



ON THE APPLICATION OF FLO_K AND
PPTE TO EXTRACT THE PERMITTIVITY
AND PERMEABILITY TENSORS OF SPLIT
RING RESONATOR STRUCTURES

THESIS

O. Wesley Petree, Capt, USAF
AFIT-ENG-MS-17-M-058

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Degree of Master of Science in Electrical Engineering

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Abstract

Recent developments in material parameter extraction techniques have been made, allowing for full tensor extractions of the effective permittivity and permeability of anisotropic materials from off-axis scattering data. The technique of interest in this work is the Permittivity and Permeability Tensor Extraction (PPTE) method, which in its current implementation requires the use of computational electromagnetic (CEM) simulations for visible and infrared wavelength applications. A rigorous study of the CEM meshing requirements for resonant structures was conducted using a government developed full-wave solver for periodic structures, FLO_K, to ensure that the complex field interactions of the modeled micro-structures adequately represented the physics and scattering phenomena of the modeled geometries. It was determined that mesh convergence alone was insufficient for an accurate solution. Floquet aperture stand-off was found to be required to correctly place resonance peaks, but only small fractions of an incident wavelength stand-off distances were required. This study concluded by successfully validating FLO_K against a semi-analytic method, Rigorous Coupled Wave Analysis (RCWA).

PPTE has been fully validated for the extraction of effective permittivity tensors of anisotropic media, but not for the extraction of other-than-unity permeability tensors for magnetic materials or structures. The technique was applied to an isotropic magnetic medium and split ring resonators (SRRs), which exhibit a magnetic resonance, to further test the cases to which this technique can be applied. PPTE was shown to extract intrinsic material parameters from isotropic materials with a high level of accuracy. The SRR case demonstrated more constraints. The current implementation of PPTE includes assumptions regarding material anisotropy, making

any bi-anisotropic results an approximation. Nonetheless, even an approximation is useful for guiding measured ellipsometry based material parameter extraction. So, evaluation geometries were tested which minimized the electric and magnetic field coupling, and thus bi-anisotropic effects, exhibited by the SRRs under test. It was determined that the bi-anisotropy of a planar array of SRRs could be constrained for PPTE application, in some cases. However, a comparison of the extracted parameters with other literature proved inclusive, due to ambiguities in the reported extraction processes.

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O. Wesley Petree

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List of Acronyms

AFIT	Air Force Institute of Technology
AFRL	Air Force Research Laboratories
CEM	Computational Electromagnetics
CRC	Coherent Resonant Cavity
ECT	Extraordinary Coherent Transmission
EM	Electromagnetic
FEM	Finite Element Method
IR	Infrared
IR-VASE	Infrared Variable Angle Spectroscopic Ellipsometer
HPC	High Performance Computers
LORE	Low Observable RADAR and Electromagnetics
MPL	Membrane Projection Lithography
PPTE	Permittivity and Permeability Tensor Extraction
RCWA	Rigorous Coupled Wave Analysis
SNL	Sandia National Laboratories
SRR	Split Ring Resonator
SPP	Surface Plasmon Polariton
TE	Transverse Electric Polarization

TM Transverse Magnetic Polarization

USAF United States Air Force

V&V Verification and Validation

ON THE APPLICATION OF FLO_K AND PPTE TO EXTRACT THE PERMITTIVITY AND PERMEABILITY TENSORS OF SPLIT RING RESONATOR STRUCTURES

I. Introduction

1.1 Motivation

In 1999, Pendry proposed a periodic structure, called the split ring resonator (SRR), which he claimed had the potential to achieve a simultaneous negative permittivity and permeability [35]. This led to multiple branches of research into a class of engineered materials broadly termed metamaterials, which are engineered to exhibit some properties that may not be found to occur in natural materials, with the intent to describe these materials by effective permittivity and permeability values. SRR structures have numerous potential applications including magnetic media within the optical regimes, negative index of refraction, and cloaking within both the microwaves and infrared (IR) [22, 25, 30, 32, 35, 38, 40, 45], making them of particular interest to the United States Air Force (USAF).

The classical design process highlights some of the difficulties in fabricating and employing this type of material. If a material is to be designed for a specific purpose, some method must be used to predict the scattering, typically a first principles approach. Once the desired scattering, based on the geometry, has been determined, the material is then fabricated, usually through a costly and time intensive process. Once the material has been realized, the scattering is measured and assessed. The measured scattering may or may not match the first principles method, which may

indicate the need for a redesign. In general, these materials exhibit responses that are too complex to be described accurately by first principles. So, if the measured scattering does not match design intent, the material designer will vary some geometric parameter in the hope of achieving the desired response. It may be necessary to iterate this process many times, at prohibitive cost in time and materials, to achieve the desired end state. This drives the need for more complex models to correctly compute the scattered fields in the design phase.

While many full-wave electromagnetic computational models exist, they all have their limitations. For instance, method of moments would require a specific Green's function for each unique geometry, the development of which is non-trivial. Finite difference time domain solvers have been employed, but this method introduces difficulties in temporal convergence. A finite element method (FEM) model can converge to an accurate solution for this type of structure, if sufficient computational resources are available. For these reasons, FLO_K, a periodic FEM solver developed by Air Force Research Laboratories (AFRL), was used on high performance computing (HPC) resources to compute the scattered fields of the SRR structures.

With the availability of better than first principles modeling capabilities, the design loop may be improved to include more accurate predictions of the scattered fields. This allows for the initial design of the material to match the scattering more closely, within fabrication tolerances. However, the designed material still requires a material parameter extraction to ensure that the purpose of the material has been realized. The method that is generally employed within the optical and IR regimes is ellipsometry. However, ellipsometry is inherently underdetermined and is often quite difficult to adequately characterize these parameters, especially for these complex structures. This led to a method developed by Dr. Michael Benson, called Permittivity and Permeability Tensor Extraction (PPTE) that is based on the underlying theory of el-

lipsometry, but employs data from simulated scattered fields to produce a complete, rather than under-determined, solution to the material parameter extraction process.

In this refined design loop the predicted scattered fields drive PPTE material parameter extractions, the results of which may induce re-design or parameter variation in simulation, until the desired material parameters are achieved, prior to any fabrication. After the entire computational process has been completed, the material can be fabricated and measured by ellipsometry under experimental conditions matching the modeled material parameter extraction configurations. Since the material parameters were found via PPTE, the ellipsometry extraction can be guided by this appropriate and *a priori* knowledge, thus improving the solution of the ill-posed ellipsometry material parameter extraction problem. The unique pairing of FLO_K, HPC resources, PPTE, and ellipsometry allows the design loop to be substantially refined for government applications.

1.2 Goals and Scope

During the development of PPTE, Dr. Benson validated that PPTE could be used to retrieve both an intrinsic permittivity and an effective permittivity of a biaxial anisotropic medium [7, 8], but its effectiveness for intrinsic or effective permeability extraction had yet to be validated. This research seeks to determine under what conditions PPTE can be applied to these magnetic materials.

Because PPTE requires the use of simulated scattered fields, specifically from FLO_K, this research seeks to characterize both the meshing requirements and the accuracy of the computed fields from FLO_K from resonant structures. To do this, three resonant structures were chosen which have known solutions that can be found by a semi-analytic method, Rigorous Coupled Wave Analysis (RCWA). This work is presented in Chapter III.

The next phase of this research examined PPTE’s ability to retrieve the permeability tensors of magnetic media. Three realized 3-D SRR material samples, shown in Figure 4 in the following chapter, were provided by Sandia National Laboratories (SNL). These realized samples provided the objective space of the research, specifically, to determine if PPTE could be applied to these structures to gain insight into the effective material parameters prior to ellipsometric extractions.

To determine if PPTE could be applied to magnetic media, two media were chosen: an isotropic medium where the material parameters were defined and a planar array of SRRs based on *Magnetic Response of Metamaterials at 100 THz* by Stefan Linden [30]. Both are presented collectively in Chapter IV. An isotropic slab with defined material parameters tested PPTE’s ability to extract a material’s intrinsic permeability. The SRRs provided an anisotropic case to test PPTE’s ability to extract a material’s effective permeability, defined by the structured geometry of the medium. Chapter II provides more detail of the differences in effective and intrinsic material parameters.

First, to determine if PPTE could extract an intrinsic permeability within the range of those reported by Linden [30], the material parameters were defined within the same range. Next, a simpler case of SRRs than those provided by SNL was examined, specifically a planar array of SRRs based on Linden’s work [30], to determine if PPTE could be applied to SRRs in general. This literature was chosen because the geometry, materials and their parameters, scattering, and permittivity and permeability in two orientations were reported. The comparison of the scattered fields first ensured the geometric model adequately represented the physics. This allowed for direct comparison of both the scattered fields from FLO_K and the extracted permittivity and permeability from PPTE against other methods.

One potential problem that needed to be addressed was that these SRRs exhib-

ited bi-anisotropic behavior upon examining the scattered fields. Bi-anisotropy lies outside the domain of the problem space to which PPTE can be applied. This led to careful examination of the scattered fields to determine if the bi-anisotropy could be sufficiently minimized for application of PPTE to extract the material parameters.

The result of the work presented in Chapter III led to further verification and validation (V&V) of FLO_K as it is still relatively young software. The work presented in Chapter IV, specifically the isotropic test, resulted in validating PPTE against intrinsic magnetic media. Another, perhaps not as obvious contribution, lies in outlining the entire process from modeling to material parameter extraction. The tools necessary for modeling, to include parameter variation, computing the scattered fields, and retrieving the permittivity and permeability tensors can be accomplished using government tools, thus allowing for government researchers to study these interesting, but complex, structures.

II. Background and Literature Review

This chapter reviews the pertinent theoretical background governing the presented research. In addition, a comprehensive literature review provides insights into development and state of the art in the areas addressed. This provides a foundation of understanding where this research fits into current science.

This chapter first examines the nature of light, presented in terms of electromagnetic fields, and defines the material parameters that govern the interaction of the fields within a given material. These relations are further explored in terms of the complex index of refraction, to consider the material differences between the optical and microwave regimes. This development establishes the motivation for engineering materials. A brief discussion on engineered materials in general concludes with a thorough discussion on Split Ring Resonators (SRRs), on which a large portion of this research will be centered. Finally, the most relevant of the current methods for extracting the material parameters of optical materials will be reviewed to conclude this chapter.

2.1 Material Interaction with Electromagnetic Fields

2.1.1 Maxwell Equations and Constitutive Relations.

In order to first discuss electromagnetic interaction with materials, one must first discuss Maxwell's Equations 1–4 that describe electromagnetic fields, presented here in differential form. These equations are the foundation of electromagnetics and are generally found within the first few pages of any electromagnetics textbook. The specific textbook cited for the development in this section is *Advanced Engineering Electromagnetics* by Balanis, [6].

$$\nabla \times \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{B}(\vec{r}, t) \quad (1)$$

$$\nabla \times \vec{H}(\vec{r}, t) = \vec{J} + \frac{\partial}{\partial t} \vec{D}(\vec{r}, t) \quad (2)$$

$$\nabla \cdot \vec{D}(\vec{r}, t) = \rho(\vec{r}, t) \quad (3)$$

$$\nabla \cdot \vec{B}(\vec{r}, t) = 0 \quad (4)$$

Where, $\vec{E}$ is the electric field, $\vec{H}$ is the magnetic field, $\vec{D}$ is the electric flux density, $\vec{B}$ is the magnetic flux density, and $\vec{J}$ is the current density. These equations are commonly known as the Maxwell-Minkowski equations. These equations are coupled, since the electric field is defined in terms of the magnetic field and vice versa. The two divergence Equations 3 and 4 can be derived from the two curl Equations 1 and 2, but this leaves an ill-posed set of equations. So, to find a complete solution, the constitutive relations are employed, which are a set of equations that describe how the material effects either the magnetic or electric fields by relating them to their respective flux densities, thus allowing for decoupling of the fields ($\vec{E}$ from $\vec{H}$). Generally, there are two such parameters; permittivity (ϵ) and permeability (μ). Permittivity refers to a material's ability to store electrical energy while permeability refers to a material's ability to store magnetic energy.

The way these constitutive parameters relate the fields to their respective flux densities vary with the type of material. There are four general types: isotropic, bi-isotropic, anisotropic, bi-anisotropic. In the simplest of these cases, isotropic, the material parameters are scalar quantities. This implies that the fields remain in the same alignment they were prior to being incident on the surface. The next case, anisotropic, has the same relative relationships, but the constitutive parameters are diadic, or tensors. That is, they are no longer scalars and can, in general, affect the

alignment of the fields in the material. The next two cases follow the same structure, scalar parameters for bi-isotropy and tensors for bi-anisotropy, but in these two cases the fields are coupled by the terms, ζ and ξ . As before, the bi-isotropic ζ and ξ are scalar while the bi-anisotropic $\bar{\zeta}$ and $\bar{\xi}$ are tensors. The following points outline these generalizations, while equations 5–12 that follow show the mathematical relationships.

- *isotropic*: materials in which $\vec{D}$ is related to $\vec{E}$, $\vec{B}$ is related to $\vec{H}$, and $\vec{J}$ is related to $\vec{E}$, with the field directions in each pair remaining aligned.
- *anisotropic*: materials in which the pairings are the same, but the fields in each pair are generally not aligned.
- *bi-isotropic*: material in which the fields $\vec{D}$ and $\vec{B}$ depend on both $\vec{E}$ and $\vec{H}$, but with no realignment.
- *bi-anisotropic*: material in which the fields $\vec{D}$ and $\vec{B}$ depend on both $\vec{E}$ and $\vec{H}$ with an arbitrary realignment of either or both fields.

The mathematic relationships are given by:

Anisotropic

$$\vec{D} = \bar{\epsilon}\vec{E} \quad (5)$$

$$\vec{B} = \bar{\mu}\vec{H} \quad (6)$$

Bi-anisotropic

$$\vec{D} = \bar{\epsilon}\vec{E} + \bar{\xi}\vec{H} \quad (7)$$

$$\vec{B} = \bar{\zeta}\vec{E} + \bar{\mu}\vec{H} \quad (8)$$

Isotropic

$$\vec{D} = \epsilon\vec{E} \quad (9)$$

$$\vec{B} = \mu\vec{H} \quad (10)$$

Bi-isotropic

$$\vec{D} = \epsilon\vec{E} + \xi\vec{H} \quad (11)$$

$$\vec{B} = \zeta\vec{E} + \mu\vec{H} \quad (12)$$

Where,

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix}, \bar{\mu} = \begin{bmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{bmatrix}, \bar{\zeta} = \begin{bmatrix} \zeta_{xx} & \zeta_{xy} & \zeta_{xz} \\ \zeta_{yx} & \zeta_{yy} & \zeta_{yz} \\ \zeta_{zx} & \zeta_{zy} & \zeta_{zz} \end{bmatrix}, \text{ and } \bar{\xi} = \begin{bmatrix} \xi_{xx} & \xi_{xy} & \xi_{xz} \\ \xi_{yx} & \xi_{yy} & \xi_{yz} \\ \xi_{zx} & \xi_{zy} & \xi_{zz} \end{bmatrix}.$$

It should be noted that anisotropy is a generalization of isotropy. Specifically, if ϵ and μ are scalars, then

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{yy} & 0 \\ 0 & 0 & \epsilon_{zz} \end{bmatrix} \quad \text{and} \quad \bar{\mu} = \begin{bmatrix} \mu_{xx} & 0 & 0 \\ 0 & \mu_{yy} & 0 \\ 0 & 0 & \mu_{zz} \end{bmatrix},$$

where $\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}$ and $\mu_{xx} = \mu_{yy} = \mu_{zz}$ can be simplified to

$$\epsilon \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \epsilon \bar{I} \quad \text{and} \quad \mu \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \mu \bar{I},$$

where $\bar{I}$ is the identity matrix,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Similar observations can be made with the ζ and ξ coupling terms between bi-isotropy and bi-anisotropy. Although anisotropy can be shown to be generalized for isotropy and bi-anisotropy generalized for bi-isotropy, bi-anisotropy can also be shown to be the generalization of all cases, by simply allowing the ζ and ξ terms go to zero when there is no field coupling. This will be an important observation in Chapter IV, when

the bi-anisotropic nature of SRRs is explored. Figure 1 summarizes the relationships between field coupling and directional dependence of these cases.

Non-coupled Fields	
Directionally Dependent	<u>Anisotropic</u> tensor $\bar{\epsilon}$, $\bar{\mu}$
	<u>Isotropic</u> scalar ϵ , μ
Directionally Independent	<u>Bianisotropic</u> tensor $\bar{\epsilon}$, $\bar{\mu}$, $\bar{\xi}$, $\bar{\zeta}$
	<u>Biisotropic</u> scalar ϵ , μ ξ , ζ
Coupled Fields	

Figure 1. Quadrant diagram of materials that exhibit field coupling and directionally dependent responses. Materials in quadrant I are isotropic and are directionally independent without field coupling. Materials in quadrant II are anisotropic and are directionally dependent but without field coupling. Materials in quadrant III are bi-anisotropic and are directionally dependent with field coupling. Materials in quadrant IV are bi-isotropic and are directionally independent but exhibit field coupling.

One final relationship to consider is that of the relative permittivity and permeability, ϵ_r and μ_r , given by

$$\epsilon = \epsilon_0 \epsilon_r \quad (13)$$

$$\mu = \mu_0 \mu_r, \quad (14)$$

where ϵ_0 is the free space permittivity, $\approx 8.854 \times 10^{-12}$ F/m, and μ_0 is the free space permeability, $4\pi \times 10^{-7}$ H/m, [6]. It is this relative permittivity and permeability, ϵ_r and μ_r , that will be the primary focus for the rest of this document.

2.1.2 Complex Index of Refraction.

With the material parameters defined mathematically, the next obvious discussion point is the physical effects these parameters have on the fields. The material parameters govern dispersion, or the wavelength dependent complex index of refraction, $\tilde{n}(\lambda)$, defined by

$$\tilde{n}(\lambda) = \sqrt{\epsilon_r(\lambda)\mu_r(\lambda)} = n(\lambda) + ik(\lambda), \quad (15)$$

where, the real part of $\tilde{n}$, n , is the index of refraction and the imaginary part, k , is the extinction coefficient [6, 42]. Both govern different physical effects. The index of refraction, n , determines how the incident wavelength is either compressed or stretched upon entering the material, depending on whether the differences in the two indices at the interface were from lower to higher or vice versa, as described by Snell's Law of Refraction [6]. The extinction coefficient, k , determines the losses associated with the material and has the overall effect of having attenuation applied to the fields [6].

However, in many optics textbooks, here *Optics* by Hecht [21], the equation is given as

$$\tilde{n}(\lambda) = \sqrt{\epsilon_r(\lambda)} = n(\lambda) + ik(\lambda). \quad (16)$$

The reason that μ is not seen in Equation 16 is due to the fact that magnetic materials simply are not found to occur naturally at the higher, optical frequencies [21, 42]. As such, Equation 15 is the more complete representation that will be used in this document. Overcoming this limitation led to the study of metamaterials, those materials that have been engineered to have properties that may not exist in nature, specifically here, magnetic materials within the infrared (IR) regime.

2.2 Metamaterials

Metamaterials, as used in the context of this work, are engineered materials that exhibit electromagnetic properties not found in nature. The simplest description of this effect is found in effective medium theory [42]. This theory is used to describe the overall effect of what is observed macroscopically in terms of what is happening microscopically. In the case of interest, the permittivity and permeability of multiple material constituents in microscopic terms are combined to express an effective permittivity and permeability which can be extended to describe the material macroscopically [42]. To design a material for a particular purpose, a metamaterialist defines a single unit cell, sometimes called a meta-atom [2], that has particular properties on the microscopic level. This individual cell then gets repeated in a periodic fashion, similar to the crystal lattice structures of solid state materials. The overall effect is that these unit cells behave like the molecules of a new material when the incident wavelength is sufficiently large to interact with the cell as a whole and not the individual constituent components that were used to make up the cell [6]. This is what is known as homogenization, and the material can be approximated as an effective material [42] which allows for the material to be represented using bulk constitutive parameters ϵ_{eff} and μ_{eff} [6]. There is a general rule that homogenization occurs when the wavelength to cell size is 10:1, but has been shown to be as small as 3:1 [8]. If however the wavelength is not sufficiently large and is small instead, the material must be examined using periodic analysis, such as Floquet Theorem [6].

2.2.1 Split Ring Resonators.

Split Ring Resonators, first developed by Pendry [35], are metallic inclusions that are of a ring shape with at least one discontinuity. Applications of SRRs range from creating a Frequency Selective Surface (FSS) [32] to negative index of refraction

[22,30,35,40,45] , to cloaking [25,38]. Predominantly, the research found in literature focuses on the potential for, and claims of achieving a negative index of refraction, and the validity of these claims is passionately debated [34]. However, it is the potential for generalized control of the electromagnetic properties, which is of interest to the USAF. The research presented here exploits the SRR as magnetic material and focuses on understanding the field interactions in an attempt to accurately extract the effective material parameters, ϵ_{eff} and μ_{eff} .

While the designs of these SRRs can be wildly complex [4, 11, 12, 17–19, 26, 32, 41, 43], the most basic and general of these designs are variations of those shown in Figure 2. Of these two basic geometries, round and square, the research presented here will focus on those that are square or ‘U’ shaped.

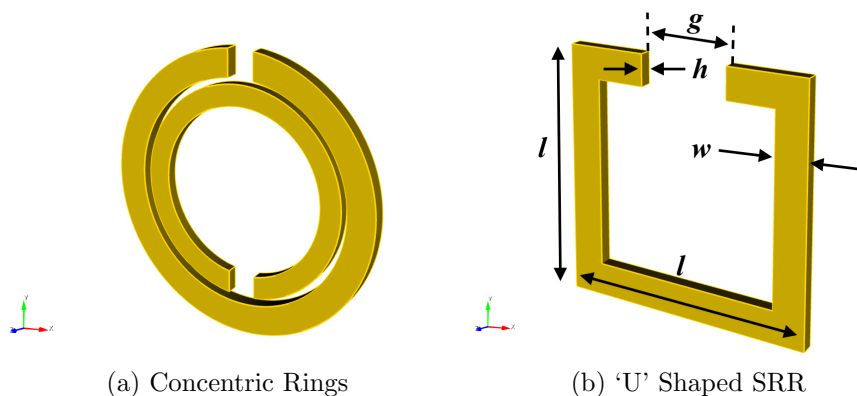


Figure 2. Basic SRR geometries. (a) Concentric rings, as developed by Pendry [35], which are common in the microwaves. (b) ‘U’ shaped SRRs that are common in designs for the IR. Geometric parameters: g is the gap, h is the metal height, w is the tracewidth, and l is the length.

Literature is littered with models attempting to describe the resonances associated with SRRs [5, 15, 18, 27, 28, 30]. While many models exist, they all generally use a lumped parameter equivalent circuit model, describing the ring as an inductor with inductance, L , and the gap of the SRR as a capacitor with capacitance, C . The following model, from Corrigan *et al.* [15] , is the simplest of these proposed

models and provides physical insight into the mechanisms driving the electromagnetic responses.

In order to determine the resonant frequency of the SRR, consider first the resonant frequency of the simple LC circuit, shown in Figure 3a. In this model, the inductance, L , can be found by

$$L = \frac{n\mu_0 A}{h} \quad (17)$$

where h is the height of the metal, A is the area of the loop, given by $A = l^2$, where l is the length of the SRR, and n is the number of turns, one, shown in Figure 2b. This leads to

$$L = \frac{\mu_0 l^2}{h}. \quad (18)$$

Similarly for the capacitance, C ,

$$C = \frac{\epsilon_0 A}{g}$$

where A is now given by $A = wh$, where w is the tracewidth and g is the capacitive gap width as shown in Figure 2b. This leads to

$$C = \frac{\epsilon_0 wh}{g}. \quad (19)$$

The product, LC , is given by

$$LC = \frac{\epsilon_0 \mu_0 l^2}{g} \quad (20)$$

and the resonant frequency can be found by

$$\omega_{LC} = \frac{1}{\sqrt{LC}} \quad (21)$$

$$\Rightarrow f_{LC} = \frac{1}{2\pi\sqrt{LC}} = \frac{\sqrt{g}}{2\pi\sqrt{\epsilon_0\mu_0 l^2 w}} = \frac{c}{2\pi l} \sqrt{\frac{g}{w}}, \quad (22)$$

where c is the speed of light, given by $c = \frac{1}{\sqrt{\epsilon_0 \mu_0}}$. The resonant wavelength, λ_{LC} , is then readily found by

$$\lambda_{LC} = \frac{c}{f_{LC}}. \quad (23)$$

This model provides intuition into understanding the physics driving the scattering mechanisms. However, it should be noted that the model is highly simplified and only accounts for the capacitance of the gap of a single SRR within a single unit cell. That is, it does not account for coupling between SRRs of neighboring unit cells. There are two additional observations that will be further explored in Chapter IV. First, the resonance found by this model is independent of ring height. Second, this simplified model does not account for a dielectric substrate near the capacitive gap, unlike the more complex models developed by Corrigan [15] and Shelton [39]. The implication is that Equations 22 and 23 can only be applied to free space SRRs, and not those that are physically realizable, i.e. those on or in a substrate.

An intuitive approach can be used to understand how the SRR LC circuit is excited. When a component of the oscillating electric field, $\vec{E}$, aligns parallel to the gap of the SRR, an oscillating potential develops across the capacitor. This oscillating potential drives a time changing current around the loop and creates a magnetic dipole, $\vec{M}$ [3]. Similarly, when a component of the oscillating magnetic field, $\vec{H}$, is aligned with the normal created by the plane containing the loop, a time-changing current is driven through the loop and creates a potential across the capacitive gap, leading to an electric dipole moment, $\vec{P}$ [3]. This is illustrated in Figure 3b. One not so obvious effect is that the fields can become coupled, leading to bi-anisotropy [3]. While some literature acknowledges this [3, 23, 27, 33, 48], others seem to ignore it completely [22, 30, 35, 40]. Even Pendry claims that SRRs of the form seen in Figure 2a are anisotropic [35]. Granted, the structure in Figure 2a is uniquely different the structure in Figure 2b, namely that the electric dipole moments created at the two

gaps are opposite (cancelling), the fact remains that the magnetic field can drive a response that is observed in the electric field. The implication is that the material is, at a minimum, potentially bi-anisotropic. Careful consideration of this potential bi-anisotropy will be considered in the development of the research presented in Chapter IV.

