 
Figure 8.5: Simulated reflection for the bottom plasmonic disk metasurface array used in the device for the design parameters $\Delta = 4.24 \mu m$ $t_{Ge} = 0.2 \mu m$ $t_{Au} = 0.15 \mu m$. There is a first order plasmonic absorption resonance with a wider bandwidth than desired by the device seen for $0.5 \mu m < r < 0.8/\mu m$. The next order plasmonic resonance begins to appear at $r > 1.4/\mu m$. The radius selected lies in between these two resonances to allow an evanescent mode to enhance the absorption.

Although the plasmonic metasurface operates in an evanescent sub-resonant regime, it still exhibits novel metamaterial properties. In particular the structure supports spoof plasmons, which arise when there is a periodic array of perturbations or evanescent localized cavity modes on a metal surface[29]. The computed eigenmode solutions shown in Fig.8.6 display a $\omega - k$ dispersion curve with characteristics similar to a surface plasmon. For low
phase values, where the phase equals $k_x \Delta$, the solver has difficulty converging. However, for higher phase the dispersion curve follows the lightline and then bends at high phase approaching a constant surface plasmon frequency which is a function of the plasmonic disk cutoff frequency. Thus the spoof plasmon mode varies with disk radius. This is another mode that was considered in the choice of disk radius dimensions. If there was a spoof plasmon resonance in the spectral range of interest, the device would again lose its tunable response.

![Figure 8.6: Simulated $\omega - k$ dispersion diagram for bottom plasmonic meta-surface. The surface mode follows the lightline for lower phase ($k$) and then approaches the spoof surface plasmon frequency which is dependant on disk radius.](image)
8.2 Dual Metasurface Simulated Results

The combined structure unit cell containing both metasurface elements is illustrated in Fig.8.7. The variable parameter $h$ tunes the frequency of the absorption resonance. The full device was simulated and the predicted reflection and absorption obtained for various values of the height $h$. These results are shown in Fig.8.8. The absorption at the resonant frequency is above 98\% in the wavelength range of 8.5 – 10\mu m. For the lower wavelength range approaching 8\mu m the absorption begins to decrease, but stays well above 90\%. This is due to the slight wavelength dependent responses of the metasurfaces which results in an envelope function bounding the device maximum absorption response over the whole range.
Figure 8.7: Illustration of the device unit cell combining the top aperture array metasurface and the bottom plasmonic disk metasurface.

Figure 8.8: Simulated reflection (solid) and absorption (dashed) of the proposed device for multiple gap heights. The maximum in absorption changes smoothly with the gap height and remains above 90% percent for the entire interval.
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To obtain the response bandwidth we examine the absorption FWHM of the device as a function of the height $h$. The predicted absorption curves shown in Fig.8.8 were use to obtain the predicted FWHM for the same values of the height $h$. These values are shown in Fig.8.9. This plot shows that the FWHM remains between 1 and 1.35% for the whole range which is significantly lower than the initial target of 5%. The resonance shows a broadening at lower gap heights (higher frequencies). This is another aspect that arises due to the fixed nature of the metamaterial geometry; as the wavelength changes relative to the fixed geometry the response undergoes slight deviations. To minimize such effects, the design was optimized at the center frequency.

Figure 8.9: Simulated FWHM/Max of the proposed device for multiple gap heights. Although there is some variation of the FWHM/Max over the interval it remains below 1.35%.
Figure 8.10: Simulated loss distribution of the proposed device for multiple gap heights. Although there is some variation of the absorption over the interval it remains above 90% and is split almost equally between the top and bottom metasurfaces throughout the range.

The distribution showing the simulated loss in the top aperture array metasurface, the bottom plasmonic disk metasurface, and the total absorption at the resonant frequencies for the above heights are shown in Fig. 8.10. For a Fabry-Perot resonator with a non-patterned bottom metal mirror, over two thirds of the incident energy is absorbed at the top layer. By introducing the plasmonic array metasurface we are able to achieve a more equal distribution between the two surfaces in the Fabry-Perot resonator even though a light ray passes through the top layer twice for each interaction with the bottom layer. This is due to the evanescent plasmonic mode that causes the light to effectively pass through the bottom layer more than once in each
8.3 Fabrication

Efforts were made to produce a test device for optical characterization. The device was fabricated in two stages, one for each metasurface. The fabrication process for the bottom metasurface is illustrated in Fig. 8.11. Silicon wafers were cleaned. A 5 nm adhesion layer of chrome followed by 100 nm of Au was deposited using thermal vapor deposition. Two layers of resist was spun and baked, first 30 nm of DS-k101 followed by 300 nm of UV210. This was followed by a UV photolithography mask exposure using an ASML 300C DUV Stepper followed by development. Thermal deposition of 100 nm of Ge and 100 nm of Au was followed by lift off in 1165 sonication bath. At this stage, the samples had a fully fabricated lower metasurface. Scanning electron microscope images of various stages of fabrication of the first layer are shown in Fig. 8.12.
(a) Silicon wafers are cleaned

(b) Thermal deposition of Au

(c) Photolithography step

(d) Thermal deposition of Ge and Au

(e) Liftoff process

Figure 8.11: Fabrication process for bottom metasurface
The fabrication process for the top metasurface is illustrated in Fig. 8.13. In order to fabricate the top metasurface at a fixed height above the substrate metasurface, a layer of polyimide was spun at 4500, 4750, and 5500 rpm to achieve thicknesses of 4.7, 4.0, and 3.8 um followed by curing in a YES polyimide oven. To fabricate the top metasurface layer another liftoff process was attempted. Two layers of resist was spun and baked, first 30 nm of DS-
k101 followed by 300 nm of UVN30, a negative resist. This was followed by a UV photolithography mask exposure using an ASML 300C DUV Stepper and development. Thermal deposition of 100 nm of Au was followed by lift off in 1165 sonication bath. At the this stage attempts at remove the underlying polyimide layer via plasma etching proved unsuccessful. The top metasurface exhibited extensive warping, ruining the sample. Scanning electron microscope images of various stages of fabrication of the top layer are shown in Fig. 8.14. Various etching parameters were altered in the process to attempt to remove the excessive heating causing the warping but was not successful. Due to the excessive warping, we were unable to obtain a functioning sample for testing.
Figure 8.13: Process for top metasurface
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(a) SEM image of top metasurface resist after exposure and development  
(b) SEM image of top metasurface post lift off  
(c) View of top metasurface post plasma etch.

Figure 8.14: SEM images of top metasurface. Significant warping occurred in the last process step ruining the sample.

8.4 Conclusion

An altered Fabry-Perot resonator incorporating metasurfaces to act as effective interfaces was proposed and simulated. This dual metasurface device is predicted to achieve absorption above 90% with a FWHM less than 1.35%
in the $8 - 10 \mu m$ range. Such a device may improve current hyperspectral sensors. However, there are significant challenges in fabricating this device due to thinness of the suspended layers as well as possible sensitivity issues with low temperature changes due to the smaller amount of effective energy absorbed in a narrow bandwidth.
Chapter 9
Conclusion

In this work we have presented various forms of photon sorting metasurfaces implementing multiple meta-atoms as the physical mechanism for selectivity. By altering the meta-atom types and configuration in the unit cell we were able to design novel selective properties. The metasurface structures discussed in the previous chapters were able to spatially sort, absorb, and distinguish between linear polarization, elliptical polarization, and frequency properties of the incident beam respectively. With further research, these novel photon sorting metasurface properties may be incorporated into future sensor designs to enhance resolution and performance.
Bibliography