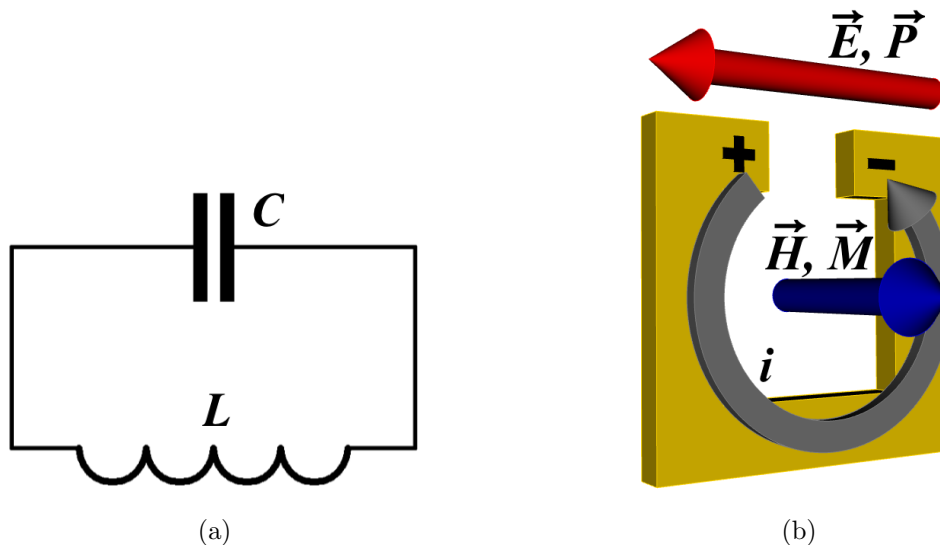


Figure 3. (a) LC circuit model schematic with the capacitance, C , representing the gap and the inductance, L , representing the ring. (b) An electric dipole moment, $\vec{P}$, and a magnet dipole moment, $\vec{M}$, are formed when the SRR is excited by either the electric field, $\vec{E}$, or the magnetic field, $\vec{H}$.

2.2.2 Fabrication.

While most of the research found uses e-beam lithography and nano-imprint lithography to make the SRRs small enough for the IR, these can only be made into planar, and or stacked materials [43]. Although some literature proposes SRRs oriented on sidewalls [35], fabrication techniques did not exist until recently for allowing for SRRs to be created both small enough for implementation within the IR and out-of-plane of the substrate [43]. Membrane Projection Lithography (MPL), developed by Sandia National Laboratories (SNL), has been used over the last few

years to deposit SRRs in cavities on various different substrates [9, 11–13]. These cavities can be of various shapes including rectangular, hemispherical, and hemi-ellipsoidal [46]. This research will only examine SRRs out of plane within rectangular cavities, fabricated by SNL using MPL.

The process of MPL is to first etch out the cavities. Once the cavities are etched out, they are then backfilled with a material that can be easily removed. Next, the material is planarized mechanically. A masking layer is then applied to the top of the planarized material. It is within this masking layer that the SRR shape is defined. Next, the backfilled material is removed, leaving hollow cavities with a masked membrane across the top. Next, the metallic SRRs are deposited on the walls via sputtering as projections from the masked layer. Lastly, the masked membrane is removed, leaving the hollow cavities with metallic SRRs affixed to the sidewalls or base [12], examples of which are shown in Figure 4.

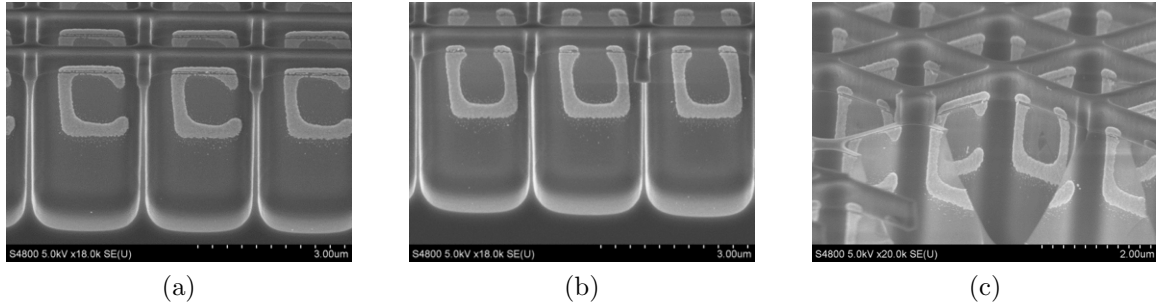


Figure 4. SEM images of MPL out-of-plane SRR samples within Si cavities. (a) Single SRR oriented with the gap to the right. (b) Single SRR oriented with the gap up. (c) Two SRRs combining both gap right and gap up on adjacent walls.

Several samples were provided by Dr. Bruce Burckel of SNL for study within the scope of this research. These samples were of three geometries: 1. a single SRR oriented with the gap to the right as shown in Figure 4a, 2. a single SRR oriented with the gap up as shown in Figure 4b, and 3. the combination of both gap right and gap up on adjacent walls as shown in Figure 4c. These physically realized samples

defined the objective space for evaluating PPTE.

2.3 Material Parameter Extraction

Much of the literature on SRRs presented thus far has used the material parameter extraction outlined by Smith [40]. Certain limitations of this technique require the illuminating and observed fields to be at normal and grazing incidence. As such, only certain tensor elements can be obtained. Additionally, this method does not address any field coupling terms. *Magnetic Response of Metamaterials at 100 THz* [30], is one such piece of literature that implements this method and reports two of the tensor elements making no mention of any bi-anisotropic coupling terms.

Other methods for both measured and modeled data do exist that make observations at oblique incidences, namely spectral ellipsometry and Permittivity and Permeability Tensor Extraction (PPTE). Both are able to retrieve full permeability and permittivity tensors. Chapter IV of this document models the geometry laid out by Linden [30], simulates the scattering, and applies PPTE for direct comparison between these two methods.

2.3.1 Ellipsometry.

Ellipsometry is a common method of characterizing the optical properties of layered materials [24]. An ellipsometric system illuminates a sample with circularly polarized light (fields) and measures the polarization of the reflected light (fields) [44]. In this way, the sample could be considered as a transfer function that alters the input as the incident light into the output as the reflected light. The ellipsometric system then characterizes the transfer function, giving insight about the sample.

Before a more in-depth discussion on ellipsometry can take place, a common definition of polarization of the fields must first be established. In the various fields that

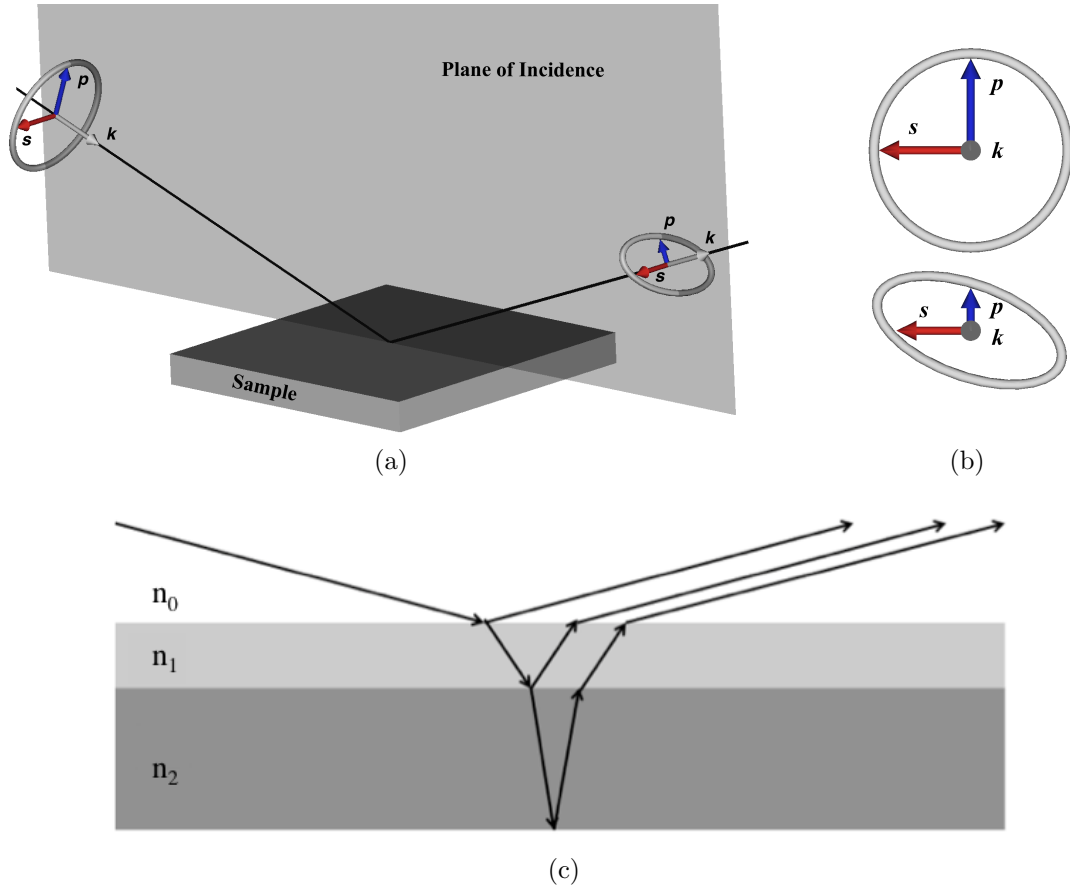


Figure 5. (a) shows circular polarized light incident on a sample and reflecting as elliptically polarized light. The incident and reflected light create a plane of incidence with the p polarization being parallel to the plane and the s polarization perpendicular to the plane. (b, top) shows the incident circularly polarized light while (b, bottom) shows the reflected elliptically polarized light. The parallel (p) polarization is depicted in blue while the perpendicular (s) polarization is depicted in red. The wavevector, k , shows the propagation direction. (c) shows how the index of refraction of each layer refracts the light before reflecting back out of the sample and being coherently added back to the incident light.

study electromagnetics, polarization states can be described in many ways. When the light is propagating in free space, it can be referred to as horizontal and vertical with respect to a reference θ (vertical) and ϕ (horizontal) in polar coordinates [6]. When the light is incident on a surface, the incident and specularly reflected fields define a plane of incidence [6], as shown in Figure 5a. Descriptors of the polarization states in this case are sometimes called parallel and perpendicular with respect to the incident plane, as well as transverse electric (TE) and transverse magnetic (TM) [6]. All the previous polarization states generally are linear, though they can be used to describe circular and elliptical states as well. Circular and elliptical polarization states are polarization states that rotate, i.e. they do not just oscillate vertically or horizontally, but both. When the vertical component is equal to the horizontal component and they are in phase with each other, the light is said to be circularly polarized [6]. When they are not equal or are out of phase with each other, the light is elliptically polarized [6]. Figure 5b provides visual reference of circular and elliptical polarizations. It is common in ellipsometry to use parallel, p , and senkrecht, s , which is German for perpendicular, to describe the polarization state [8]. This research will generally use TE and TM polarizations to describe the polarization states of the fields in terms of the plane of incidence, except in instances referring specifically to the spectral ellipsometer, such as the infrared variable angle spectroscopic ellipsometer (IR-VASE).

The IR-VASE illuminates a sample with circularly polarized light over the spectral band from 1.2–40.5- μm from a black body source [44]. The intensities of the reflections from the sample are measured in the s - and p -polarizations [44]. The IR-VASE assumes Fresnel reflections and as such takes measurements close to the Brewster angle, where the s - and p -polarizations are most separated allowing for the best resolvability [7]. Figure 5c shows how the coherent sum of the incident light and

the refracted light is the reflected light that gets measured, producing a means of predicting their phase difference [44]. The measurements are reported as a ratio of the magnitudes of s - and p -polarizations as well as the phase difference between them for further processing. The change in the polarization states upon reflection, in general, causes the circularly polarized light to become elliptically polarized, as shown in Figure 5. The ratio of magnitudes and phase differences Ψ and Δ , respectively, are found by $\rho = \frac{r_p}{r_s} = \tan(\Psi) \exp(i\Delta)$, where r_p and r_s are the p - and s -polarizations of the reflected light [7].

Like all ellipsometry systems, the IR-VASE also employs a modeling process to address the ill-posed material parameter extraction process [44]. In addition to materials which already exist in the database, new materials can be created using various oscillator models, including Drude and Lorentz [44]. The software is also capable of creating inhomogenous layers, called effective medium approximation (EMA) layers, which can allow the user to create layers that consist of more than one material at various ratios [7, 44]. The IR-VASE can take advantage of *a priori* knowledge of the n and k of the layers to determine the thicknesses or conversely use the thicknesses to determine n and k , but it is generally difficult to determine n , k , and thickness without this knowledge [8].

This is an important observation. The IR-VASE extraction software faces the problem of two measurements while trying to determine three unknowns, n , k , and layer thickness [8]. Which is to say that it is attempting to solve an underdetermined system. The accuracy of the resulting extractions depend on taking measurements at different incident angles and by sample rotations. However, if there are multiple layers and/or unknowns in the sample, the degree of underdeterminedness of the system can be quite difficult to overcome. The more information which is known about the sample prior to taking measurements, the better the system is able to

determine the material parameters.

The previous development assumes mostly isotropy. However, the IR-VASE can also be used to characterize samples that range from anisotropy to bi-anisotropy [47]. This makes the IR-VASE especially suited for taking measurements on the out-of-plane SRR samples provided by Dr. Burckel. Samples of this type have been studied extensively by Burckel and Adomanis [1, 10], but have yet to have full ellipsometric extractions performed on them. However, it would be of great benefit to extract the material parameters using the method developed by Dr. Michael Benson to gain insight into the material parameters, effectively guiding the ellipsometric process. This method, which is based on ellipsometry, is outlined in the following section.

2.3.2 Permittivity and Permeability Tensor Extraction.

Permittivity and Permeability Tensor Extraction (PPTE) is a powerful method used to extract material parameters from computed scattered fields. It was developed by Dr. Michal Benson and is based on ellipsometry, solving a fully posed ellipsometry problem from computed scattered fields, because it is currently impossible to measure the absolute phase and magnitude of the fields at optical wavelengths [8].

The development of PPTE is quite extensive. Benson provides a brief description in an IEEE paper [7], while a more thorough development is found in his dissertation [8], which resulted in the conferment of a Doctorate of Philosophy for Dr. Benson. This research made no alterations or changes to the development of PPTE, save for its limited application to multilayered materials. The conceptual development of which was included in Benson's dissertation [8], but was never implemented within the software nor tested. See Section 4.2.2.10 for more detail of the multilayered development and results. Because of this, the mathematical development of PPTE will not be included within this document, and I urge the reader strongly to read

either of the two pieces of literature mentioned, [7, 8], for more details.

The research presented in Chapter IV will apply PPTE to SRRs of the geometry outlined by Linden [30]. But first, given the nature of PPTE's dependence on simulation, the next chapter will explore the effect of various mesh refinements on resonant structures in order to characterize the required meshes and any error sources associated with the tools that will be used throughout the remaining research. In order to accomplish these simulations, the high performance computers (HPC) managed by the Air Force Research Laboratories (AFRL) are utilized.

III. Finite Element Mesh Study

This study examines three metallic (gold) resonant structures using a Finite Element Method (FEM) model. This provides insight into the meshing requirements of resonant structures, helps to ensure meshes are generated efficiently, and ensures that unambiguously modeling of the scattering from the structures to which PPTE will be applied are produced. Thus, any issues or errors that may be observed can be isolated from the geometry-based model. The results from the FEM model will be compared to results using Rigorous Coupled Wave Analysis (RCWA). The RCWA results are considered to be truth data, with solutions converged to less than 0.001% deviation for the given geometries. The research presented throughout this document will depend heavily on FEM modeling, and therefore, a thorough understanding of how this FEM model behaves with regards to resonant structures must be developed. By comparing the FEM results to the RCWA truth, an adequate characterization of the FEM model can be developed.

3.1 Methodology

The geometries, and corresponding meshes, will be generated using Cubit, a geometry and meshing package developed by Sandia National Laboratories (SNL). The simulations will be run using FLO_K, a frequency domain computational electromagnetics (CEM) solver which uses a floquet modal expansion to represent scattering from infinitely periodic structures. Although many grating orders can be found using FLO_K, the research will solely explore the specular mode (0,0), for which complex reflection and transmission coefficients are calculated, which is the necessary input for PPTE.

The FEM model will be meshed using various methods to determine the cell-per-

wavelength requirement for solutions to converge. First, the model will be meshed with a constant finite element cell size that will vary from course to fine, and examine the relationship between the number of cells-per-wavelength before converging to a solution. A general rule of thumb states ten cells-per-wavelength are necessary to converge a solution. Here it will be determined exactly how many cells-per-wavelength are necessary, as it pertains to specific resonant structures. Next, after determining when the global mesh size converges, the geometry will be meshed just outside of the converged region with specific refinement techniques to determine if the mesh needs to be finer around interfaces in order to capture the phase differences between material boundaries accurately. Lastly, it was discovered that the floquet apertures required some standoff from the structures to not measurably contaminate the far field data. The standoff distance was determined for each geometry through iteration. It should be noted that Cubit allows for scripting the geometry, allowing the use of variables and conditional logic, which aids in the parameter variation that was required through this work.

The mesh refinement will consist of three different approaches, refinement of the metallic region, refinement of the free space region, and using an additional geometry with refined mesh at the interface between the metallic and free space regions. The first two of the refinement techniques make no changes to the geometry, only the underlying mesh. The third however, adds additional geometry to localize the refinement only at the interface between the metallic region and the free space region. The additional geometry will have free space material parameters (ϵ_0 and μ_0) ensuring that no additional interfaces are presented in the simulation. One potential problem with using any discrete model is that the nodes at the interface between two different materials must be either one material or the other and may not always adequately capture the interface boundary conditions. By adding an additional geometry at

the boundary and refining the mesh at this region, this effect should be minimized. The ultimate goal of this study is to determine where to most efficiently use mesh, particularly when dealing with a resonant structure.

3.1.1 Geometries.

The three resonant structures that will be examined are shown in Figures 6–8, labeled here Frill structure, extraordinary coherent transmission (ECT) structure, and coherent resonant cavity (CRC) structure. All three consist of gold structures that are invariant in the $\hat{y}$ -direction and periodic in the $\hat{x}$ -direction. The Frill and ECT geometries are somewhat similar in that there is an invariant discontinuity (free space cavity) that allows for transmission, despite being sub-wavelength. The CRC geometry is a variation of a square-welled grating which has a controlled depth to the grating wells for a specific resonance response, but transmission is not allowed due to the depth of the metal.

The Frill has a unit cell period of $1.75\ \mu\text{m}$, ECT unit cell period $2\ \mu\text{m}$, and the CRC unit cell period $3.5\ \mu\text{m}$, as shown in Figures 6–8. Because the geometries are invariant in the $\hat{y}$ direction, the unit cell was kept at a minimum in this dimension to save overall mesh assignment and reduce computational time. Figures 6a, 7a, and 8a show a 3×100 expansion of the unit cell for visual reference, while Figures 6b, 7b, and 8b depict the specific dimensions of the individual unit cells.

While the focus of this chapter is to study the meshing requirements needed for resonant geometries, a brief discussion on the electromagnetic mechanisms governing the observed responses of these structures is necessary. These types of structures have been studied extensively in their application to plasmonics and metamaterials, [20]. The underlying mechanisms driving the resonant responses has been associated with surface plasmons polaritons (SPPs), spoofed SPPs, and evanescent fields, as

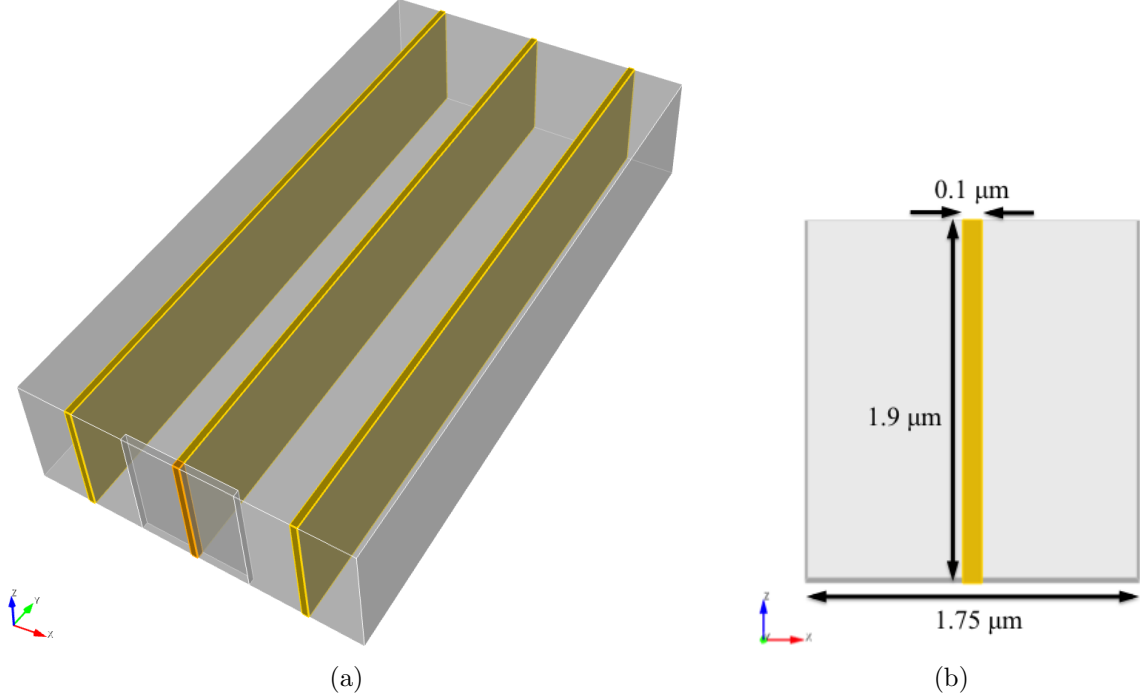


Figure 6. Frill geometry. (a) depicts a 3×100 expansion with the unit cell highlighted in the front. (b) depicts the dimensions of a single unit cell.

described by Pendry [36]. Pendry proposed that these spoofed SPPs formed from the structured surfaces, can be useful to create plasma frequencies for non-metals at desired frequencies for modeling at the lower, microwave frequencies [36]. Pendry concluded the effective permittivities of these structured materials follow the plasma form described by metals, $\epsilon = 1 - \omega_p^2/\omega^2$, where ω_p is the plasma frequency [36].

The resonances associated with the ECT and Frill are driven by two mechanisms, with the geometry controlling the width of the slit and the periodicity determining the coupling of the SPPs from adjacent surfaces [29]. In particular, the geometry controls a mechanism described by Fabry-Pérot-like resonances which are constructive and destructive interference (or coherence) [29]. Fabry-Pérot resonances are usually associated with geometries where half-wave and quarter-wave reflections cause constructive and destructive interference. Both the ECT and the Frill, when probed by fields, have surface waves that couple with those from adjacent discontinuities and

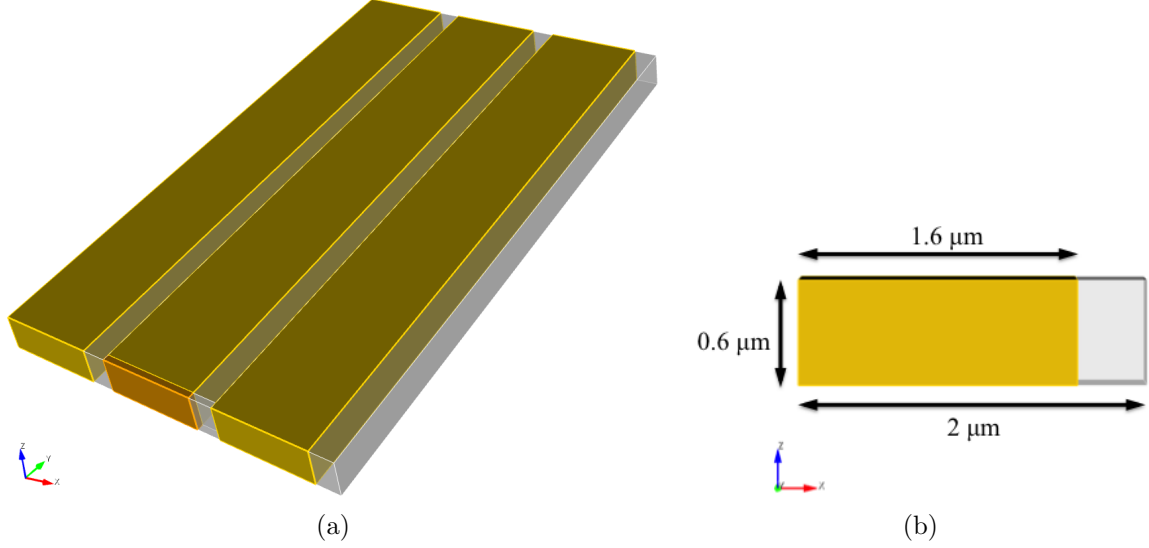


Figure 7. ECT geometry. (a) depicts a 3×100 expansion with the unit cell highlighted in the front. (b) depicts the dimensions of a single unit cell.

can cause the free space region to be excited in waveguide-like modes. These modes then couple to the backside, where SPPs and evanescent fields can create surface currents to reradiate the fields. These fields can be extraordinarily high despite being sub-wavelength in size [20, 29, 36].

Although the mechanisms driving the CRC are also very similar, there is no transmission due to the continuous metal at the bottom of the resonant well. Instead, the effect is unusually high absorption, or perfect absorption [14]. The resonant frequency is uniquely determined by the geometry and material of the cavity [16]. Localized fields exist inside the cavities which originate from coupled SPPs from the cavity walls [16].

Because these structures are metallic, the only polarization that will be of interest in this study is the TM polarization, when the electric field is oriented across the gaps. The TE polarization will quickly be extinguished due to the boundary conditions, effectively being shorted across the metal.

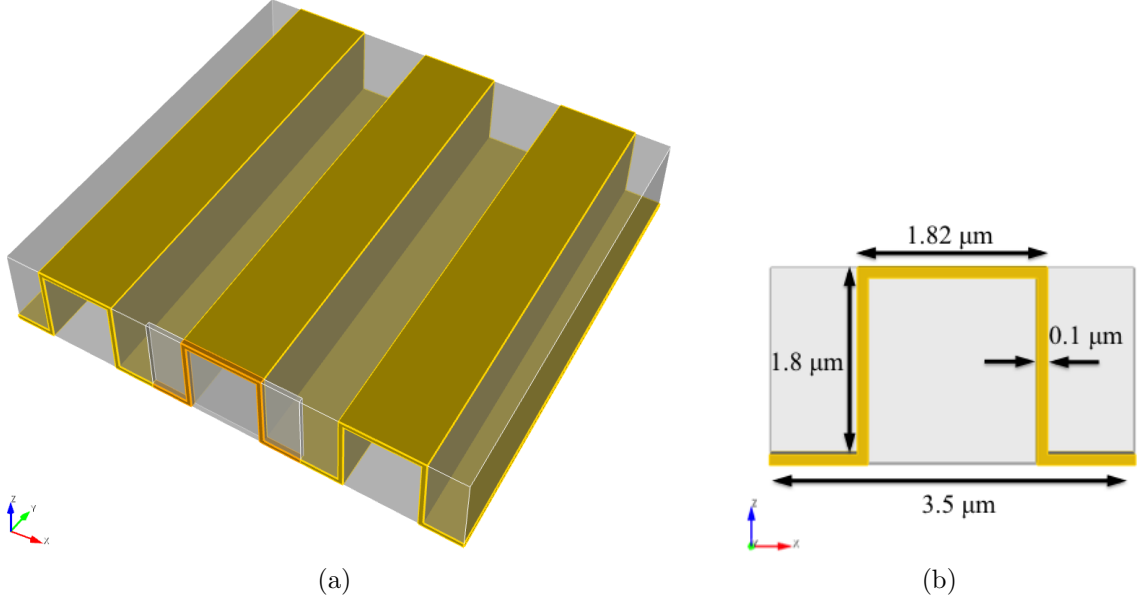


Figure 8. CRC geometry. (a) depicts a 3×100 expansion with the unit cell highlighted in the front. (b) depicts the dimensions of a single unit cell.

3.1.2 FLO_K Experimental Setup.

The U.S. government has developed a suite of tools under the CREATE program, of which SENTRi is useful as a finite element, boundary integral solver. FLO_K, a derivative of SENTRi's FEM solver for periodic structures, is the primary CEM tool for examining the electromagnetic responses of the structures throughout this research. FLO_K simulates a plane wave on the positive $\hat{z}$ -surface and is based on the angles of incidence and wavelengths defined for each experiment. FLO_K then computes all of the like-polarized (co-pol) and cross-polarized (x-pol) reflection and transmission coefficients for the propagating orders.

The simulations presented within this chapter are set up in the same way and only vary based on geometry. The Frill geometry is illuminated at an incident angle of 60° measured from the surface normal in the $\hat{z}$ direction toward the $\hat{x}$ direction at wavelengths 3–4 μm. The ECT geometry is illuminated at normal incidence at wavelengths 2–2.6 μm. The CRC geometry is illuminated at normal, but at wavelengths

3.4–3.6 μm . A summary of this information can be found in Table 1. The resonant wavelengths of each geometry from the RCWA work are listed as well.

Table 1. FLO_K Experiment Setup

Geometries	Illumination Wavelengths (μm)	Incident Angle ($^\circ$)	$\lambda_{\text{resonant}}$¹ ($\mu\text{m}$)	Unit Cell Period (μm)
Frill	3–4	60	3.262	1.75
ECT	2–2.6	0	2.21	2
CRC	3.4–3.6	0	3.5	3.5

3.2 Global Meshes

As with any FEM model, the accuracy of the solution depends on whether or not the mesh was fine enough to accurately capture the phase changes between the different cells. This global mesh study was conducted to determine the mesh requirements to converge solutions for these resonant structures. The mesh cells chosen for the geometries were of hexahedron shape, which allows for more uniform meshing regardless of the geometries and for compatibility with FLO_K. The hexahedron cells were chosen with 20 nodes per cell, called a HEX20 cell, and places a node at all vertices and midpoints between the vertices of the hexahedron.

Cubit allows for a global mesh to be generated using a floating point variable between 1–10 with the lower number being the finer mesh. The HEX20 cells of each geometry correspond to the meshing variable differently due to the geometries being of different sizes, but choosing common variables to implement allows Cubit to mesh each geometry in a similar and predictable way. Values of 1.0, 3.0, 5.0, and 7.0 were chosen for the mesh variable, each corresponding to a different cell-to-wavelength ratio for each geometry. It is generally considered that at least ten cells/ λ are needed to

¹provided from RCWA

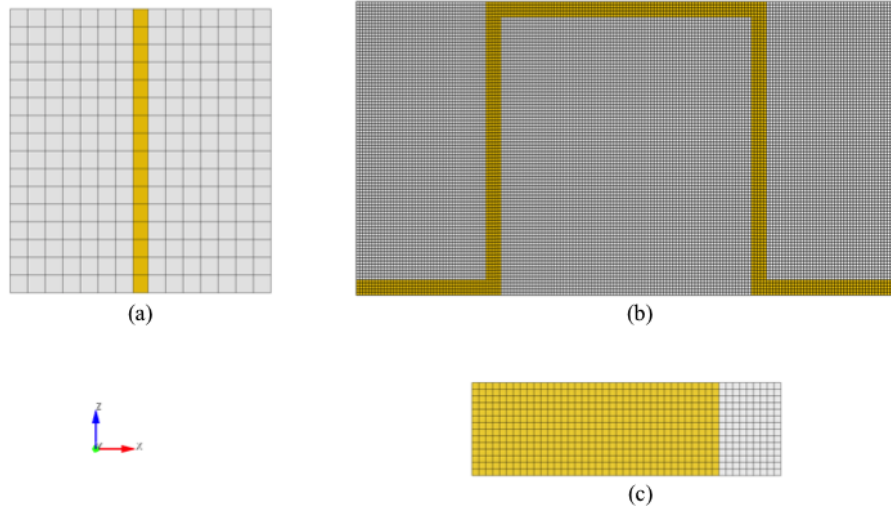


Figure 9. Global meshes of the resonant geometries. (a) Frill geometry meshed with global mesh variable 7.0. (b) CRC geometry meshed with global mesh variable 1.0. (c) ECT geometry with global mesh variable 5.0. The three different geometries are kept to relative sizes of each other.

Table 2. Global HEX20 Cell Summary for all Geometries			
Geometry	Global Mesh Variable	Cell Size (nm)	$\frac{\text{Cells}}{\lambda}$
Frill	7.0	116.7	25.7
	5.0	51.5	58.3
	3.0	23.6	126.9
	1.0	16.5	181.7
ECT	7.0	100	20
	5.0	44.4	45
	3.0	20	100
	1.0	13.9	144
CRC	7.0	140	24.3
	5.0	63.6	53.5
	3.0	28.7	118.5
	1.0	20.1	169

converge to a solution. Figure 9 shows examples of 1.0, 5.0, and 7.0 globally meshed geometries. Table 2 summarizes the cell sizes and cell/ λ ratios of each geometry and global mesh. The cell/ λ ratios were determined from the smallest wavelength illuminating each geometry.

Figures 10–12 depict the magnitudes of the complex reflection and transmission coefficients computed from FLO-K from the globally meshed geometries. These figures also include the deviations from the curves that have converged. This convergence is determined when the amount of deviation from each curve has been made arbitrarily small. These figures report the amount of deviation in absolute error and considers the curve associated with the finest mesh converged. Though this curve may be arbitrarily close to the actual truth, or may not as will be shown later, the goal is to show self-convergence to a single solution.

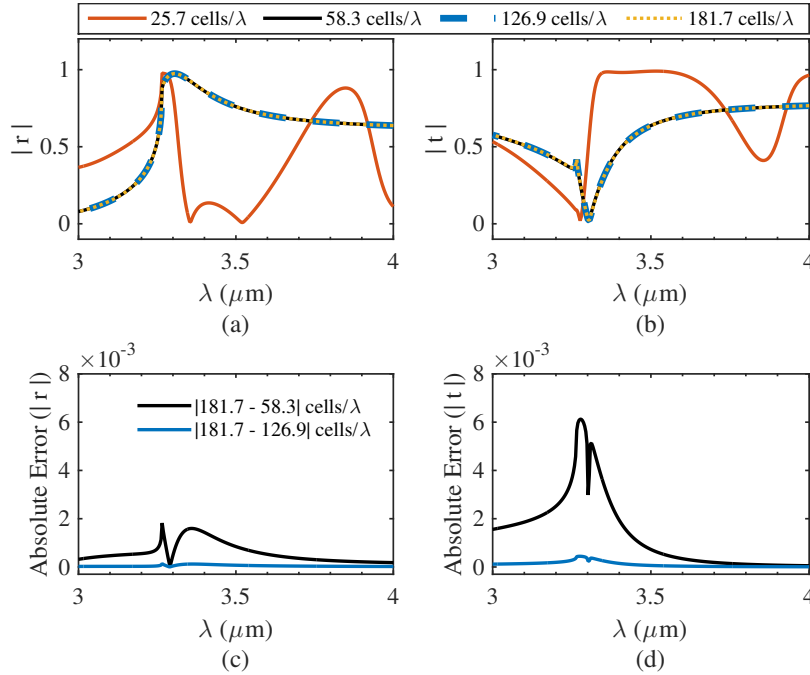


Figure 10. Magnitudes of the complex (a) reflection and (b) transmission coefficients from global Frill meshes. Absolute error for (c) reflection and (d) transmission with the 181.7 cells/ λ curve assumed to be the truth in the error calculation.

Figure 10 depicts the complex reflection and transmission coefficients from globally

meshing the Frill geometry. Of the four simulations, three converge to the same curve. The unconverged curve was with a cells-per-wavelength ratio of 25.7, more than doubling the general rule of thumb requirement of ten. The deviation associated between the converged curves is depicted in Figure 10c and d as absolute error, due to the range of values lying between zero and one. While the deviations associated with the courser mesh solution (58.3 cells-per-wavelength) are higher than those associated with the moderate mesh solution (126.9 cells-per-wavelength), the deviation, shown in Figure 10c and d, is less than 1% with a maximum at 0.006, indicating that the courser mesh is adequate. This mesh is more than five times the required ten cells-per-wavelength for non-resonant geometries. It is noted that while the deviations from the curves associated with the courser mesh (58.3 cells-per-wavelength) are small, the moderately fine mesh (126.9 cells-per-wavelength) has exceptionally low deviation from the finest mesh (181.7 cells-per-wavelength), less than 0.0004 at maximum, shown in Figures 10c and d. While the courser mesh is adequate, the finer meshes show that the error can be driven lower by refining the overall mesh, the upper limit of which is controlled by the amount of RAM on the machine running the simulation.

Figure 11 depicts the complex reflection and transmission coefficients from globally meshing the ECT geometry. Of the four simulations, three again converge to the same curve. The unconverged curve was with 20 cells-per-wavelength ratio, doubling the general rule of thumb requirement of ten. The deviation associated between the converged curves is depicted in Figure 11c and d again as absolute error. The courser mesh solution (45 cells-per-wavelength) again has a maximum deviation less than 1%, shown in Figures 11c and d, with a maximum ~ 0.004 , indicating this mesh is again adequate. This mesh is slightly less than five times the ten cells-per-wavelength required. It is noted that while the deviations from the curves associated with the courser mesh (45 cells-per-wavelength) are small, the moderately fine mesh

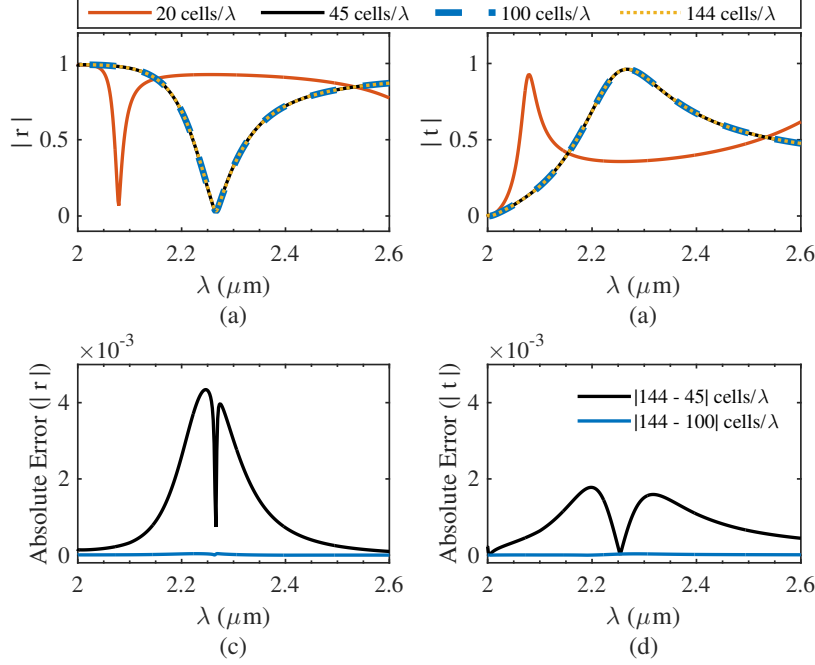


Figure 11. Magnitudes of the complex (a) reflection and (b) transmission coefficients from ECT global meshes. Absolute error for (c) reflection and (d) transmission with the 144 cells/ λ curve assumed to be the truth in the error calculation.

(100 cells-per-wavelength) has, again, incredibly low deviation from the finest mesh (144 cells-per-wavelength), less than 4×10^{-5} at maximum, shown in Figures 11c and d.

Figure 12 depicts the amplitude of the complex reflection coefficients from globally meshing the CRC geometry. Again, of the four simulations, three converge to the same curve. The unconverged curve was with a 24.3 cells-per-wavelength ratio, more than doubling the general rule of ten required. The deviation associated between the converged curves is depicted in Figure 12b. This geometry has the highest deviation, seen in 12b. Of the three geometries, this is the most resonant. The deviation associated with the courser mesh is again less than 1%, shown in Figure 12b, with a maximum of ~ 0.0055 , again indicating this mesh is adequate. The deviations from the curves associated with the courser mesh (53.5 cells-per-wavelength) are small, but the moderately fine mesh (118.5 cells-per-wavelength) deviation from the finest

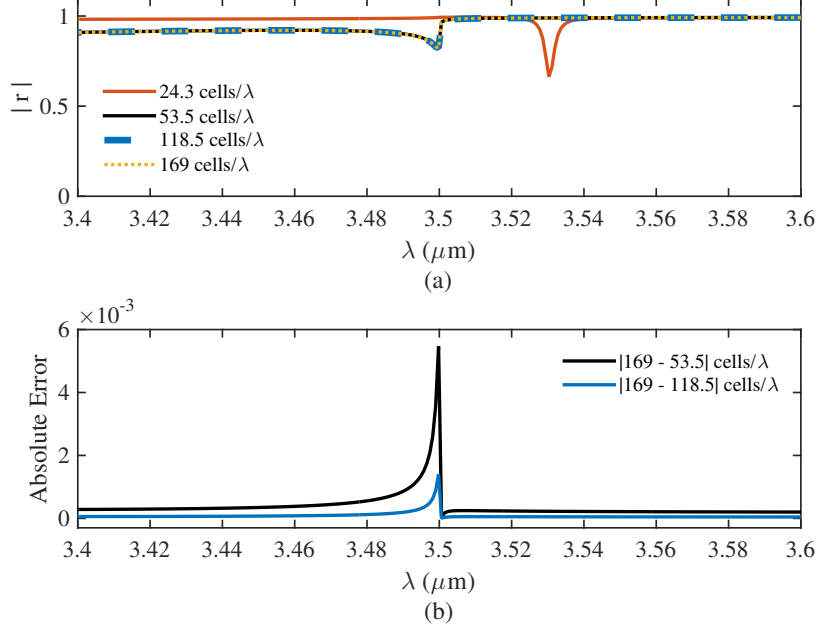


Figure 12. Magnitudes of the complex (a) reflection coefficients from global CRC meshes. Absolute error for (b) reflection with the 169 cells/ λ curve assumed to be the truth in the error calculation.

mesh (169 cells-per-wavelength) is not orders of magnitude smaller as the previous two geometries, shown as ~ 0.0014 at maximum in Figure 12b.

Interestingly, in all geometries, the solutions converged with a mesh variable of 5.0 and smaller. The number of cells-per-wavelength required for each geometry is 58.3, 45, and 53.5 for Frill, ECT, and CRC, respectively. This is an interesting observation as the general rule calls for 10 cells-per-wavelength is required to converge to a solution. FLO_K will also report an error if the edge length of a cell is larger than three cells-per-wavelength. The results indicate that at least four and half times as many cells-per-wavelength are required for converged solutions for resonant geometries, than those geometries that are non-resonant. It is also noted that once the solution converges, the amount of deviation between the coarsest converged mesh and the finest mesh of all geometries was less than 1%.

3.3 Localized Mesh Refinement

While the previous section sought to determine how fine a global mesh was required to converge a steady solution for these resonant structures, this section aims to determine the sensitivities of these resonant structures to localized mesh refinement. After the mesh variable required for convergence has been determined to be 5.0 from the previous section, that global mesh variable is backed off slightly to be in the region that is out of convergence, chosen as 6.0. Then, three different localized refinement approaches are implemented – Au refinement, free space refinement, and interface refinement. While the first two do not alter the geometries, the third approach adds an additional layer of material at the interface. This additional geometry is modeled as free space, thus not changing the underlying problem, but allowing for that layer’s mesh to be refined, and more specifically confined, only to that interface. Table 3 summarizes the resulting HEX20 cells and cells-per-wavelength relationships.

Figures 13, 15, and 17 show the localized mesh refinements while Figures 14, 16, and 18 depict the magnitudes of the complex reflection and transmission coefficients computed from FLO_K for those refinements. The refined meshes utilized for the Frill geometry are shown in Figure 13. Figure 13a depicts the metallic region refinement, Figure 13b shows the free space refinement region, and Figures 13c and d show the additional free space geometry and corresponding mesh refinement of that additional geometry, respectively.

The magnitudes of the complex reflection and transmission coefficients from FLO_K are shown in Figures 14a and b, respectively. Here, it is clearly observed that none of the refinement techniques, as applied to this geometry, have any effect on converging to the same solution found from the global mesh study. The black curves in both Figures 14a and b depict the converged solution found from the globally course mesh for comparison. Although none of the meshes show any tendency to converge to the

Table 3. Localized HEX20 Refinement Cell Summary for all Geometries

Geometry	Global Mesh Variable	Refinement	Cell Size (nm)	$\frac{\text{Cells}}{\lambda}$
Frill	6	None	83.3	36
		Au	33.3	90
		Air	27.5	109.1
		Interface	16.7	180
ECT	6	None	66.7	30
		Au	22.2	90
		Air	22.2	90
		Interface	33.3	60
CRC	6	None	94.6	35.9
		Au	32.1	105.9
		Air	30.9	109.9
		Interface	33.3	102
	5.5	None	77.8	43
		Au	26.4	129
		Air	25.3	134.4
		Interface	33.3	102
	5.2	None	68.6	49.5
		Au	24.4	139.3
		Air	21.4	158.8
		Interface	33.3	102

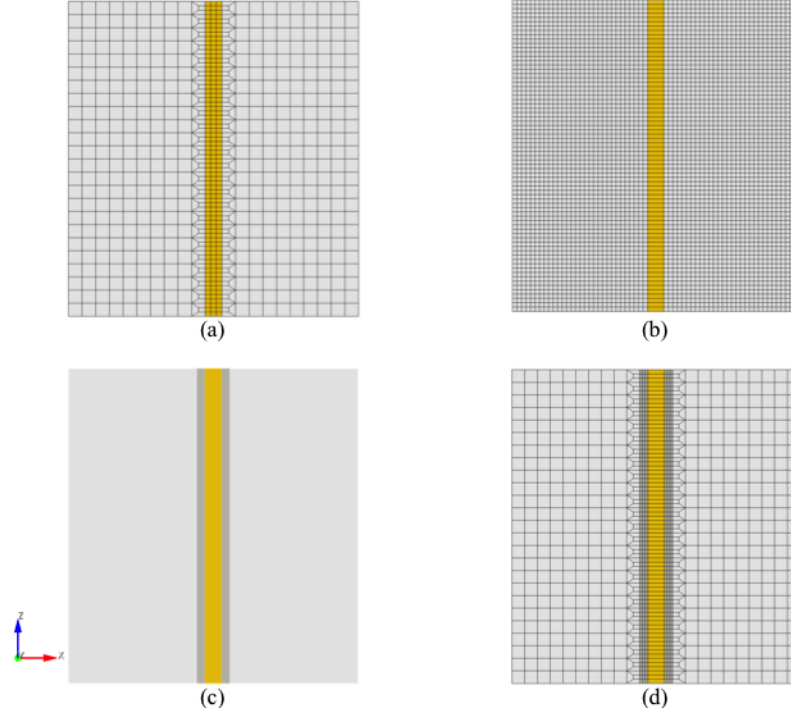


Figure 13. Frill localized mesh refinement. (a) Metallic region refinement. (b) Free space region refinement. (c) Additional free space geometry for (d) localized refinement of the interface.

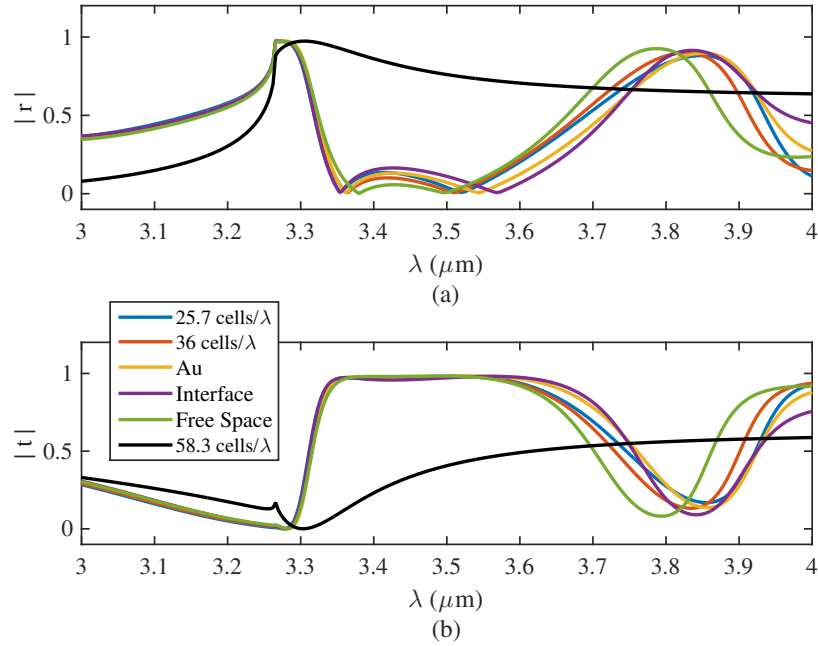


Figure 14. Mesh Refinement of Frill (a) $|r|$ and (b) $|t|$. Black curves in (a) and (b) indicate the converged solution from global mesh.

steady solution found using the global meshes, it is interesting to note that the trend in the solutions is similar, implying the underlying mechanism driving the failed solutions is seen as approximately the same in all of these cases, specifically low frequency breakdown.

The refined meshes utilized for the ECT geometry can be seen in Figure 15. Figure 15a depicts the metallic region refinement, Figure 15b shows the free space region refinement region, and Figures 15c and d show the additional free space geometry and corresponding mesh refinement of that additional geometry, respectively.

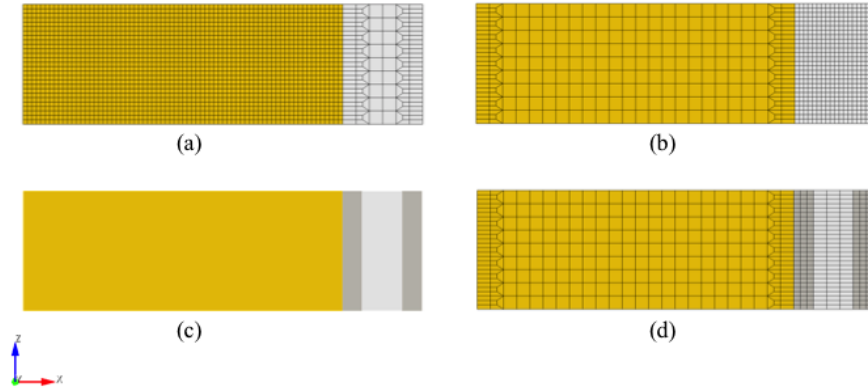


Figure 15. ECT localized mesh refinement. (a) Metallic region refinement. (b) Free space region refinement. (c) Additional free space geometry for (d) localized refinement of the interface.

The magnitudes of the complex reflection and transmission coefficients from FLO_K for the refined meshes of the ECT are shown in Figures 16a and b, respectively. Again, here it is clearly observed that none of the refinement techniques, as applied to this geometry, have any effect on converging to the same solution found from the global mesh study. The black curves in both Figures 16a and b depict the converged solution found from the globally course mesh for comparison. It is noted that the same mechanism observed in Figure 14 is driving the same errors here, again low frequency breakdown. Here, all the unconverged solutions are even more uniform than in the Frill geometry. This could create drastically incorrect results if it were assumed that

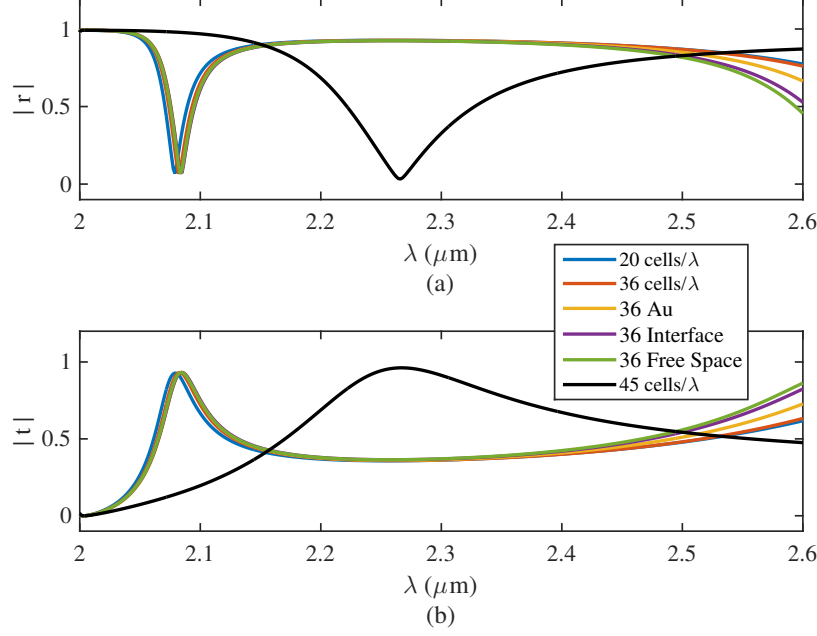


Figure 16. Mesh Refinement of ECT (a) $|r|$ and (b) $|t|$. Black curves in (a) and (b) indicate the converged solution from global mesh.

these curves were indeed self converged.

The refined meshes utilized for the CRC geometry can be seen in Figure 17. Figure 17a depicts the metallic region refinement, Figure 17b shows the free space refinement region, and Figures 17c and d show the additional free space geometry and corresponding mesh refinement of that additional geometry, respectively.

The magnitudes of the complex reflection coefficients from FLO_K for the refined meshes of the CRC are shown in Figure 18. Here, unlike the previous two geometries, it is clearly observed that the refinement techniques, as applied to this geometry, do indeed have an effect on converging to the same solution found from the global mesh study. It is observed that the resonance peaks are indeed moving toward the black curve resonance peak, seen in Figure 18, though the depths of the resonance peaks are notably larger. Given that this geometry is sensitive to the localized mesh refinements presented, the meshes will be further refined in order to determine if the solutions will converge.

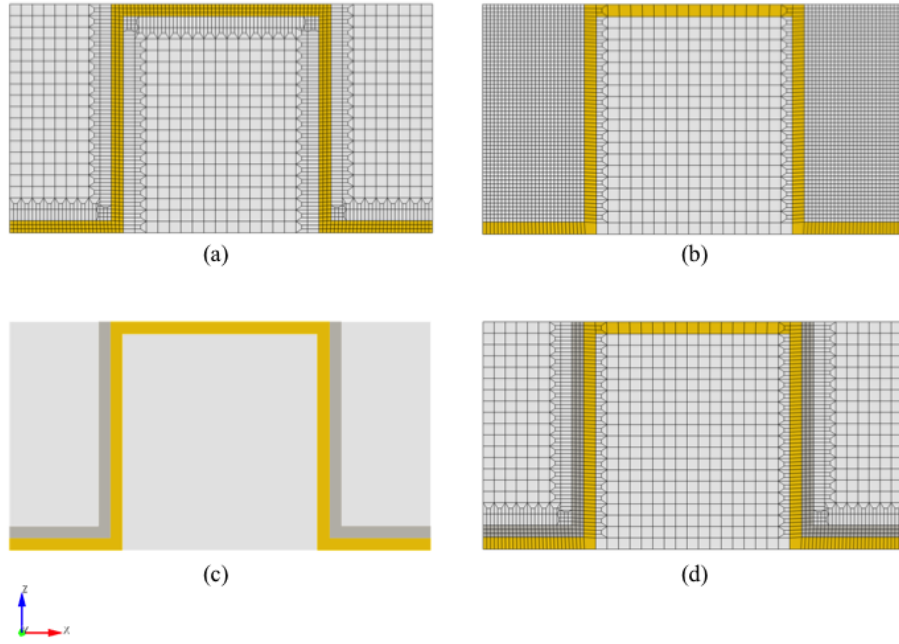


Figure 17. CRC localized mesh refinement. (a) Metallic region refinement. (b) Free space region refinement. (c) Additional free space geometry for (d) localized refinement of the interface.

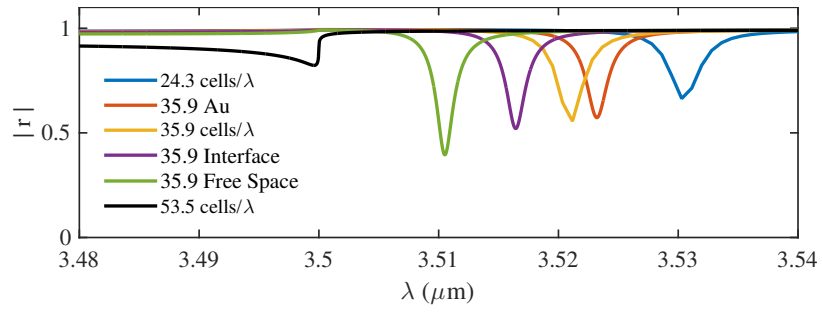


Figure 18. Mesh refinement of CRC $|r|$. Black curve indicates the converged solution from global mesh.

The global mesh variable of the CRC geometry was further refined from 6.0 down to 5.5 and 5.2, noting that the previous study showed a steady, converged solution when the mesh variable was 5.0. These variables result in global cell-per-wavelength ratios of 35.9, 43, and 49.5, respectively. The converged solution from the 5.0 mesh variable had a 53.5 cell-per-wavelength ratio. More details in numerical results are presented in Table 3. Figure 19 illustrates the results computed with FLO_K under these refined mesh conditions. Figure 19 is arranged by refinement with (a) being the metallic refinement, (b) the interface refinement, and (c) showing the free space refinement. The overall trend when separating them this way is that the free space refinement has greatest effect, which should come as no surprise. The unit cell is approximately half free space, when this region is refined, it has the effect of almost globally refining the mesh. It should be noted that despite these sensitivities, none of the solutions indeed converged.

It is interesting to note that for both the Frill and ECT geometries, all unconverged solutions seem to match similar curves, implying that these two geometries are not sensitive to localized mesh refinement, and therefore require a global mesh fine enough to converge. This will be an important factor when meshing the SRRs that will be modeled in Chapter IV, specifically, a global mesh refinement is necessary.

3.4 FEM Compared to RCWA

After all geometries have been converged, the next step is to compare these converged solutions to the RCWA truth values. Figures 20–22 show the results of this comparison. These results do not agree as closely as originally desired. Figures 20a and b depict the FEM solutions found from FLO_K for the Frill geometries and compares them with those found from RCWA to determine if FLO_K is correctly computing the scattered fields. It is observed that while the general shapes of the

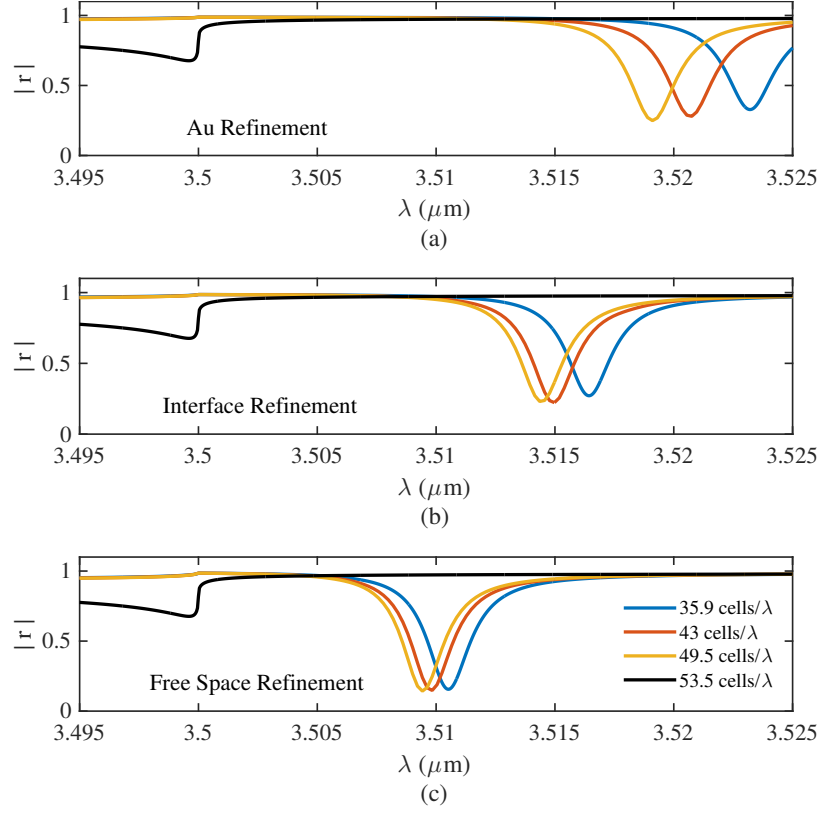


Figure 19. Further mesh refinement of CRC $|r|$ for (a) metallic region refinement, (b) interface refinement, and (c) free space refinement. Black curves in (a), (b), and c indicate the converged solution from global mesh.

curves are very similar, the resonance peaks are noticeably shifted, the amount of which is depicted in Figures 20c and d. The values reported in (c) and (d) are shown as absolute error which provide a measure for how far the FLO_K curves deviate from those from RCWA.

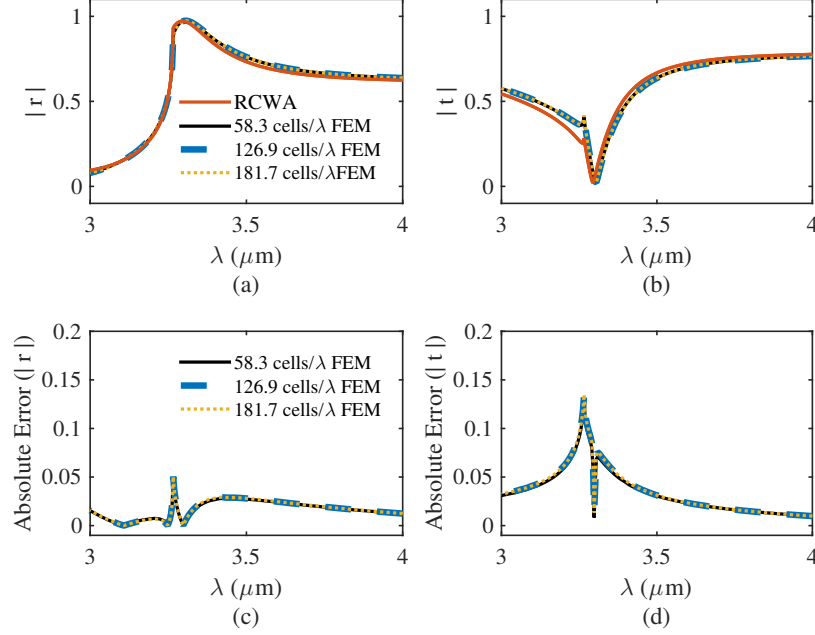


Figure 20. Frill FEM compared to RCWA. (a) $|r|$ and (b) $|t|$ curves shown with RCWA in red. Absolute error for (c) reflection and (d) transmission given with RCWA considered to be truth.

A comparison of the results found from FLO_K and RCWA for the ECT geometry are shown in Figures 21a and b, again to determine if FLO_K is correctly computing the scattered fields. As was the case for the Frill, it is clear that while the general shapes of the curves are very similar, the resonance peaks are noticeably shifted, the amount of which is depicted in Figures 21c and d. The values reported in (c) and (d) are shown as absolute error which provide a measure for how far the FLO_K curves deviate from those from RCWA. The fact that the Frill and the ECT curves are similar, but with resonances shifted further illustrates that these two geometries are very similar with similar underlying mechanisms driving the results.

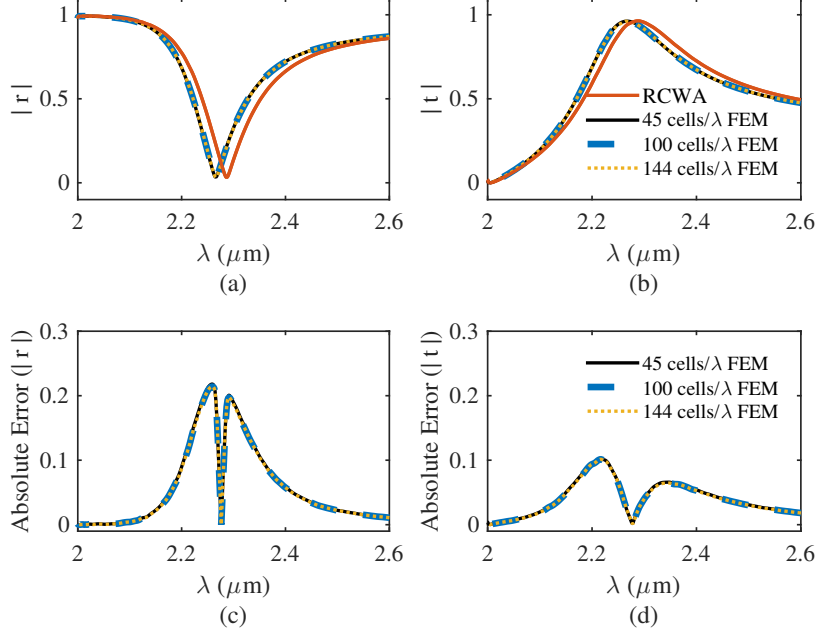


Figure 21. ECT FEM compared to RCWA. (a) $|r|$ and (b) $|t|$ curves shown with RCWA in red. Absolute error for (c) reflection and (d) transmission given with RCWA considered to be truth.

A comparison of the results from FLO_K and RCWA for the CRC geometry is depicted in Figure 22a to determine if FLO_K is computing the scattered fields correctly. Here, while the curves are again similar, as the previous two scenarios were, the resonance is where it should be, but does not appear to be as absorptive as the RCWA results predict. The fact that the resonance is in the same location is a good indicator that the geometry is correct, but further analysis was required to determine the cause of the errors seen in all three geometries.

These deviations in the converged FEM results when compared to RCWA led to further analysis of the meshed geometries. After much troubleshooting with the geometries, it was found that the geometries were indeed dimensionally correct, as initially thought in the CRC case, but FLO_K was experiencing port contamination due to the high evanescent fields near the aperture. This is due to the floquet apertures being placed at the surface of the metal. In short, FLO_K was capturing the

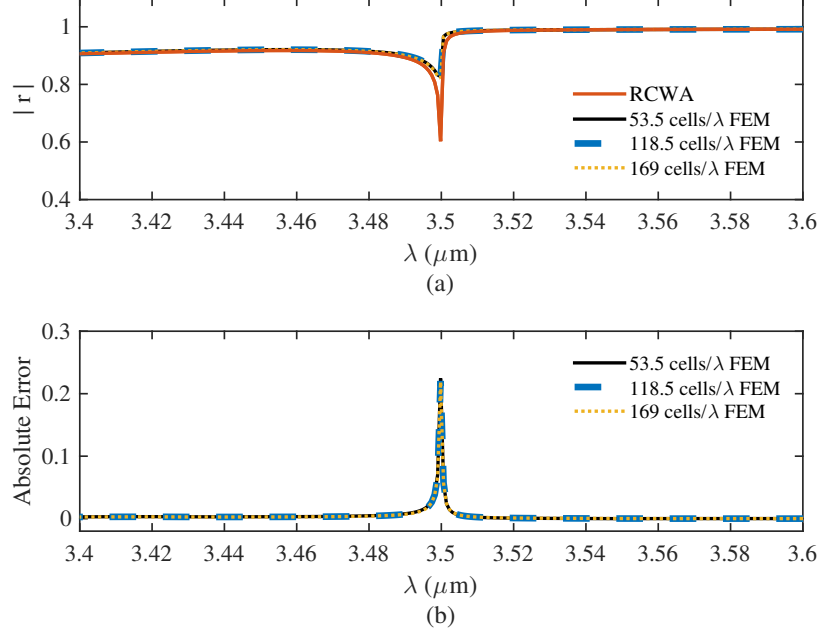


Figure 22. CRC FEM compared to RCWA. (a) $|r|$ curves shown with RCWA in red. Absolute error for (b) reflection given with RCWA considered to be truth.

near field interactions, contaminating the specular reflection and transmission on far field expansion. The solution to overcome the contaminated fields was to include additional free space cells above and below the geometry, which effectively pushed the floquet apertures far enough away from the evanescent fields to avoid measurably contaminating the results.

3.4.1 Free Space Padding.

The amount of free space padding that was needed was determined through iteration. Each iteration of the simulation included more free space between the metallic surface and the floquet apertures. This process was repeated until the resonance peaks no longer moved. Lastly, the results from adding the air padding were compared to those from RCWA.

These results are presented together to highlight the convergence found when less of the evanescent fields were being captured. Figures 23, 25, and 27 show how adding

different amounts of free space padding on the top and bottom of the unit cell affect the $|r|$ and $|t|$ curves, notably that they converge to the correct solution found from RCWA. Figures 24, 26, and 28 show the results after determining the required free space padding, including the deviations between the FEM and RCWA solutions.

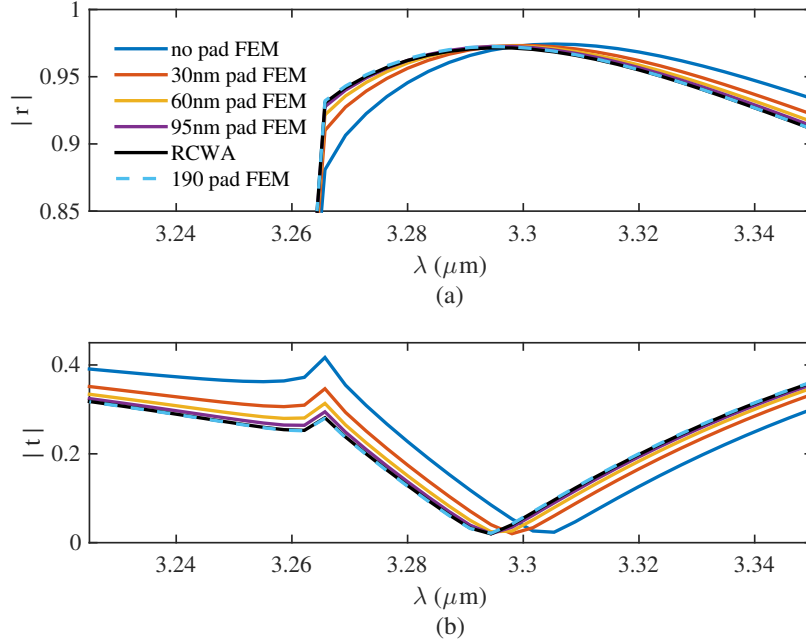


Figure 23. Frill geometry with varying amounts of air padding used from 0–190 nm padding resulting in the (a) reflection and (b) transmission shown.

Figures 23a and b show the $|r|$ and $|t|$ curves, respectively, for the Frill geometry with varying amounts of free space added above and below the resonant geometry. The scale of these plots is zoomed to illustrate how the curves shift to the correct value when not being contaminated with the evanescent fields. The Frill geometry found that 190 nm free space padding above and below the metal surface was sufficient distance to no longer have measurable effects contaminate the results. The 190 nm is an exceptionally small fraction of the incident wavelengths (3–4 μm).

After the 190-nm free space padding was applied to the Frill geometry, the curves were observed to match with much better agreement, as shown in Figure 24. Absolute

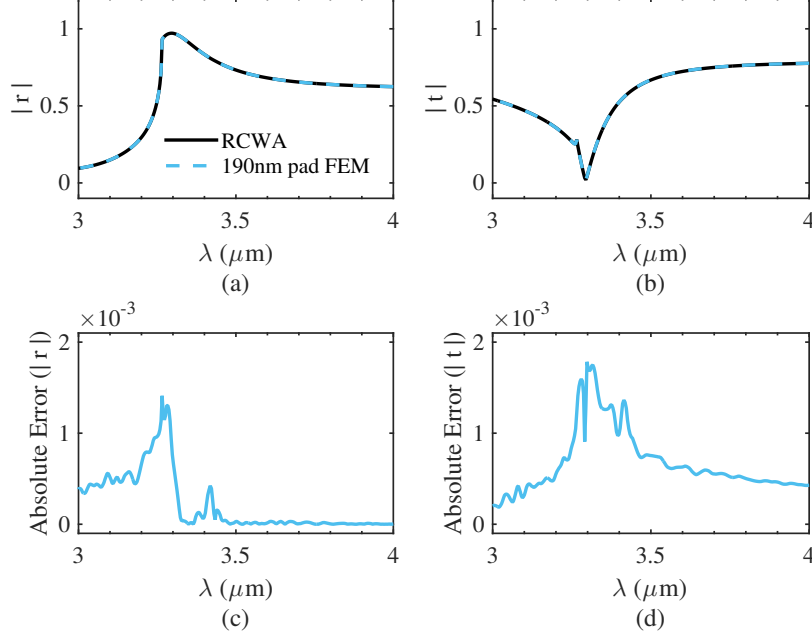


Figure 24. Converged Frill FEM vs RCWA with (a) reflection and (b) transmission curves shown with RCWA in black. Absolute error for (c) reflection and (d) transmission.

error reported for both the reflection and transmission was found to be less than 0.002 as shown in Figures 24c and d, respectively.

The convergence of the ECT curves with free space padding is shown in Figure 25. Again, the scale of these plots is zoomed in to show how varying the free space padding affects the amount of evanescent fields being captured. Here, it was observed that 200 nm of free space padding yielded the best results. Again, this 200 nm is a very small fraction of the incident wavelengths (2–2.6 μm). Much better agreement was observed when comparing the 200-nm free space padded FEM to RCWA, shown in Figure 26. Again absolute error is reported, seen in Figures 26c and d. The maximum error reported is less than 0.003 for the transmission and 0.002 for the reflection and shows very good agreement between the results from the FEM model compared to RCWA.

When free space was added to the CRC geometry, it was observed that the pre-

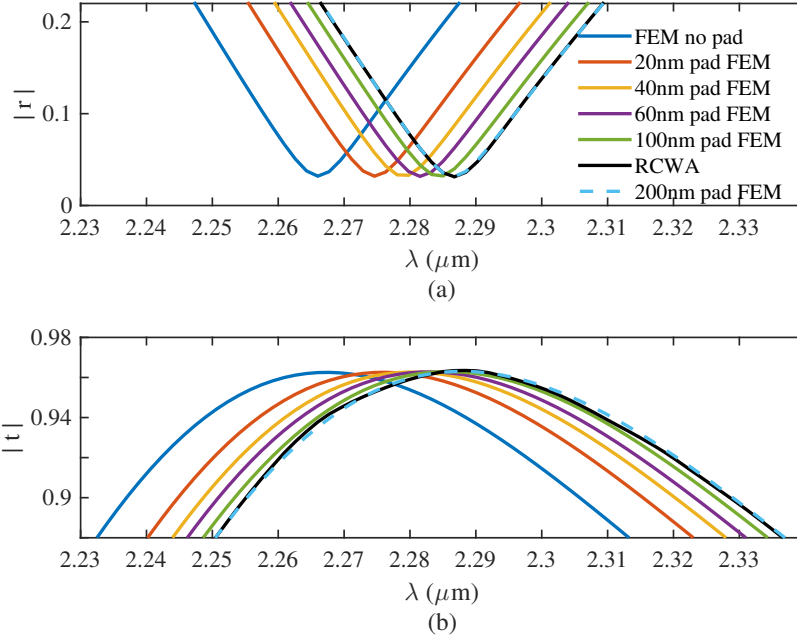


Figure 25. ECT geometry with varying amounts of air padding used from 0–256 nm padding resulting in the (a) reflection and (b) transmission shown.

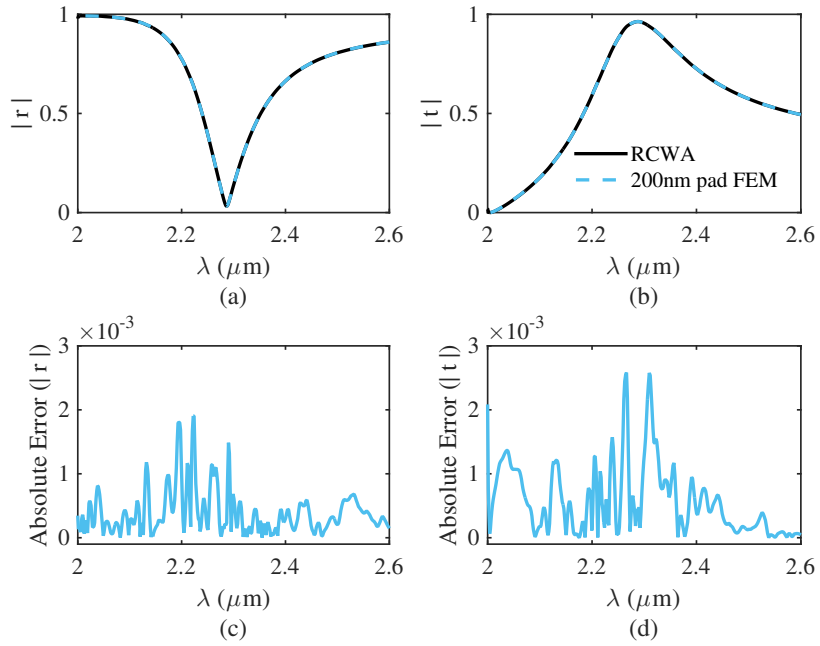


Figure 26. Converged ECT FEM vs RCWA with (a) reflection and (b) transmission curves shown with RCWA in black. Absolute error for (c) reflection and (d) transmission.

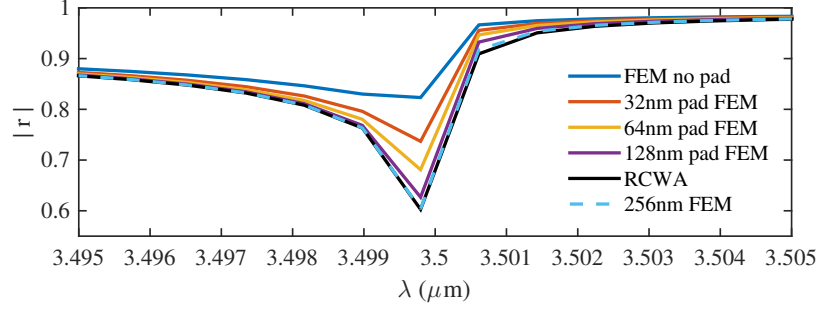


Figure 27. CRC geometry with varying amounts of air padding used from 0–256 nm padding resulting in the reflection shown.

viously less absorptive FEM solution became more absorptive, showing better agreement with the RCWA solutions. Figure 27 illustrates this. For this geometry, 256 nm of free space padding was needed. Again, 256 nm is a very small fraction of the incident wavelengths (3.4–3.6 μm). The fact that all three geometries required such a small fraction of the incident wavelengths implies that while the apertures are not impervious to contamination, they are certainly very resilient.

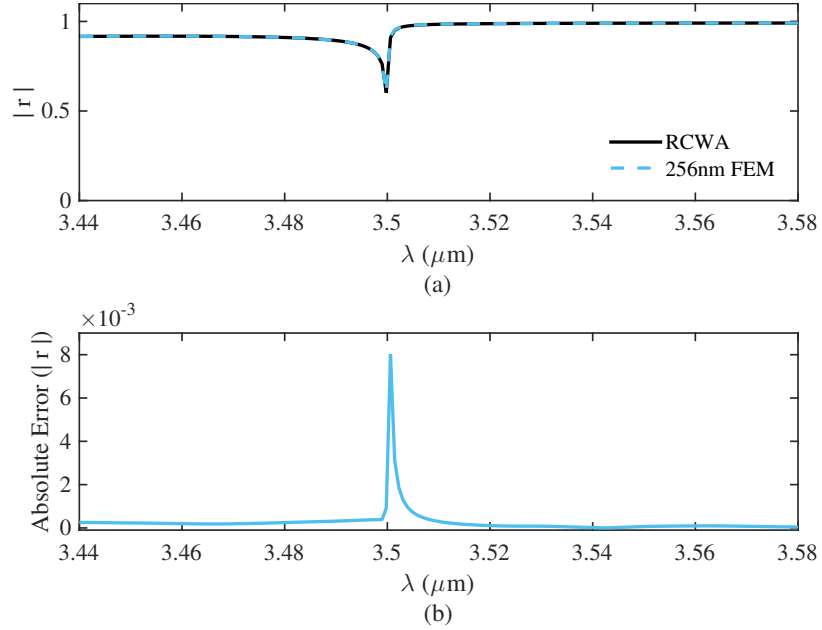


Figure 28. Converged CRC FEM vs RCWA with (a) reflection curves shown with RCWA in black with (b) absolute error.

Figure 28 shows the final FEM solution with 256 nm of free space padding compared to RCWA. As before, the absolute error was calculated and shown in Figure 28b with a maximum value of 0.008 at the resonance peak.

The FEM solutions for these free space padded geometries used global mesh variables of 3.0, giving cell-per-wavelength ratios of 126.9, 100, and 118.5 for the Frill, ECT, and CRC, respectively. These were the moderate meshes, neither the fine nor the course meshes. As has been shown in previous sections, using the finer global meshes would result in even less deviation from the RCWA values, but the moderate value was chosen due to lower deviation than course mesh. However, when considering computational time, significantly less time is needed for the moderate as compared to the fine meshes, as can be seen in Table 4. Unless extremely low error is required, generally the moderate mesh gives the best cost/benefit for computational time versus error. It is also important to note that many workstations would not be able to handle the RAM requirements of the finest mesh.

Table 4. HPC vs Local Workstation Computational Comparisons

Geometry	$\frac{\text{Cells}}{\lambda}$	HPC Time (hrs)	Local Time Equivalent (Hrs)	Max RAM (GB)
Frill	58.3	0.4	7.5	3
	126.9	2.2	38.7	25
	181.7	4.5	80.4	92.2
ECT	45	0.2	3	2
	100	1.8	32.1	16
	144	6.4	114.3	56
CRC	53.5	0.4	5.6	3.2
	118.5	2.9	39.9	22.6
	169	12.5	174.5	57.8

3.5 Conclusion

In conclusion, three FEM geometries have been simulated using FLO_K using both global meshes and locally refined meshes. The CRC was the most sensitive to localized mesh refinement, but all required a global mesh of at least 45 cells-per-wavelength, as seen with the ECT. It was discovered that simply ensuring self convergence was insufficient for correct results due to evanescent fields contaminating the specular results. Free space padding needed to be placed above and below the resonant geometry to effectively push the floquet apertures far enough away to not contaminate the results. The amount of free space needed was observed to be a very small fraction of the incident wavelengths, which implies that while the FLO_K apertures are not impervious to the evanescent fields, they are highly resilient. The results of the self convergence, including the free space above and below the geometry, showed a high level of agreement when compared to the RCWA as the truth data.

The meshing requirements learned from this study will directly affect modeling that will be conducted in Chapter IV, to isolate any issues that may come up while applying PPTE to SRRs.

IV. Permittivity and Permeability Tensor Extraction of In-Plane Split Ring Resonators

The goal of this chapter is to evaluate the accuracy of the Permittivity and Permeability Tensor Extraction (PPTE) method to extract the anisotropic permeability of an engineered magnetic material. The material chosen to examine is the Split Ring Resonator, which is inherently magnetic. PPTE was developed for generalized anisotropy. However, the SRR structure is known to be bi-anisotropic [3,23,27,33,48], which ultimately limits the potential of using this technique. The nature of the bi-anisotropy of the particular orientation of the SRRs was unknown at the start of this research. While most literature acknowledges the bi-anisotropy, others ignore it entirely, [22,30,35,40]. Linden’s paper, *Magnetic Response of Metamaterials at 100 THz*, is one such piece of literature that ignores the bi-anisotropy and reports a permittivity and permeability for two orientations of incident fields [30]. This chapter models the geometry and materials reported by Linden [30] in order to determine if PPTE can be used to evaluate these SRRs when they are oriented in-plane with the surface of the substrate material.

This chapter first explores PPTE’s effectiveness on an isotropic sample with defined permittivities and permeabilities within the range of those reported by Linden [30]. Although this shows PPTE’s ability to extract intrinsic magnetic permeabilities (those other than unity), it is not sufficient to determine if the full tensors (18 tensor elements) extracted using PPTE are accurate from this simple, isotropic test medium. Next, it is shown, through simulated scattering, the bi-anisotropic nature of the SRR geometry when it is constrained to free space in order to determine under what conditions the bi-anisotropy may be ignored. PPTE is then applied to extract the permittivity and permeability tensors in this free space example at three different aspect angles, showing how the bi-anisotropy alters the extracted permittivity and

permeability tensors. After this is completed, the research shows how the scattering is altered by the inclusion of a substrate which induces a change in the SRRs capacitance. Finally, PPTE is applied to extract the permittivity and permeability tensors and compare those values to what was reported by Linden [30].

During Dr. Benson's work in developing PPTE, it was tested against several cases to show its effectiveness in retrieving effective permittivity from an isotropic sample, a biaxial anisotropic sample, and an unaligned anisotropic sample [7,8]. The isotropic case is the simplest and easiest to check given that the permittivity and permeability are defined prior to the experiment. The same method will be applied here. His work was shown to have a very high level of agreement on a biaxial anisotropic material when compared to extractions made by other researchers here at AFIT through traditional microwave techniques, [7,8]. However, lacking an amenable local experimental method to verify this, another method of checking is required, specifically, turning to literature reported by Linden [30].

The algorithm PPTE employs is invertible and provides an effective starting point. It is necessary, but not sufficient to show that the inverse algorithm, when applied to the permittivity and permeability tensors, recovers the input fields. It can at least show that the underlying assumptions upon which the method was based were not violated. However, it is insufficient in and of itself to verify the retrieved tensors correctly model the effective material. In order to sufficiently prove that the method itself is accurate, it will need to be compared to other methods. This work turned to literature for comparison, applying the same geometries and material parameters reported by Linden to determine the level of agreement in the reported permittivity and permeability in the orientations given [30].

4.1 FLO_K Experimental Setup

PPTE requires more angles of incidence than what was necessary for the mesh study in Chapter III. For this reason, and to ensure common vernacular for the angle definitions, a more thorough explanation of how the experiments were simulated is reported.

Two sets of coordinate systems are used to describe the system as a whole; the sample coordinate system and the instrument (FLO_K) coordinate system. The sample coordinate system has cartesian coordinates with the geometry generated in Cubit, as was the case in Chapter III. FLO_K has spherical coordinates with θ being the elevation angle measured off normal ($\hat{z}$) in the $\hat{x}$ direction and ϕ is the azimuthal, or rotation, angle measured from the $\hat{x}$ and has the effect of rotating the sample. Figure 29 illustrates this.

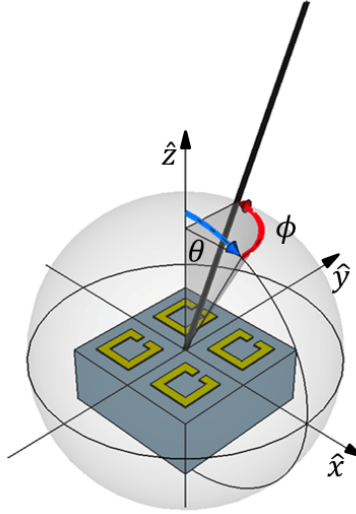


Figure 29. Sample and FLO_K Experimental Coordinate Systems. The sample has cartesian coordinates, labeled $\hat{x}$, $\hat{y}$, and $\hat{z}$, while FLO_K has spherical coordinates with θ being the elevation angle measured from $\hat{z}$ and ϕ being the azimuthal angle measured from the $\hat{x}$ axis. Here $\theta = 30^\circ$ and $\phi = 90^\circ$.

PPTE requires two orthogonal ϕ angles in order to solve for all tensor elements. For this reason, $\phi = 0^\circ$ and 90° were chosen. Additionally, some θ sweeps from 10° –

70° were performed on the free space SRR to explore the bi-anisotropy of the split ring resonators. For PPTE predictive purposes, ϕ sweeps from 0°–345° in increments of 15° were also performed.

Throughout this chapter, transverse electric (TE) and transverse magnetic (TM) will be used to describe the polarization of the fields for all cases, e.g incident, reflected, and transmitted. Figure 30 illustrates the orientation of the fields with respect to the plane of incidence. Here, TE implies that the electric field, $\vec{E}$ is transverse to the plane of incidence while the magnetic field, $\vec{H}$, lies within the plane of incidence. TM, as the name would suggest, implies that $\vec{H}$ is transverse to the plane of incidence while $\vec{E}$ lies within the plane of incidence. Co-pol will be used to describe cases where the reflected and/or transmitted fields are the same polarization as the incident fields, while cross-pol (x-pol) will be used to describe when the reflected and/or transmitted fields are aligned with the orthogonal polarization to the incident fields.

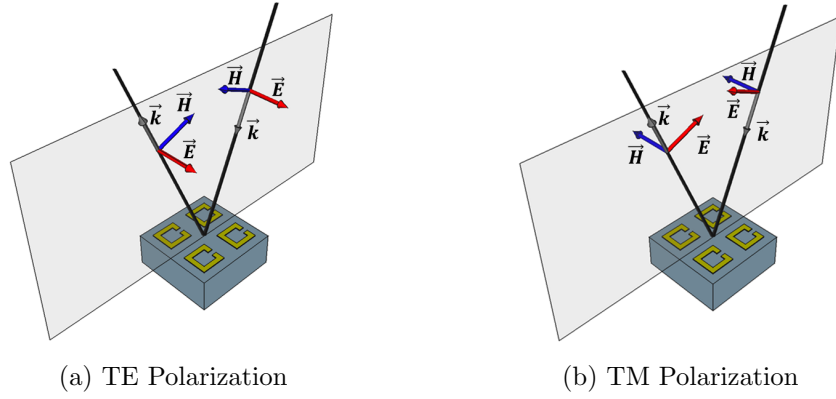


Figure 30. Polarization states of the fields with respect to the plane of incidence. (a) The magnetic field is aligned with the plane of incidence and the electric field is transverse to the plane of incidence. (b) The electric field is aligned with the plane of incidence while the magnetic field is transverse to the plane of incidence.

4.1.1 Geometries.

Three different geometries were considered in the simulations conducted in this chapter. First, a simple slab, $1\ \mu\text{m} \times 1\ \mu\text{m} \times 0.5\ \mu\text{m}$ was used for an isotropic test of defined material parameters against PPTE. The second and third consisted of SRRs of the geometry and material parameters outlined by Linden [30,31], as shown in Figure 31. The first of the SRRs consisted of the SRR in free space, as shown in Figure 31b, to observe the scattering response at multiple angles of incidence to determine the existence of any bi-anisotropy. PPTE was applied to this geometry as a baseline before moving on to the third geometry, a second SRR deposited on SiO_2 , shown in Figure 31a. The dimensions of the SRR were followed as outlined by Linden [30,31]. Specifically, the unit cell period, $T = 450\ \text{nm}$, metal height, $h = 20\ \text{nm}$, the length of the SRR legs, $l = 320\ \text{nm}$, the trace width, $w = 90\ \text{nm}$, and the gap, $g = 70\ \text{nm}$ [30,31].

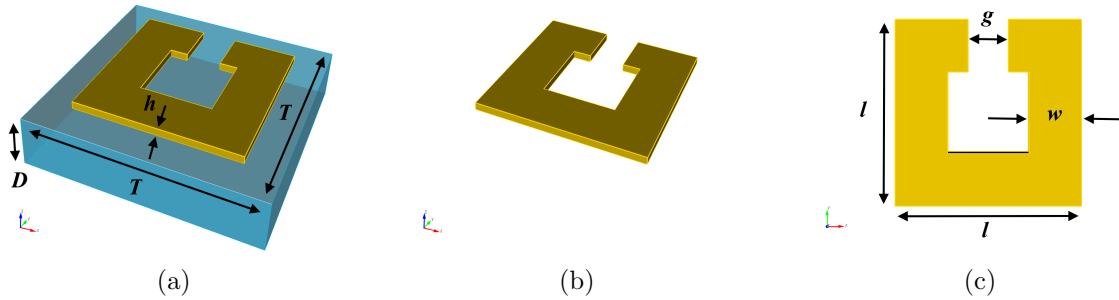


Figure 31. SRR geometries and dimensions. (a) SRR on SiO_2 substrate. The SiO_2 substrate depth, D , will be varied from $20\ \text{nm}$ to $2\ \mu\text{m}$. (b) SRR in free space. (c) SRR dimensions. The SRR geometries in (a), (b), and (c) share the same dimensions with length, $l = 320\ \text{nm}$, tracewidth, $w = 90\ \text{nm}$, gap, $g = 70\ \text{nm}$, and unit cell period, $T = 450\ \text{nm}$. The metal height, h , will be varied from $13\text{--}30\ \text{nm}$.

The material properties that were used for the SRR simulations were based off the reported values by Linden [30,31] so that a direct comparison could be made between the scattering reported and the extracted effective permittivity and permeability. The

gold properties that were used followed the drude model [30],

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega(\omega + i\omega_c)},$$

where ω_p is the plasma frequency and ω_c is the collision frequency. The specific values were reported to be $\omega_p = 2\pi \times 2.175 \times 10^{15} \text{ s}^{-1}$ and $\omega_c = 2\pi \times 6.5 \times 10^{12} \text{ s}^{-1}$ [30]. Linden also reports that the collision frequency used was 1.65 times higher to increase the absorption and to more closely match their model with their measured value [30]. The material properties that were used for the glass were not reported, except to state that a standard glass substrate was used [31]. BK7 was chosen as a standard crown glass with an index of refraction of ~ 1.5 in the 1–5 μm range and is given by the dispersion relationship

$$n^2(\lambda) - 1 = \frac{B_1\lambda^2}{\lambda^2 - C_1} + \frac{B_2\lambda^2}{\lambda^2 - C_2} + \frac{B_3\lambda^2}{\lambda^2 - C_3},$$

where $B_1 = 1.03961212$, $C_1 = 0.00600069867$, $B_2 = 0.231792344$, $C_2 = 0.0200179144$, $B_3 = 1.01046945$, and $C_3 = 103.560653$, as reported by SCHOTT [37]. This material is non-magnetic, which implies ϵ can easily be determined by

$$\epsilon(\lambda) = \frac{B_1\lambda^2}{\lambda^2 - C_1} + \frac{B_2\lambda^2}{\lambda^2 - C_2} + \frac{B_3\lambda^2}{\lambda^2 - C_3} + 1.$$

4.2 PPTE Application

With modeled fields developed and converged, PPTE is then utilized to extract the permittivities and permeabilities in three cases – an isotropic test case, SRRs in free space, and SRRs on an SiO_2 substrate. The isotropic test case has defined material parameters within the desired range of what is expected for the SRRs. Determining if PPTE can accurately extract an intrinsic permeability in this range is necessary

before moving on to the SRRs.

4.2.1 Isotropic Test Case.

Prior to the application of PPTE for material parameter extraction on complex structures like SRRs, it must first be verified that PPTE can handle an isotropic test case of varying relative permeability. For this case, material parameters were chosen to be in the range of those reported by Linden [30]. Figure 32 depicts the parameters graphically. For reference, see Figures 68a and 68c for the reported permittivity and permeability from Linden, which will be examined more closely in that section. The material parameters here have a maximum relative permittivity of ± 55 and permeability of ± 6.8 . The maximum values occur at 80 THz while the minimum values occur at 98 THz.

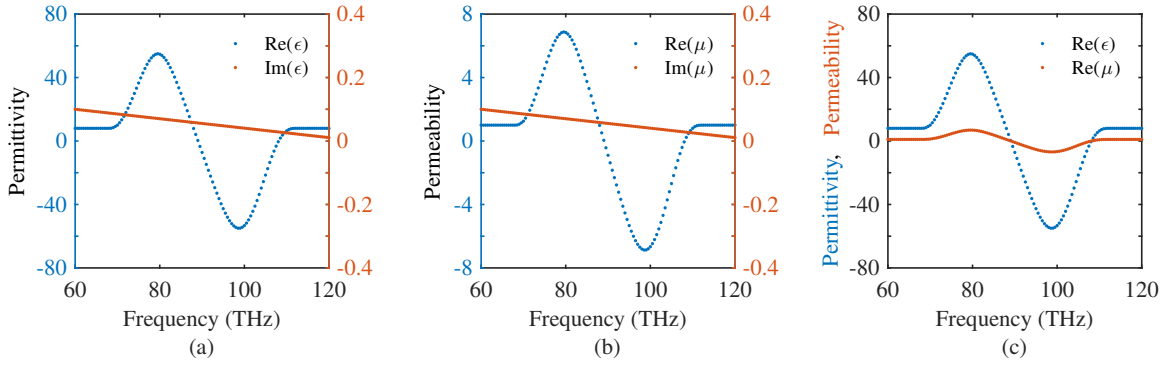


Figure 32. Material parameters defined for the isotropic test case for PPTE. These values are similar in range and shape of those reported by Linden [30], shown in Figure 68.

Using these values of permittivity and permeability, the complex index of refraction, $\tilde{n}$, was determined using Equation 15, specifically $\tilde{n} = \sqrt{\epsilon_r \mu_r}$. Here, the assumption that $n = \sqrt{\epsilon_r}$ due to μ_r being unity is not valid. The real part of $\tilde{n}$ is given as the index of refraction, n , while the imaginary part, k , is the extinction coefficient. Figure 33 shows both the index of refraction and the extinction coefficient.

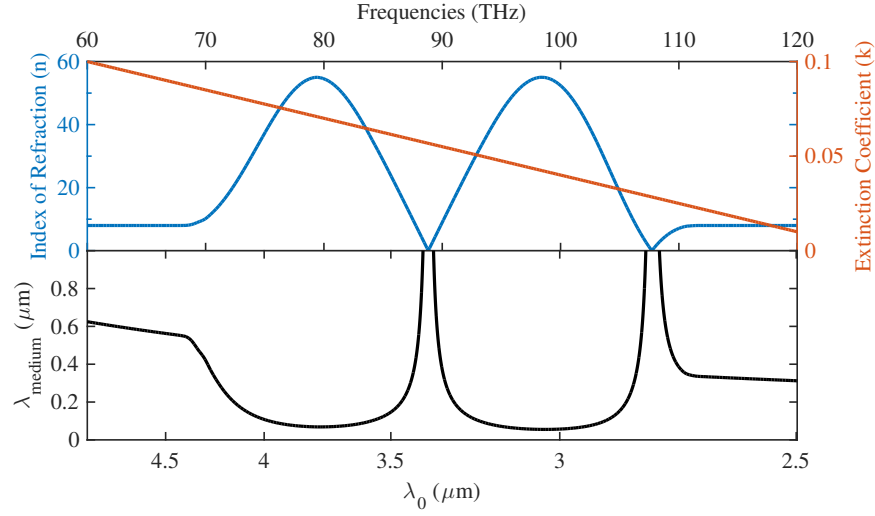


Figure 33. (Top) Index of refraction and extinction coefficient based on material parameters defined for the isotropic test of PPTE. **(Bottom)** Wavelength within the medium vs. the incident wavelength.

In order to appropriately set up the experiment, the geometry and accompanying mesh must be chosen with care. As discussed in Chapter III, the mesh size determines how accurate of a solution can be achieved. From Figure 33, it is observed that the smallest incident wavelength, $2.5 \mu\text{m}$, is indeed not the smallest wavelength within the material. Note that at the largest indices of refraction, occurring near 80 and 100 THz, the wavelength is compressed to be very small, on the order of 55 and 68 nm at 100 and 80 THz, respectively. These values are far too small to mesh and test, but the medium wavelength at the $2.5 \mu\text{m}$ incident wavelength is around 312 nm. If the mesh is to adequately capture the phase differences between cells, the cell size will need to be at most 10% of this. The mesh cell size was chosen to be 32 nm and is close to the desired one tenth of the wavelength designed for.

After simulating the scattering with FLO_K, the scattered fields were then run through PPTE and yielded the results presented in Figures 34 and 35. It is clear that PPTE was able to extract both the intrinsic permittivity and permeability and both are diagonalized with all diagonal elements being equal, as would be expected

for simple, isotropic media.

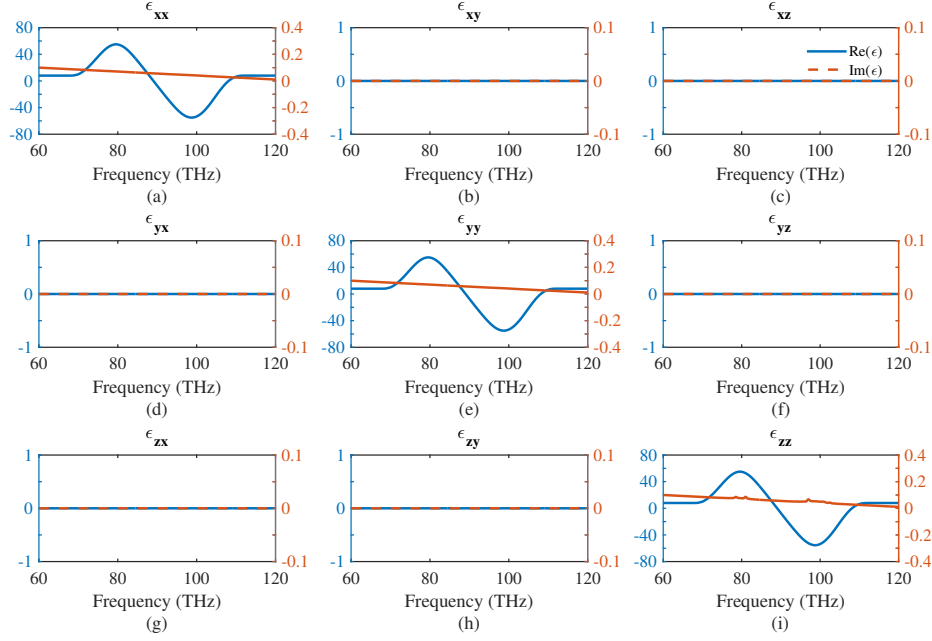


Figure 34. Extracted permittivity tensor from the isotropic test case. Note that it is diagonalized with $\epsilon_{xx} = \epsilon_{yy} = \epsilon_{zz}$ as expected for an isotropic sample.

Figure 36 shows the tensor elements along the diagonal only, along with the associated errors. The first thing to note is that the error is very small with the highest error shown to be at the wavelengths where the compression from the index of the material was highest. This is due to the fact that the experiment was set up for the 312 nm wavelength. At the shorter wavelengths, 55 and 68 nm, the mesh does not meet the required ten cells per wavelength. Also note the shape is the same as the index of refraction, which should come as no surprise as the index of refraction is the mechanism that controls the compression of the wavelengths, shown in Figure 33.

The errors reported in Figure 36 are provided as absolute error which highlights the shape of the deviation. Previous usage of the absolute error was also based on the range of values lying on the interval $[0 \ 1]$. Here, the values for the permittivity and permeability do not lie on this interval. When considering the relative errors, the maximum error for ϵ_{xx} and ϵ_{yy} is 0.09% for the real part and 2% for the imaginary part.

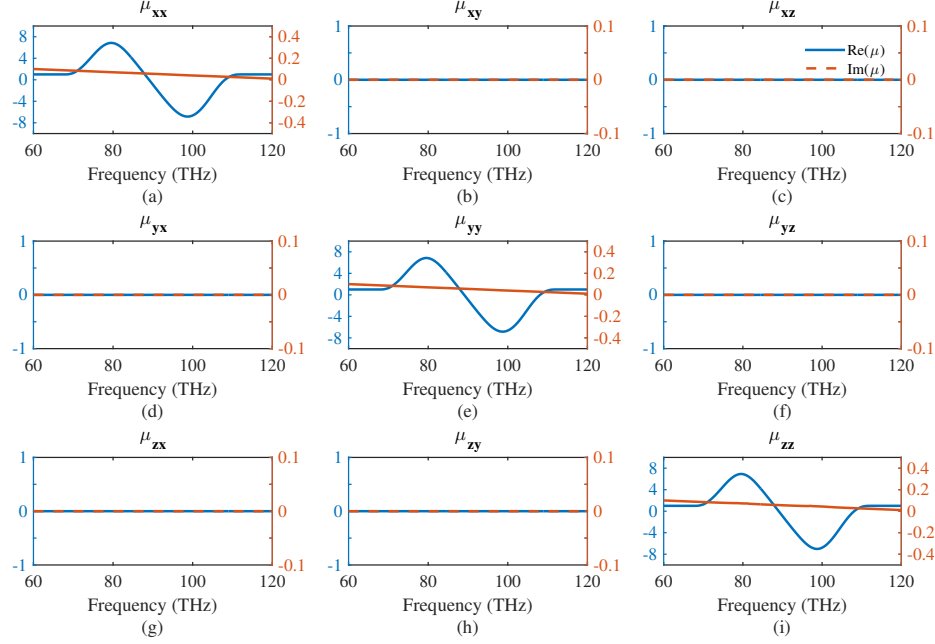


Figure 35. Extracted permeability tensor from the isotropic test case. Note that it is diagonalized with $\mu_{xx} = \mu_{yy} = \mu_{zz}$ as expected for an isotropic sample.

The relative error associated with ϵ_{zz} is 0.2% for the real part and has two sharp spikes of 54% and 28% for the imaginary part. These high spikes are associated with the mesh inadequacy due to the high index of refraction at 80 and 100 THz. Additionally, the values for k were defined to be small, implying that any observable deviation will result in a large relative error due to dividing by a small number. Errors elsewhere for the imaginary part of ϵ_{zz} are below 0.03%. The maximum relative errors for μ_{xx} and μ_{yy} are 0.1% for the real part and 1.5% for the imaginary part. The maximum relative error for μ_{zz} is 0.8% for the real part. Again, two sharp spikes of 11% and 5% are observed for the imaginary parts with 0.1% observed elsewhere. As shown in Chapter III, the error could be driven lower by using a smaller mesh cell size. However, this also increases the machine memory requirements and simulation times. The error reported here is sufficiently small, and otherwise obeys the expected mesh-error mechanism, to adequately state that PPTE can accurately retrieve intrinsic

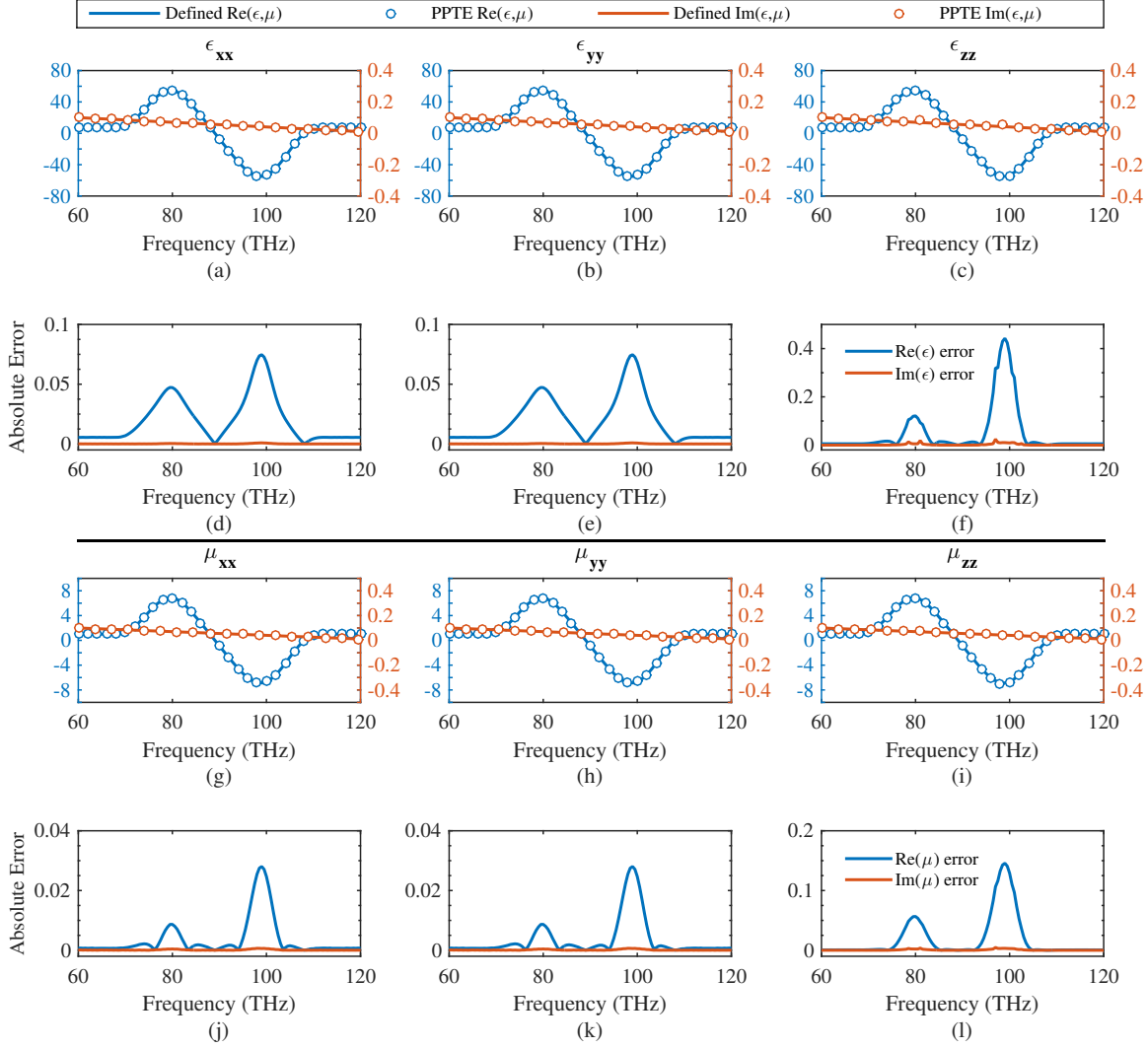


Figure 36. Diagonalized Permittivity and Permeability Tensors of Isotropic Test Case. (Top) Permittivity and associated errors. (Bottom) Permeability and associated errors. Note that the errors are maximum when λ_{medium} is the smallest as seen in Figure 33 (Bottom).

permeabilities from simple, magnetic materials, over the expected range of interest. This assumes the experiment has been sufficiently discretized to capture the necessary phase information, which was driven specifically in this case by the index of refraction.

4.2.2 SRR from Literature.

Now that PPTE has been shown to work remarkably well with simple magnetic media, the next step is to examine SRRs, which are expected to be anisotropic. This section first examines the bi-anisotropic nature of split rings when oriented in the xy-plane. This was achieved through simulation of SRRs of the size and materials reported by Linden [30] via FLO_K. First, SRRs are examined in free space with a θ sweep from 10° – 70° with increments of 10° . Next, PPTE was applied to three cases, $\theta = 10^\circ$, 40° , and 70° . After these cases have been examined, the next step was to examine how the scattering changes when the SRRs are coupled with a substrate, in this case SiO_2 . This section concludes with PPTE being applied to the SRR structure coupled with glass for direct comparison of the reported permittivity and permeability in the orientations reported by Linden [30].

4.2.2.1 SRR in Free Space.

To examine how SRRs interact with electromagnetic fields, a simplified case of a split ring in free space was evaluated. This isolated the effects of the split rings from that of any other materials, coupled or otherwise. Likewise, if PPTE is to be applied to SRRs, an assumption must be made that the material is anisotropic *without* field coupling. It should be evident in the inherent nature of the SRR that the magnetic and electric dipoles that are formed when either the capacitive gap or the inductive ring is excited, as was shown in Figure 3b in Chapter II, that there should be some field coupling under some conditions.

4.2.2.2 SRR Mesh Convergence.

Before any extensive examination of the scattering of the SRRs, it must first be determined that the meshes result in a converged solution. The methods developed in Chapter III were applied, except that it was not necessary to extensively explore the unconverged region, simply to ensure that the resulting meshes were converged and accurate. The work in Chapter III determined that all three of the structures examined during that work showed converged solutions when the mesh variable used by Cubit were 5.0 or smaller. These SRR geometries are considerably smaller at 450 nm unit cell period, resulting in inherently smaller meshes. Figure 37a depicts a global mesh generated by Cubit with a mesh variable of 5.0. The mesh resulted in a 76 cell-per-wavelength ratio, well above the 50 cell-per-wavelength ratio that was determined from Chapter III to be required. Metallic and free space refinement was also employed to determine if the meshes resulted in converged solutions. These meshes are shown in Figures 37b and c.

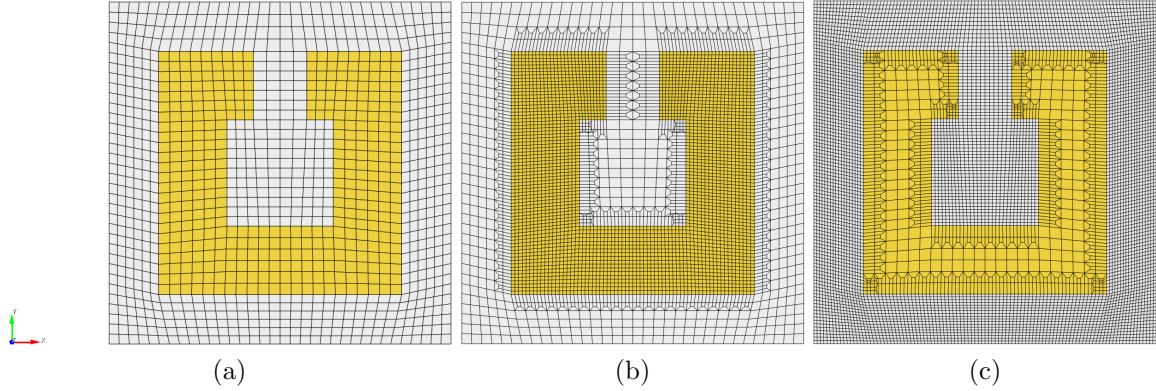


Figure 37. SRR meshes with perspective from $\hat{z}$ direction looking down to the xy-plane. (a) global mesh with 13 nm max cells resulting in 76 cells-per-wavelength. (b) metallic region refinement with 5 nm cells resulting in 206 cells-per-wavelength. (c) free space region refinement with 4 nm cells resulting in 227 cells-per-wavelength.

The resulting solutions from these meshes are depicted in Figure 38, with (a) and (b) showing the reflection magnitude of the two co-pol case found at $\phi = 0^\circ$ with 40°

incident angle. All other polarizations and transmission showed similar results. The deviation between any two of the curves is shown in Figure 38c and d. The blue curves in (c) and (d) show the deviation between global and free space refined meshes shown in (a) and (b). The yellow curves in (c) and (d) depict the deviation between the global and metallic refined meshes shown in (a) and (b). The green curves depict the deviation between the two refined meshes, free space and metallic, from (a) and (b). Notably, all deviations are below 0.004, which is in line with the deviation between the converged solutions from Chapter III. Of these meshes, the global is the simplest and resulted in the quickest of the simulation times. As such, all the meshes in the remaining sections will use this global mesh variable of 5.0.

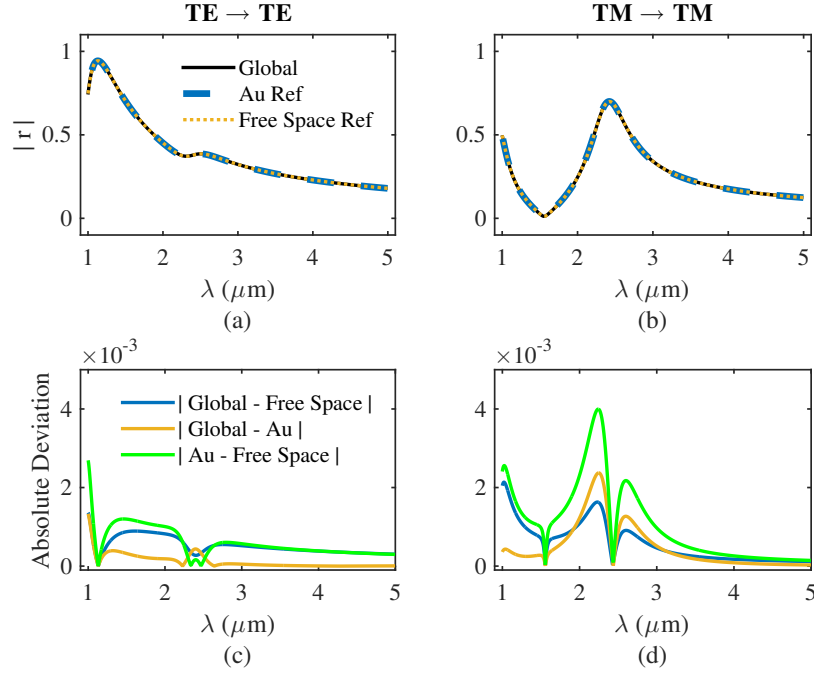


Figure 38. SRR mesh convergence. (a) and (b) depict the co-pol reflection magnitude found from $\phi = 0^\circ$ and 40° incident angle. (c) and (d) depict the deviation between any two curves from (a) and (b), shown in absolute deviation.

After determining the solutions have converged, evanescent fields must now be considered. As before, this was determined through iteration, varying the amount of free space above and below the geometry from 20–200 nm. It was determined that

only 20 nm was required for this 40° incident angle. The final result of 20 nm free space padding for this 40° incident angle is depicted in Figure 39. Higher incident angles, such as 70°, did require more free space, specifically 80 nm.

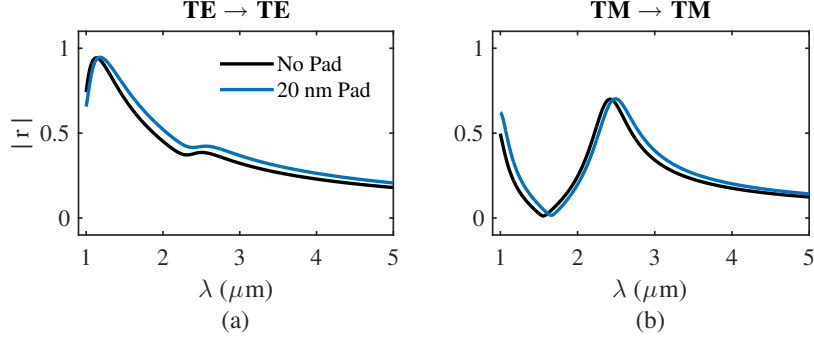


Figure 39. SRR Free space padding. Both (a) and (b) depict the co-pol reflection magnitude found from $\phi = 0^\circ$ and 40° incident angle. The black curve shows the converged solution without evanescent fields being considered while the blue curve includes 20 nm free space padding above and below the geometry to remove any contamination caused by the evanescent fields.

4.2.2.3 Minimization of Bi-anisotropic Scattering.

In order to determine exactly how bi-anisotropic the SRR is, a θ sweep at $\phi = 0^\circ$ and 90° was performed using FLO_K. A θ sweep should give an indication if the magnetic field is capable of driving an observable response in the electric field that was computed by FLO_K. Figs 40 and 41 show the results of the scattering. Of particular note, the resonance is indeed not isolated to one polarization when $\phi = 0^\circ$, as shown in Figures 40a and e, the TE co-pol reflected and transmitted fields.

The mechanisms driving the observed phenomena can be easily understood when decomposing $\vec{E}$ and $\vec{H}$ into their respective $\hat{x}$, $\hat{y}$, and $\hat{z}$ components. This can be done simply by looking at the projections onto each of the axes and comparing relative magnitudes of each component to those that are aligned with either the inductive ring or the capacitive gap. In order to decompose the fields into their respective components, first the vertical, $\hat{z}$, and horizontal, those lying in the xy-plane, components

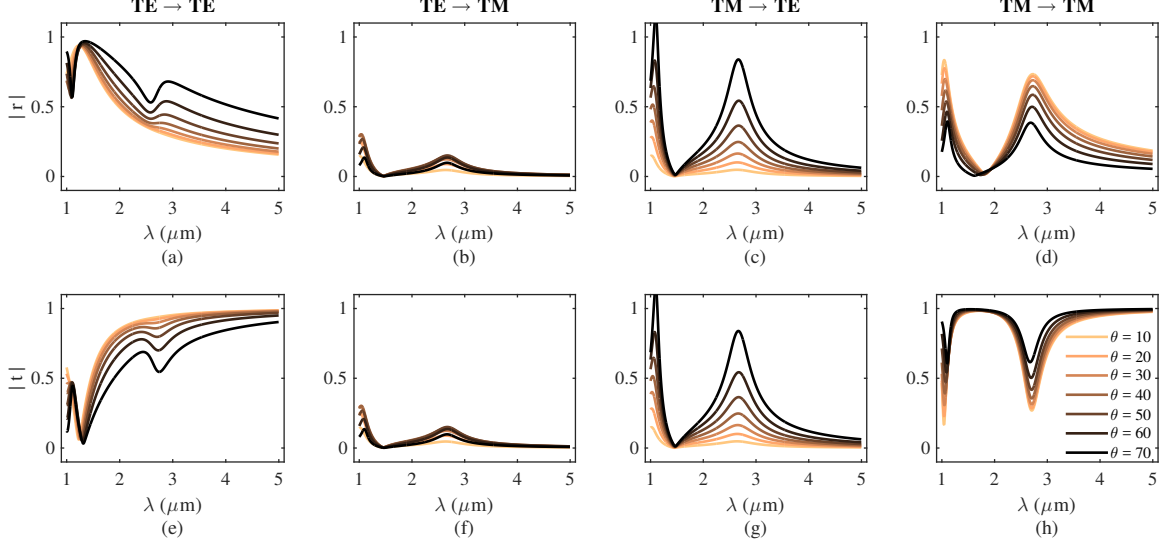


Figure 40. SRR geometry from [30] in free space with $\phi = 0^\circ$ and a θ sweep from 10° – 70° . Note that (a) and (e) show the existence of magnetic field coupling at higher θ angles.

must be found. Ignoring ϕ angle, the $\hat{z}$ component can be found by $\sin(\theta)$, while the horizontal components can be found by $\cos(\theta)$. If ϕ is one of the cardinal angles, then the horizontal component will lie entirely along either the $\hat{x}$ or $\hat{y}$ directions. If, however, ϕ is not one of the cardinal angles, then the horizontal component can be decomposed further by projecting onto the $\hat{x}$ and $\hat{y}$ axes in a similar manner – the $\hat{y}$ component is found from $\sin(\phi)$, while the $\hat{x}$ component is found from $\cos(\phi)$. If H_z is small, it does not drive enough current to give an observable response in the measured electric field. If, however, H_z is large, then the current driven through the loop is large enough to create a potential across the capacitive gap, creating an electric dipole moment, $\vec{P}$ and can realign the fields causing an observable magnitude in the x-pol cases. Similarly, if the E_x component is large, a potential is formed across the gap, which in turn drives a current through the loop and creates a magnetic dipole, $\vec{M}$, causing an observable realignment of the fields in the x-pol cases.

This same effect can also be used to describe the resonances in the co-pol cases. That is, if H_z is large, a response should be observed, regardless of whether or not

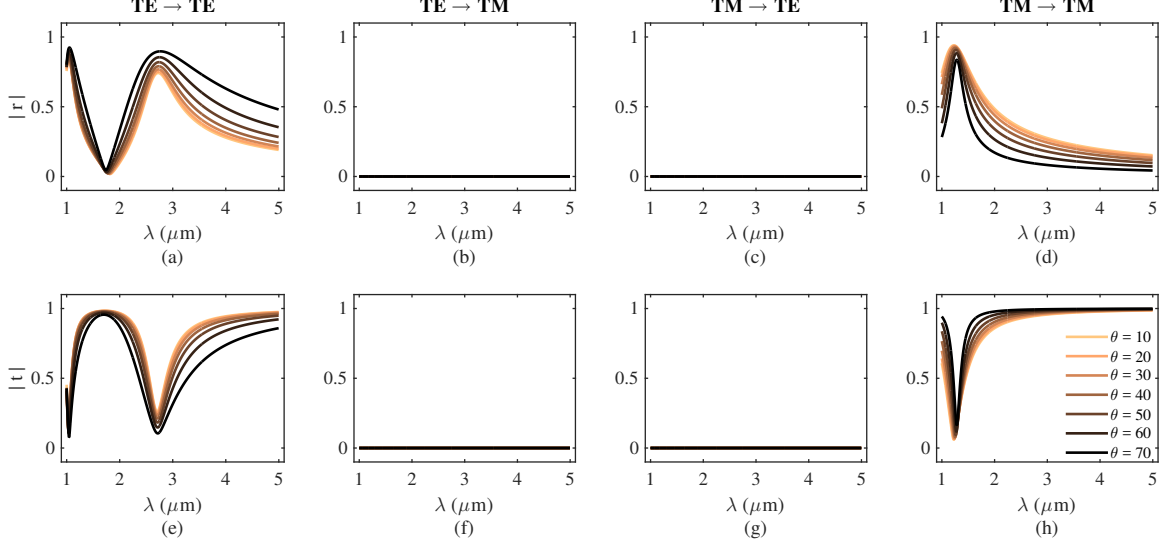


Figure 41. SRR geometry from [30] in free space with $\phi = 90^\circ$ and a θ sweep from 10° – 70° . Note that only the TE co-pol cases, (a) and (e), show the resonance. This is when $\vec{E}$ is aligned with the capacitive gap of the SRR.

E_x was large enough to drive a response. This effect is indeed observed in Figures 40a and e. When decomposing the relative magnitude of the H_z component when $\phi = 0$, as in Figure 40, $\sin(10^\circ) \approx 0.17$ while $\sin(70^\circ) \approx 0.94$. The implication is that at $\theta = 70^\circ$, the magnetic field is driving a response measured in the electric field, indicating coupling of the fields. This shows that at higher incident angles, the SRRs are indeed observably bi-anisotropic. However, when $\theta = 10^\circ$, the magnetic response is not readily observed.

Although the existence of this resonance is somewhat intuitive when considering the relative components of the fields, it is somewhat contrary to what was reported by Linden who reports that little difference was observed when taking measurements between $\theta = 10^\circ$ and 40° [30]. The evidence would indicate that the ϕ angle must have been 90° as shown by Figure 41. The attributable resonances are easily described given that the fields are either fully aligned or unaligned. That is, there are no components of either field that align with the ring in the TM polarization. This also further explains the lack of any measured x-pol at this ϕ angle.

Lastly, it is observed that the resonance is located around $2.6 \mu\text{m}$. The simplified LC circuit model presented in Chapter II yields a value of $2.3 \mu\text{m}$ from Equation 23, which provides a useful approximation and is acceptable as a first principles estimate of where the resonances should occur. Also, the simplified model is independent of metal height, but it will be shown in later sections, that this further breaks the simplified model as the resonance does indeed shift based on the height of the metal.

After examining how the fields interact with the SRR, it is observed that of these θ angles, $\theta = 10^\circ$ does not seem to have observable effects of the magnetic field coupling with the electric field. Therefore, the bi-anisotropic effects should be minimized allowing for the application of PPTE. It should be noted though, given the bi-anisotropic nature presented here, that PPTE is insufficient to fully characterize the material parameters and will be incomplete without the $\bar{\zeta}$ and $\bar{\xi}$ field coupling terms. However, the current implementation of PPTE is developed based on sample rotation and is independent of θ angle [8]. The implication is that for a given θ angle, there is a specific result that may be different and not apply at other θ angles. To further test this, PPTE will be applied to these simulated results for $\theta = 10^\circ$, 40° , and 70° .

4.2.2.4 PPTE at 10° Incident Angle.

This section examines the extractions from the SRR in free space case when the incident angle, θ is 10° . Of the θ angles examined, this case showed the least amount bi-anisotropic activity and is presented as the best case for application of PPTE. It is worth mentioning that this is the most constrained case – bi-anisotropy is minimized and simulated without a substrate layer.

As previously stated, PPTE requires two orthogonal ϕ angle experiments with corresponding backside experiments, making the total simulations required four. How-

ever, a ϕ sweep accross 0° to 360° was simulated in order to determine how well PPTE can predict the scattered fields from the extracted permittivities and permeabilities at various different sample rotations (ϕ angles).

Figures 42 and 43 show the extracted permittivity and permeability tensor elements from the $\theta = 10^\circ$ case. Of note, the existence of off-diagonal elements ϵ_{xy} , ϵ_{yx} , μ_{xy} , and μ_{yx} indicate significant optical activity outside of the primary axes of the sample, as well as significant x-pol response. This should be of no surprise and was observed in Figure 40. It is also interesting to note that the shapes of some of the curves seem to match those that were reported by Linden [30], though not matching in either tensor element location or the magnitude. Also, some shapes, specifically from Figure 42e ϵ_{yy} , this curve matches very closely in shape to what was reported as permeability [30], shown in Figure 68f later in this chapter. Obviously, all the resonance locations do not match, which is due the SRR not being coupled with a substrate. It will be shown later in this chapter how the resonance shifts due to the inclusion of a substrate. However, here, using Equation 22, yields a resonant frequency of 131.5 THz. As was shown in the scattering data from the previous section, this is useful as a first principles approach, but using the $2.6 \mu\text{m}$ resonant wavelength from the scattering data yields a value of 115 THz. This resonance is shown in the ϵ_{xx} and the μ_{zz} tensor elements. This result is consistent with the previous development that $\vec{E}_x$ and $\vec{H}_z$ are the components of the fields that drive the observed resonant response.

One of the principles of PPTE is the ability to invert the process and recover the fields. These recovered fields from inverting the process could be used to effectively predict what the fields would be at a different angle than what went into the extraction. Here ϕ angles of 0° and 90° went into the extraction process. To effectively

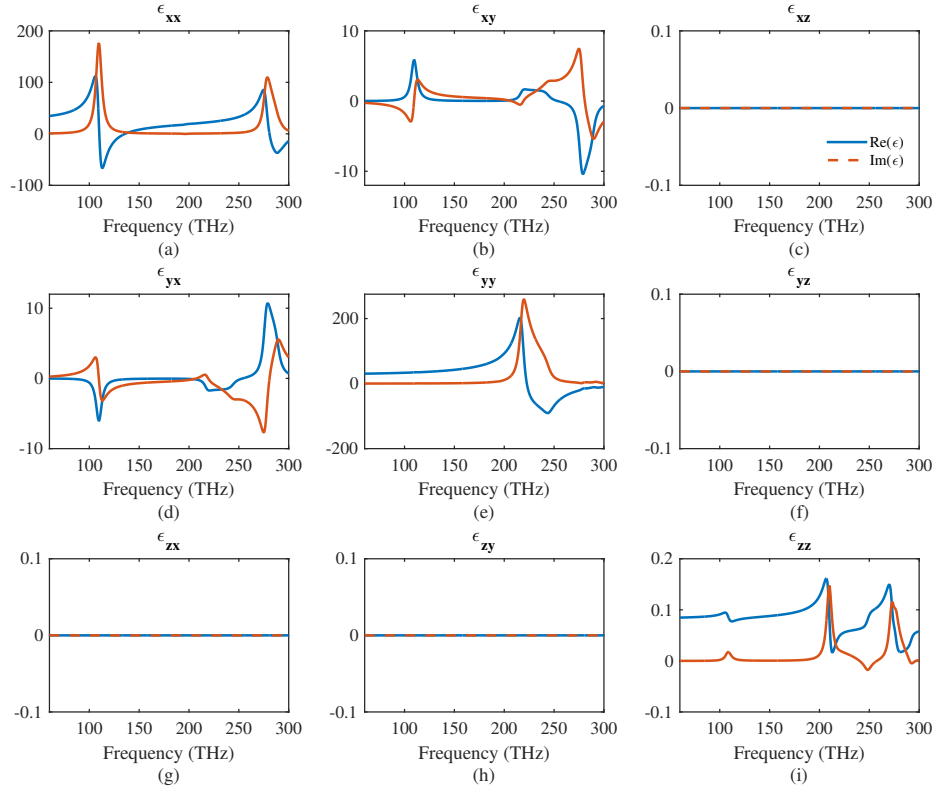


Figure 42. Extracted permittivity tensor from the literature SRR in free space when $\theta = 10^\circ$.

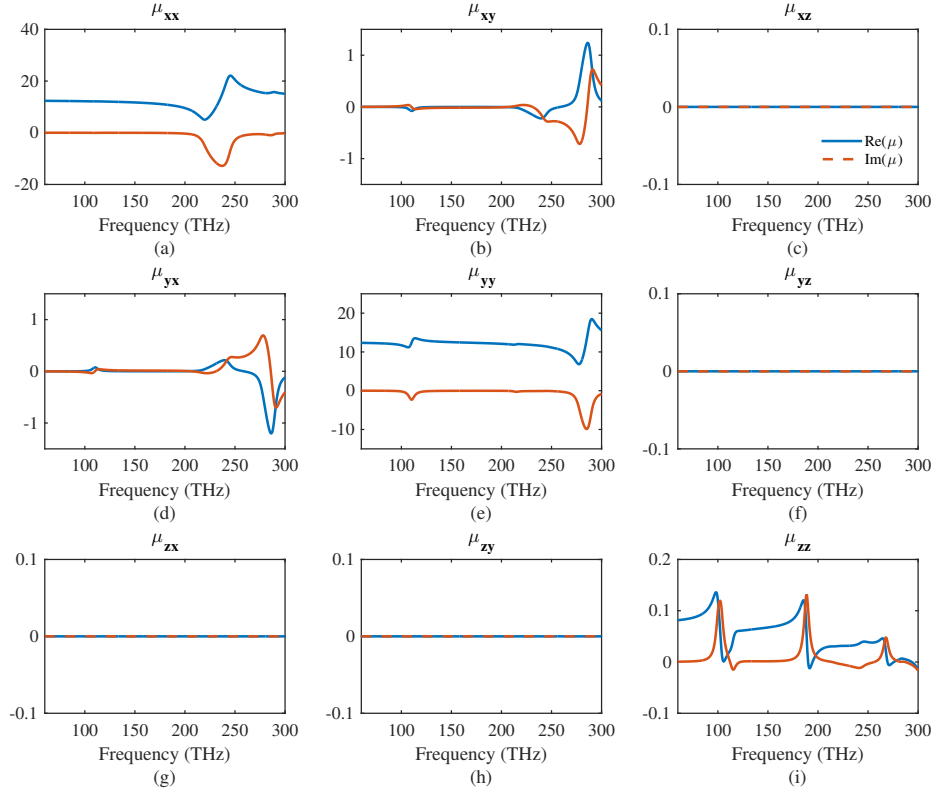


Figure 43. Extracted permeability tensor from the literature SRR in free space when $\theta = 10^\circ$.

predict what the fields would be at a different sample rotation, a rotation matrix,

$$R_z(\phi) = \begin{bmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (24)$$

is used to multiply the extracted tensors.

The results from these predictions match closely to those simulated by FLO_K. Figures 44 and 45 are two examples presented here. All other cases show similar comparisons except for the cardinal angles, $\phi = 0^\circ, 90^\circ, 180^\circ$ and 270° x-pol cases. This is due to the fields being either fully aligned or unaligned in the $\phi = 90^\circ$ and 270° , resulting zero x-pol activity, while activity exists in the $\phi = 0^\circ$ and 180° cases. PPTE seems to spread the energy from $\phi = 0^\circ$ and 90° . In this case, predictions result in half magnitude for the $\phi = 0^\circ$ and 180° , while sharing equal magnitudes with the $\phi = 90^\circ$ and 270° cases. Even in this case though, the error is still less than 1%.

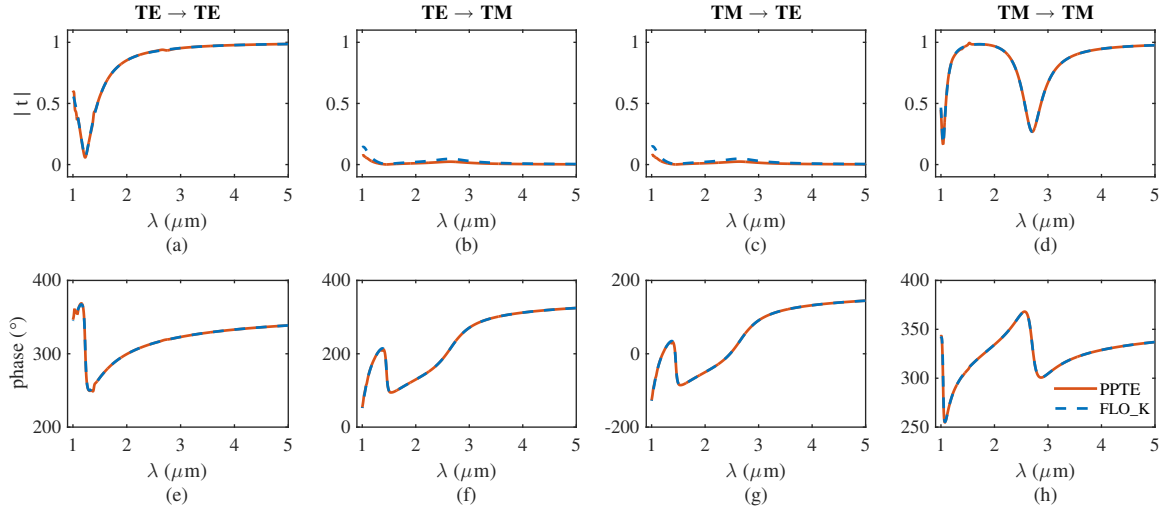


Figure 44. Literature SRR in Free Space Transmission Prediction vs FLO_K: $\phi = 0^\circ$, $\theta = 10^\circ$.

Since simulations and predictions were made over a wide set of ϕ angles, the

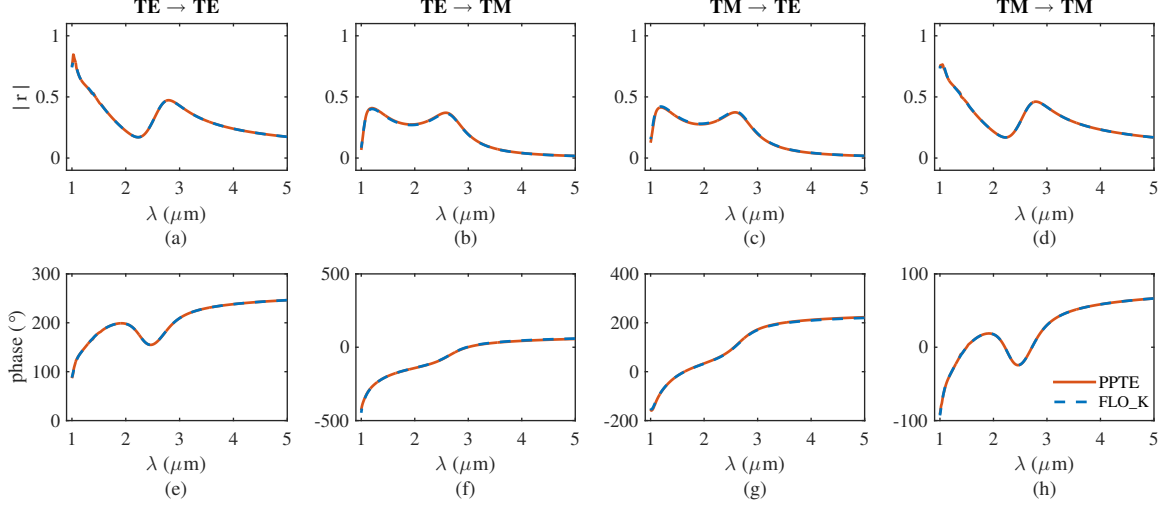


Figure 45. Literature SRR in Free Space Reflection Prediction vs FLO_K: $\phi = 45^\circ$, $\theta = 10^\circ$.

error is presented in single plots for each polarization case, seen in Figure 46. The maximum error for the co-pol cases is near 1% and occurs at the plasmonic resonance region, around $1 \mu\text{m}$ wavelength. The errors over the region surrounding the SRR resonance, around $2.6 \mu\text{m}$, are shown to be less than 0.5%, while the vast majority of the region is shown to be even lower.

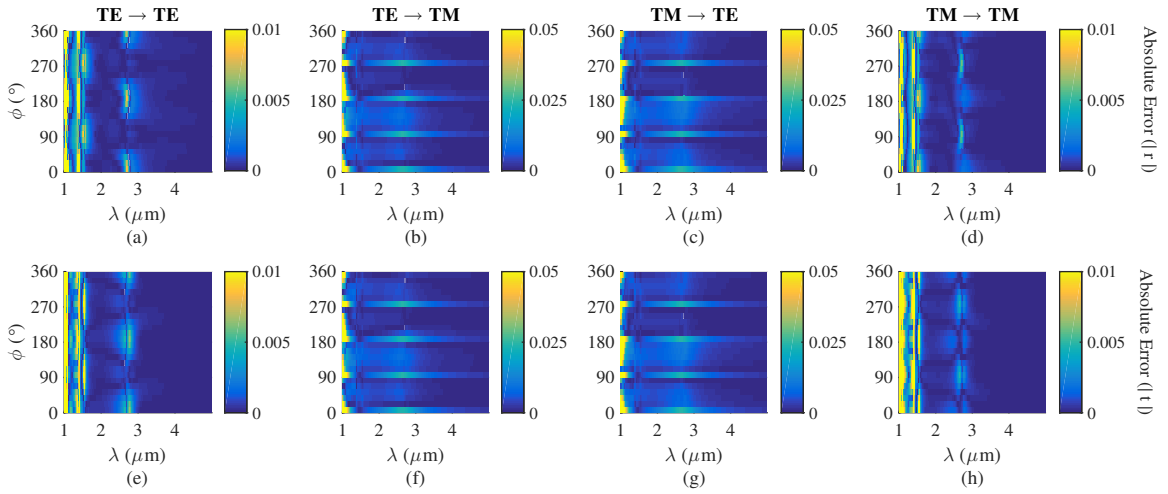


Figure 46. Literature SRR in Free Space Prediction vs FLO_K Error: $\phi = 0^\circ\text{--}360^\circ$, $\theta = 10^\circ$.

The error for the x-pol cases, depicted in Figures 46b, c, f, and g, are shown to have a slightly higher magnitude than the co-pol cases. Again, the maximum error is shown at the plasmonic resonance region, around $1 \mu\text{m}$, to be around 5%, five times higher than the co-pol cases. Also, of note, the error is shown to be higher across the entire spectral region at the cardinal angles for the x-pol cases. Again this is due to PPTE spreading the energy from the $\phi = 0^\circ$ and 180° to $\phi = 90^\circ$ and 270° . This is due to the remnant effects of the bi-anisotropy of the SRR not being completely driven to zero, but rather to only small values. Even at this shallow incident angle, there is enough of a component of either of the fields to excite the respective inductive ring and capacitive gap.

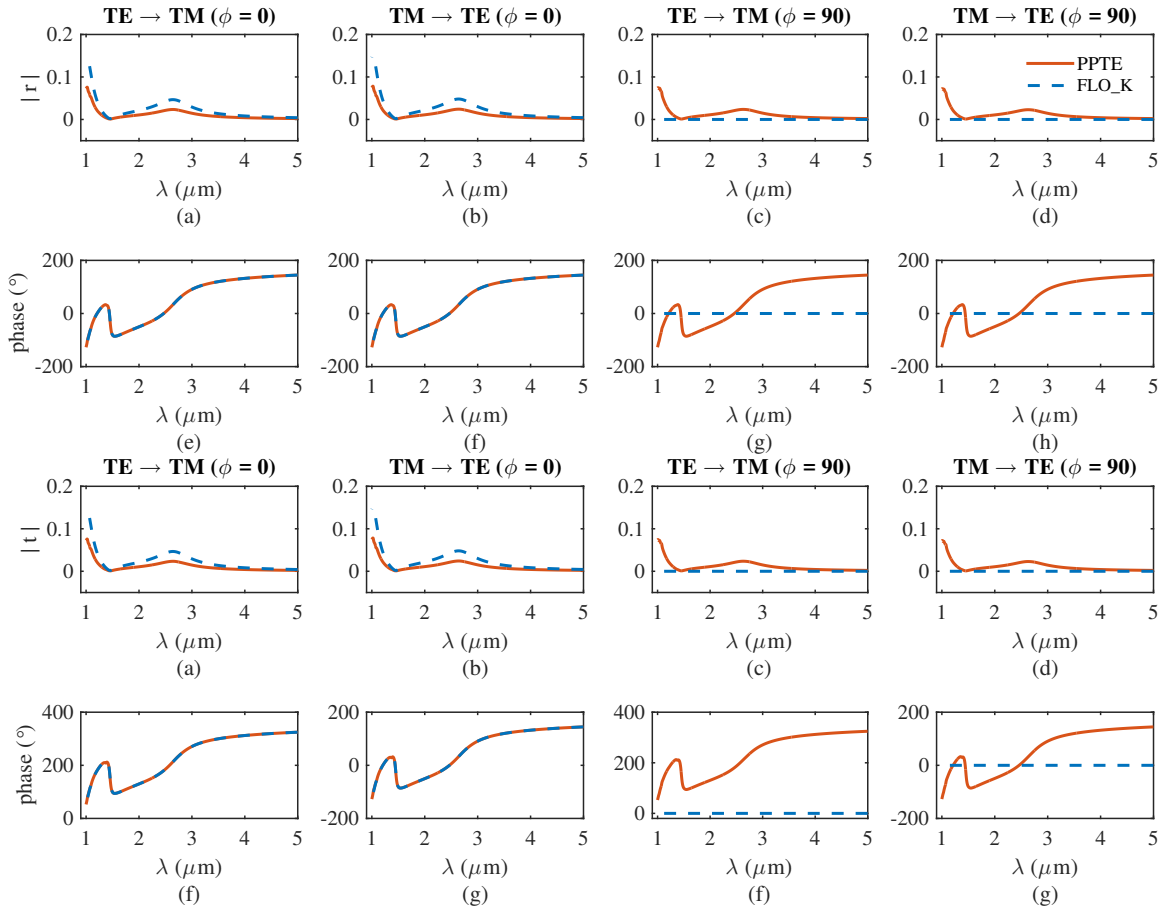


Figure 47. Literature SRR in Free Space Prediction vs FLO_K x-pol: $\phi = 0^\circ$ & 90° , $\theta = 10^\circ$.

Figure 47 shows more closely the effect of the PPTE predictions of the x-pol cases at the cardinal angles. It is interesting to note that at $\phi = 0^\circ$, while the magnitude is half that of FLO_K, the phase still matches. However, because PPTE predicts that the magnitude is shared between $\phi = 0^\circ$ and 90° , the same phases are predicted when no phase should have been. Because the magnitude is particularly small though, the error is also inherently small, but is noted as being the region with the highest error. Given that these are the only cases where PPTE did not predict as accurately as the remaining ϕ angles, and are a small subset of the overall ϕ sweep, it may be concluded that the underlying assumptions from the development of PPTE have not been violated heavily for this case.

4.2.2.5 PPTE at 40° Incident Angle.

After completing the most constrained case, $\theta = 10^\circ$ in free space, the next step is to test a case when it is expected that some of the magnetic field response will contaminate the electric field response. It may be noted, from Figure 40, that the presence of the magnetic interaction with the SRR is observable, but small. This violates the anisotropy constraint of PPTE due to the field coupling nature of the observed scattering response. Here, the fields are clearly coupled, but the effect is small and provides a good test to see how PPTE performs under these conditions.

This experiment was set up in the same way as the $\theta = 10^\circ$ case with the exception of θ . Once again, a ϕ sweep from 0° – 345° was conducted. This generates more angles than PPTE requires, and only the $\phi = 0^\circ$ and 90° cases were used to extract the permittivity and permeability tensors, but retaining the extra ϕ angles produces scattering predictions for comparison other than those where the extractions were made.

Figures 48 and 49 show the extracted permittivity and permeability tensors. The

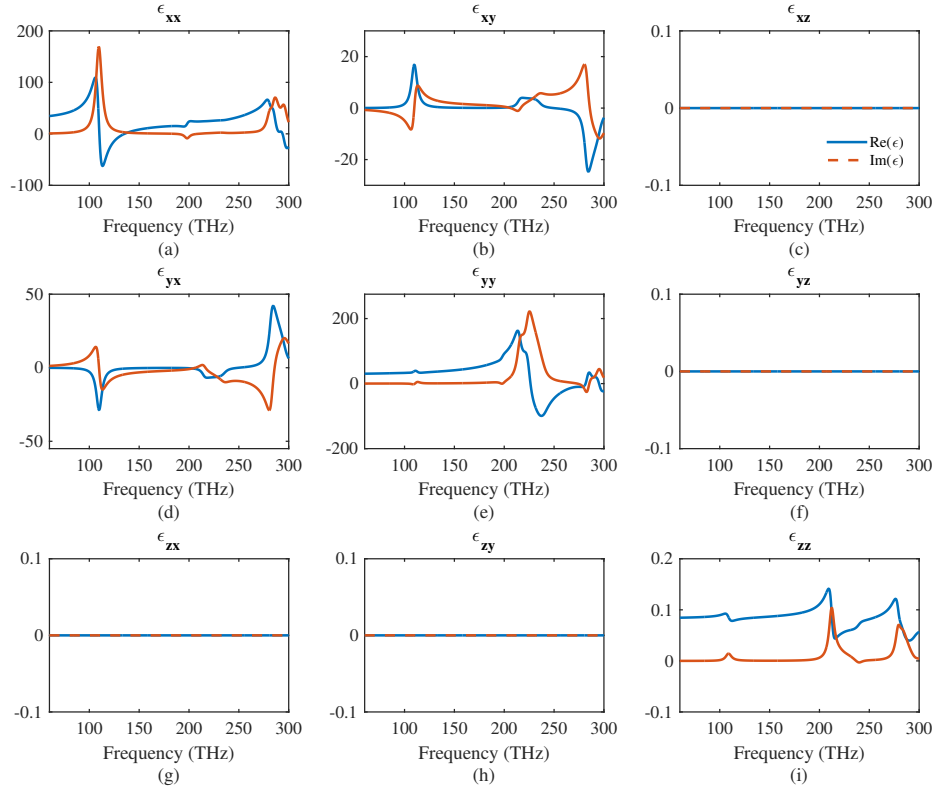


Figure 48. Extracted permittivity tensor from the literature SRR in free space when $\theta = 40^\circ$.

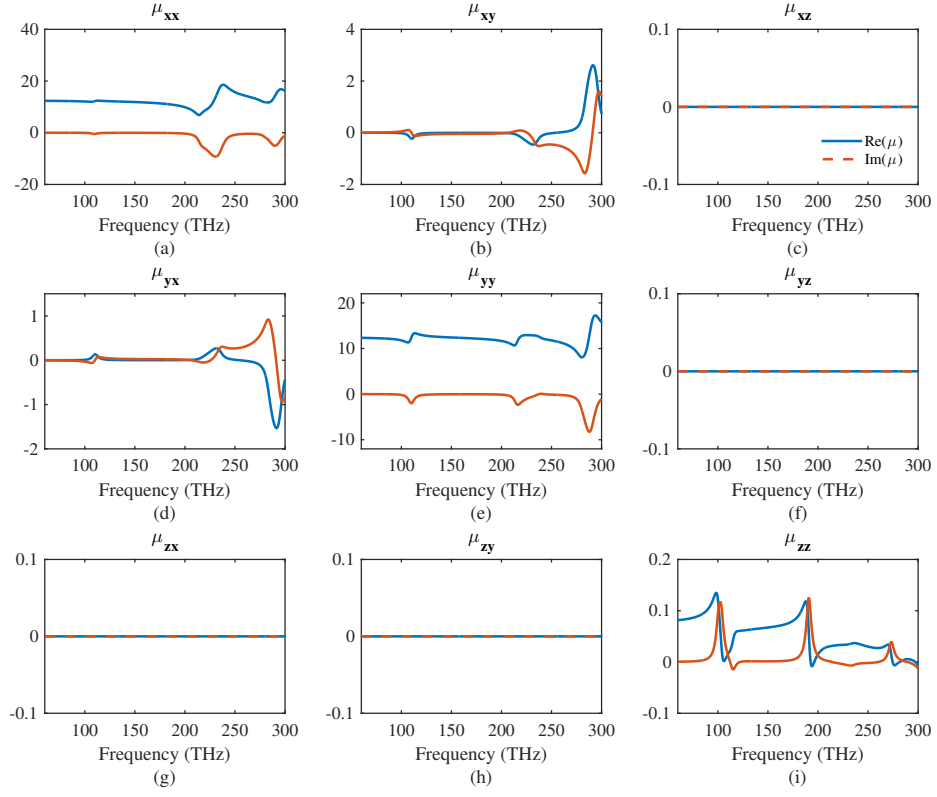


Figure 49. Extracted permeability tensor from the literature SRR in free space when $\theta = 40^\circ$.

ϵ_{xy} and ϵ_{yx} elements clearly show larger magnitudes with the ϵ_{xy} tensor element being roughly twice as large, and the ϵ_{yx} being 5 times as large as the 10° case. There are also new observable resonances in the ϵ_{xx} tensor element near 200 THz and in the ϵ_{yy} tensor element near 110 THz. These frequencies correspond to $1.5 \mu\text{m}$ and $2.7 \mu\text{m}$, the wavelengths of the plasmonic and SRR resonances. It is also noted that the resonance shape in the ϵ_{yy} element has changed slightly.

Notable differences in the permeability tensor are seen in the μ_{xy} element, where again, the magnitude has nearly doubled. A new small resonance, similar to that observed in ϵ_{xx} , is also observed in the μ_{xx} element. There is new, larger resonance occurring around 290 THz of this element as well. This corresponds to near $1 \mu\text{m}$ and is due to the plasmonic resonance.

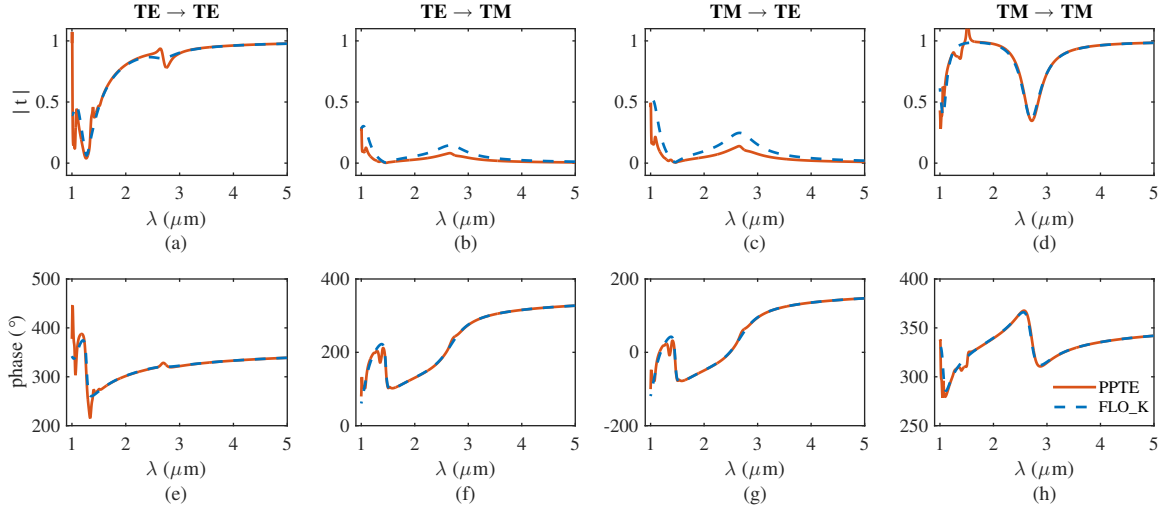


Figure 50. Literature SRR in Free Space Transmission Prediction vs FLO_K: $\phi = 0^\circ$, $\theta = 40^\circ$.

PPTE was also utilized to make predictions of the scattered fields at rotations other than those where the extractions took place to compare to the scattered fields that FLO_K computed. Cases of $\phi = 0^\circ$ transmission and $\phi = 45^\circ$ reflection were chosen as examples. As with the $\theta = 10^\circ$ case, these results are representative of the other angles. The predictions are still relatively good approximations, though

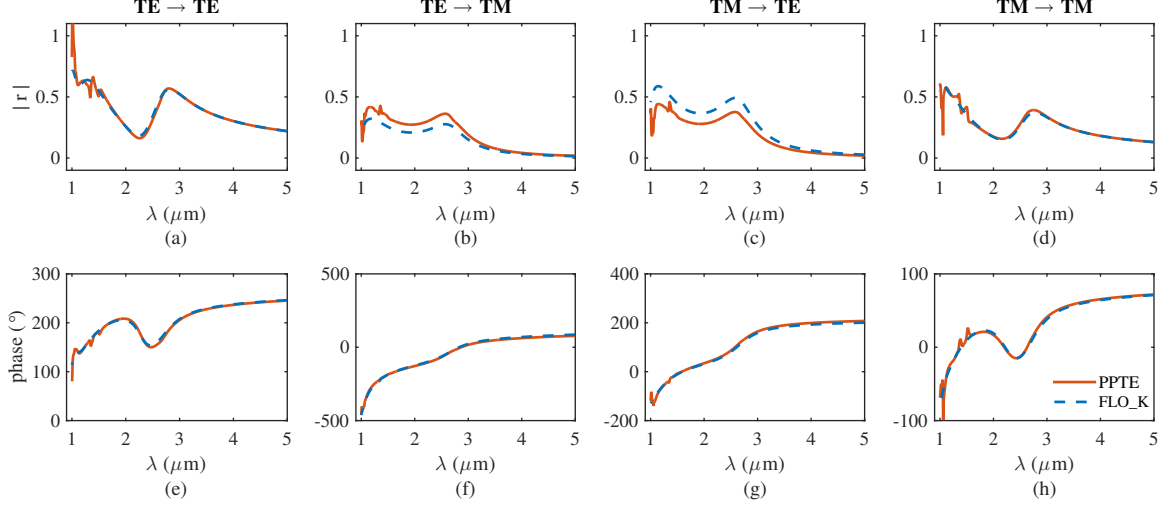


Figure 51. Literature SRR in Free Space Reflection Prediction vs FLO_K: $\phi = 45^\circ$, $\theta = 40^\circ$.

there are additional resonances observed, particularly within the plasmonic resonance region between 1–2 μm . It could be argued that the material is not homogenized within this region, implying that Maxwell's Equations would break down. This is because unit cell period is 450 nm and this plasmonic region is near 1 μm , just over two times the period. The wavelength is not sufficiently large, as compared to the period, and cannot be represented macroscopically to approximate the material in effective parameters. Also of note, where the magnetic field excited the resonance at $\phi = 0^\circ$, the resonance has been exaggerated. This effect is not observed when the ϕ angles are off the cardinal angles, shown in Figure 51. Another effect is observed in the x-pol cases (b), (c). At this θ angle, the relative magnitude of H_z in the TM reflected wave is larger than when $\theta = 10^\circ$ due to the higher incident angle. This results in a larger magnetic dipole being created that realigns the fields to this polarization. The magnitudes for the differing x-pol cases are no longer equal as they were in the $\theta = 10^\circ$ case. PPTE, however, still spreads the energy evenly between the two, causing both x-pol cases to be erroneous. This is due to PPTE assuming the material does not contain the coupling parameters, $\bar{\zeta}$ and $\bar{\xi}$, causing PPTE to incorrectly associate

whatever these values are to the permittivity and permeability tensors.

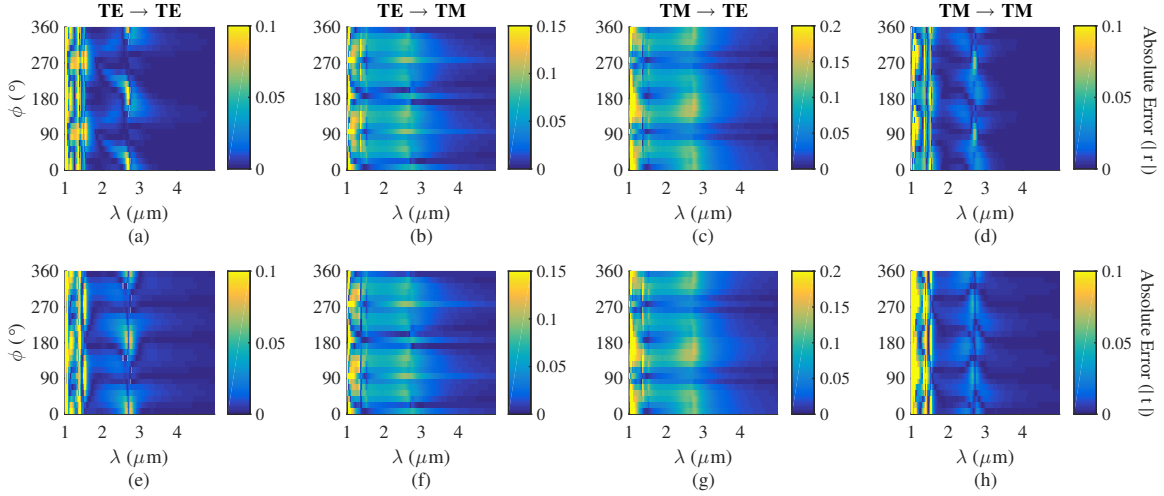


Figure 52. Literature SRR in Free Space Prediction vs FLO_K Error: $\phi = 0^\circ\text{--}360^\circ$, $\theta = 40^\circ$.

The magnitude errors were calculated for all ϕ angles and are presented collectively. While at first glance, Figure 52 may look very similar to Figure 46, the $\theta = 10^\circ$ errors, it should be noted that the scale is an order of magnitude higher. The maximum errors for the co-pol cases are approximately 10% and are greatest at the plasmonic region for all aspect angles. It should also be noted that the error at the SRR resonance, specifically for the TE incident to TE exiting case, are of the same magnitude as the errors for the plasmonic region. This was not observed for the $\theta = 10^\circ$ case. The x-pol cases have equivalent errors across the different aspect angles, where as for the $\theta = 10^\circ$ case, it was isolated at the cardinal angles. It should be noted that these errors give an indication into how much of the underlying assumptions of PPTE are broken.

4.2.2.6 PPTE at 70° Incident Angle.

The third and final free space, in-plane SRR case to be explored is when $\theta = 70^\circ$. The scattering from this case clearly shows strong coupling of the magnetic field into

the measured electrical field. The permittivity and permeability tensors show similar differences to 40° as 40° had to 10° , shown in Figures 53 and 54. Notably, the ϵ_{xy} tensor element is of similar magnitude and shape as for the 40° case, while the ϵ_{yx} element doubled the 40° case just as the 40° case did when compared to the 10° . Also, the resonance observed near 200 THz in the $40^\circ \epsilon_{xx}$ element is more prevalent in the $70^\circ \epsilon_{xx}$ element. Another key observation is in the ϵ_{zz} element, where the shapes of the resonances seem to have been compressed in magnitude. A small compression is observed in the $40^\circ \epsilon_{zz}$ element, but is not as apparent as in 70° . This is likely where including a field coupling term would more accurately represent the material.

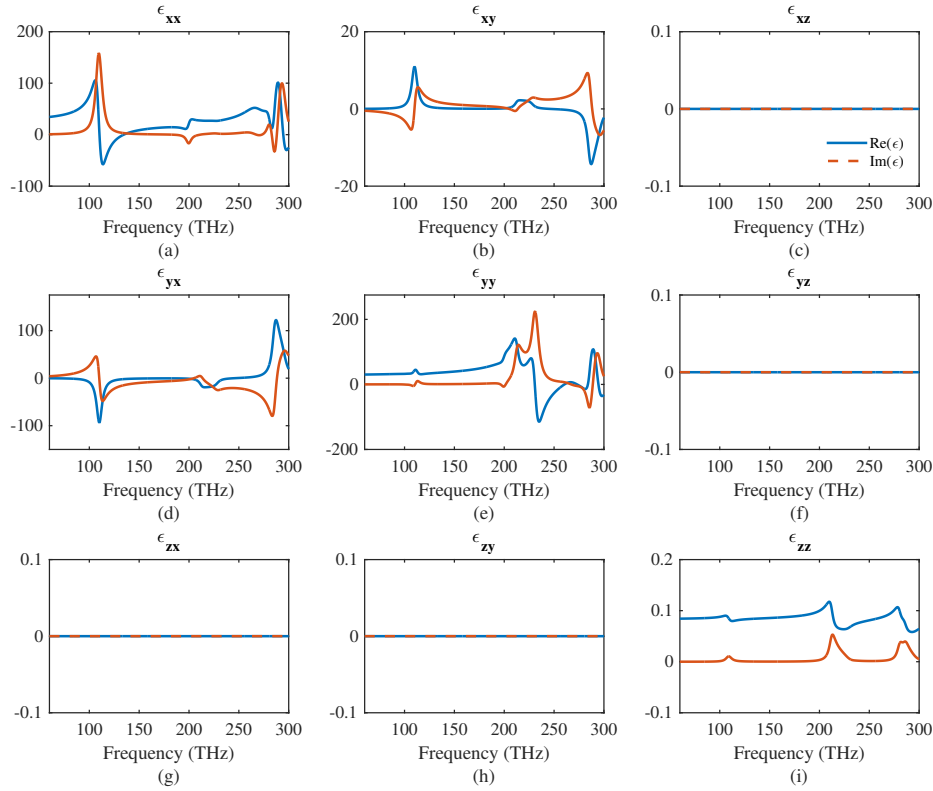


Figure 53. Extracted permittivity tensor from the literature SRR in free space when $\theta = 70^\circ$.

The observable differences in the μ_{xx} element are similar to what was previously observed between the 40° and $10^\circ \mu_{xx}$ elements, but exaggerated. The magnitudes of

the off-diagonal terms are significantly smaller, particularly in the μ_{yx} element than what was observed for the 40° and 10° cases.

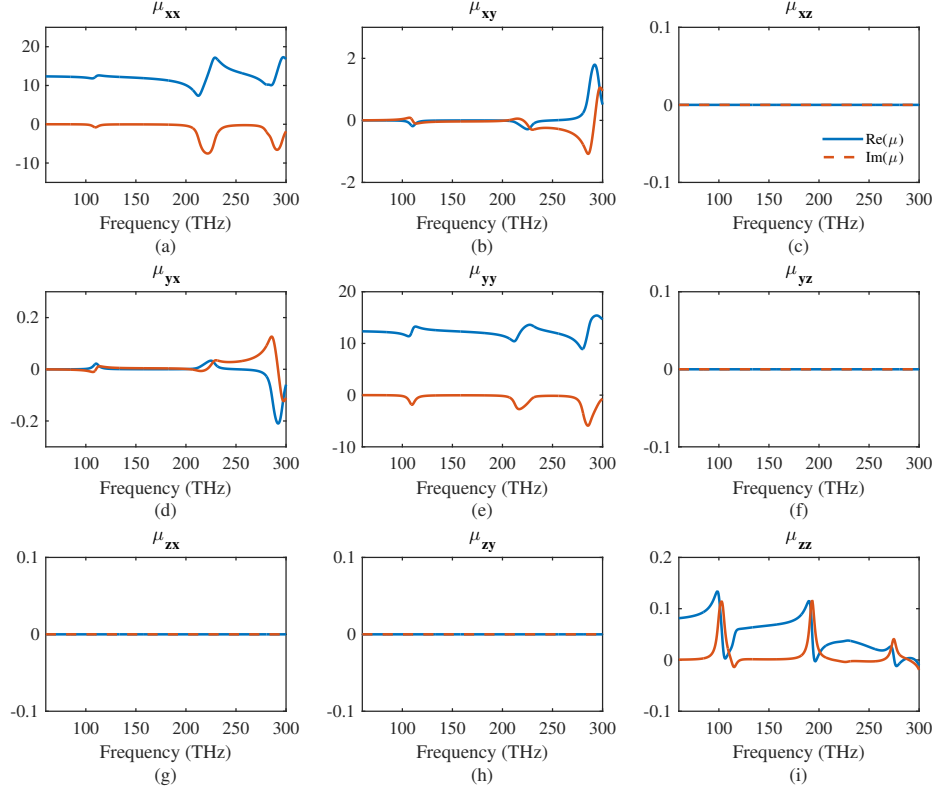


Figure 54. Extracted permeability tensor from the literature SRR in free space when $\theta = 70^\circ$.

As with the previous two cases, predictions were made for all ϕ angles simulated in order to gain an insight into how much of the underlying PPTE assumptions were broken. Noted here, the same errors associated with the 40° case are evident, but more prevalent. Figure 56 in particular shows that with the larger magnetic field component in the TM incident to TE reflecting case shown in (c), the curve predicted by PPTE does not match the curve computed with FLO_K. A similar occurrence was observed for the 40° case, but is exaggerated further due to the larger field component aligning with the inductive ring. It is interesting to note that at 0° , the worst case for $\theta = 10^\circ$ for the x-pol cases, the x-pol seems to correctly predict larger TM incident

TE exiting, but is still erroneous.

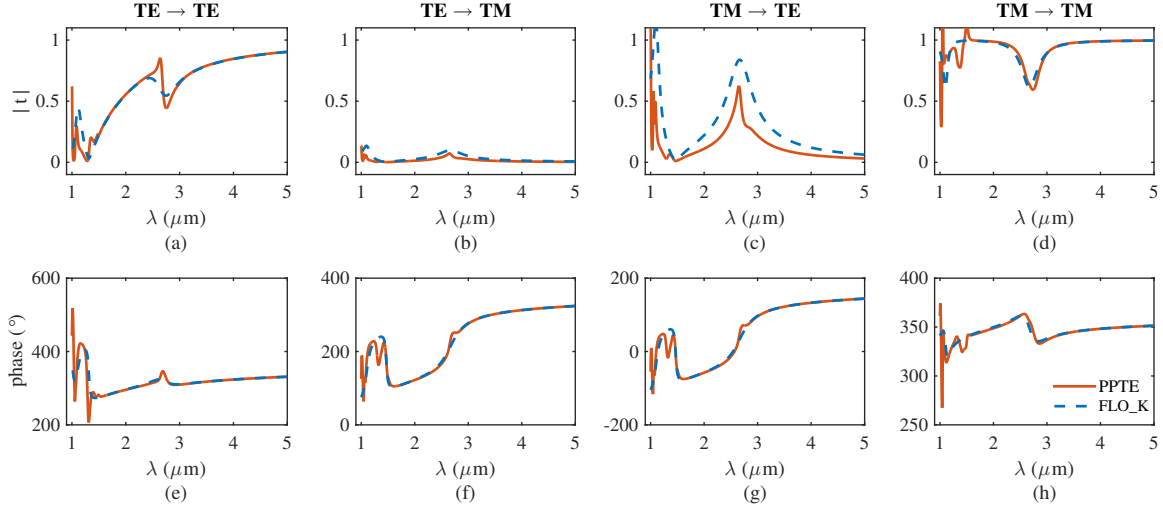


Figure 55. Literature SRR in Free Space Transmission Prediction vs FLO_K: $\phi = 0^\circ$, $\theta = 70^\circ$.

The errors associated with the predictions as compared to FLO_K are provided collectively, shown in Figure 57. As with the 40° case, it is important to note the scale on the colorbar. Although the associated errors for the co-pol cases are only slightly higher than at 40° , the x-pol, particularly TM incident TE exiting polarization, is significantly higher. It shows a maximum error of 100%, and is no longer isolated to the plasmonic resonance region.

The errors reported for the 40° and 70° incident angles clearly indicate that the assumptions of anisotropic media are clearly violated. The 10° incident angle showed the lowest error, implying that at this angle, the material is mostly anisotropic, that is $\bar{\zeta}$ and $\bar{\xi}$ are small. This is similar to the scattering reported by Linden at 10° [30]. For this reason, the scattering and extractions for the SRR on SiO_2 substrate will only consider 10° incident angle.

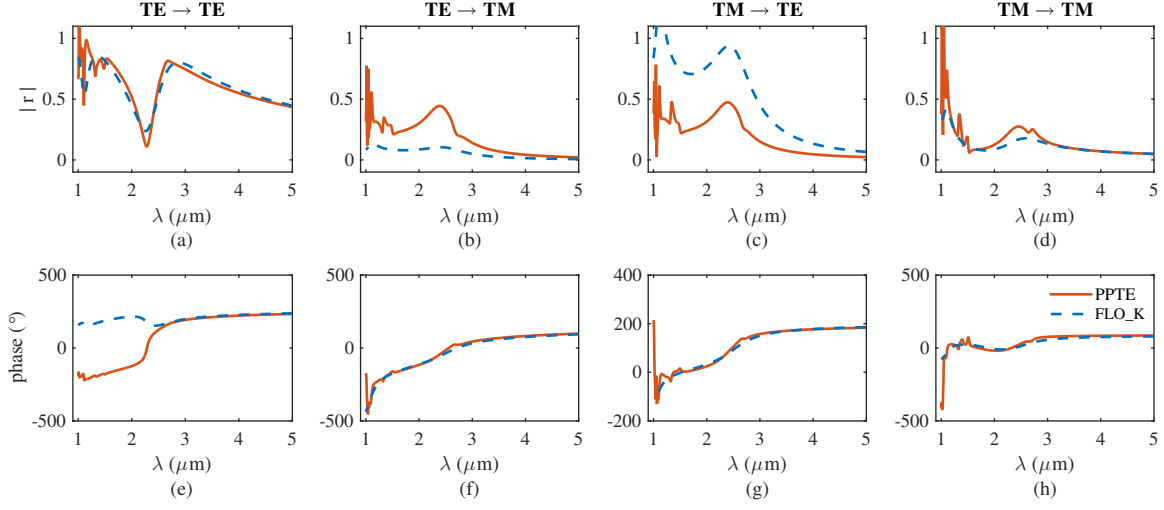


Figure 56. Literature SRR in Free Space Reflection Prediction vs FLO_K: $\phi = 45^\circ$, $\theta = 70^\circ$.

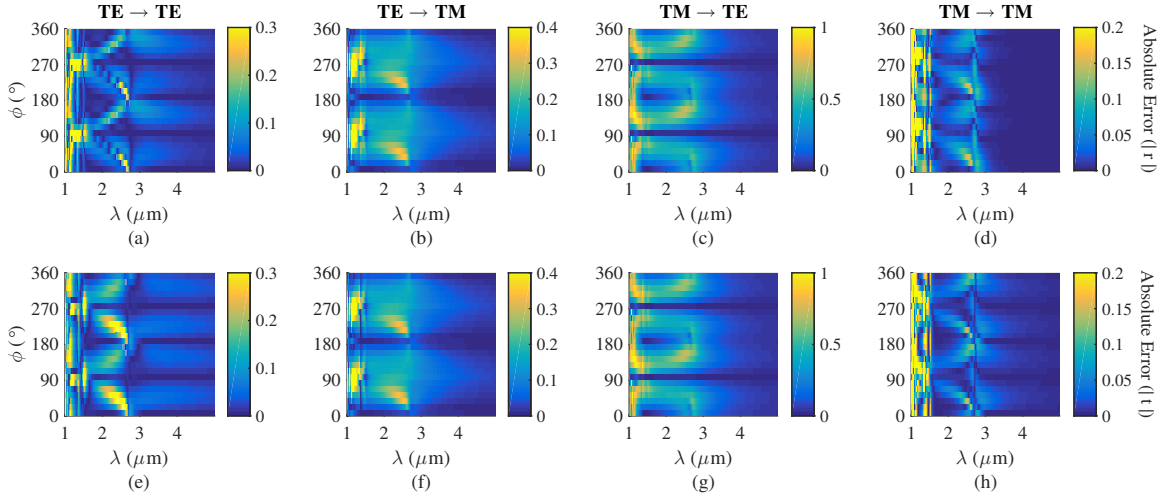


Figure 57. Literature SRR in Free Space Prediction vs FLO_K Error: $\phi = 0^\circ-360^\circ$, $\theta = 70^\circ$.

4.2.2.7 SRR on SiO₂ Substrate.

Now that an adequate baseline of behavior has been developed for the SRR in free space, the effects of including a substrate are considered. It is known that capacitance is not just a function of the geometry, but also a function of the dielectric material that is placed between the plates, [39]. Here, the gap of the split ring behaves as a capacitor and while it is obvious that a dielectric material is not between the plates of the capacitor, the substrate acts in a similar manner. This is due in part to the fields existing not only between the plates, but also curve from the cathode to the anode [39]. Figure 58 illustrates this effect. While the substrate is not within the gap, the fields are not entirely in free space either. The implication is that the dielectric substrate does indeed alter the fields, thereby changing the capacitance. The simplified LC circuit model used to describe where the resonance occurs should appropriately predict this resonance if the capacitance can be determined. However, the problem exists that it is not known how deeply the fields between the plates penetrate the substrate and therefore, no closed form solution exists. New models have been developed in literature that can more accurately predict the resonance location [15,39]. In this work, an iterative simulation approach was used.

4.2.2.8 SiO₂ Depth.

In a FEM solver, it is impossible to use the full substrate depth. The SiO₂ substrate layer depth was reported as 1 mm, while the SRR geometry has a unit cell period of 450 nm [30]. The majority of the glass has little effect on the overall scattering, which should be dominated by the SRR response, only altered by being coupled with the glass. In order to determine the necessary depth, and in effect the active near field boundary, multiple depths of glass were simulated. One potential issue with this approach is Fabry-Pérot, or quarter-wave and half-wave resonances,

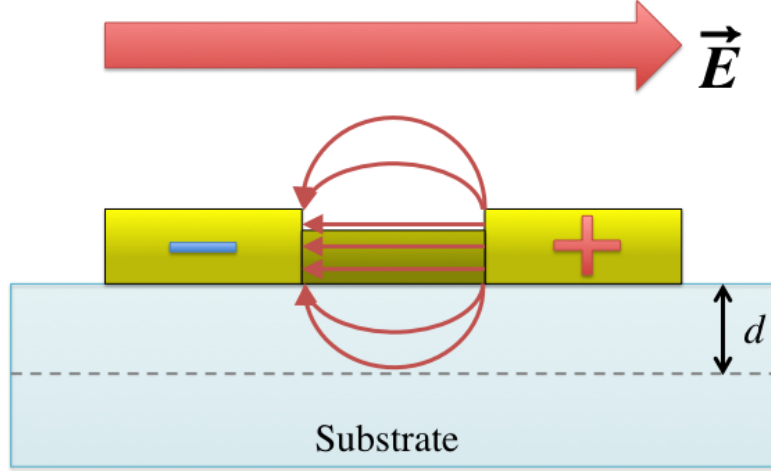


Figure 58. Electric field, $\vec{E}$, penetrates into the substrate which increases the capacitance of the SRR gap. This has the effect of shifting the resonance.

which could potentially be generated by the reflection from the bottom of the glass interfering constructively or destructively with the overall reflection and transmission. It is expected that the capacitive near field will not heavily intersect the region where Fabry-Pérot resonances occur, so that these resonances do not contaminate the scattering. If this is the case, then a comparison between the scattering from the model and what was reported in literature will provide a qualitative measure of how closely the models match.

For this experiment, simulations were executed with varying depths of glass, from 20 nm to 2 μm . Figure 59 shows the results of these simulations with red arrows indicating the orientation of $\vec{E}$ with respect to the capacitive gap. This figure, and those that follow that compare reported values from literature, report the reflection and transmission as scattered intensity, or reflectance and transmittance, denoted by $|R|$ and $|T|$. This allows for direct comparison of the values from literature. As predicted, the resonance does indeed move to the right as the depth increases. That is, including more substrate increased the capacitance which shifted the resonance. Also note that by 100 nm, the resonance does not seem to shift any further, implying

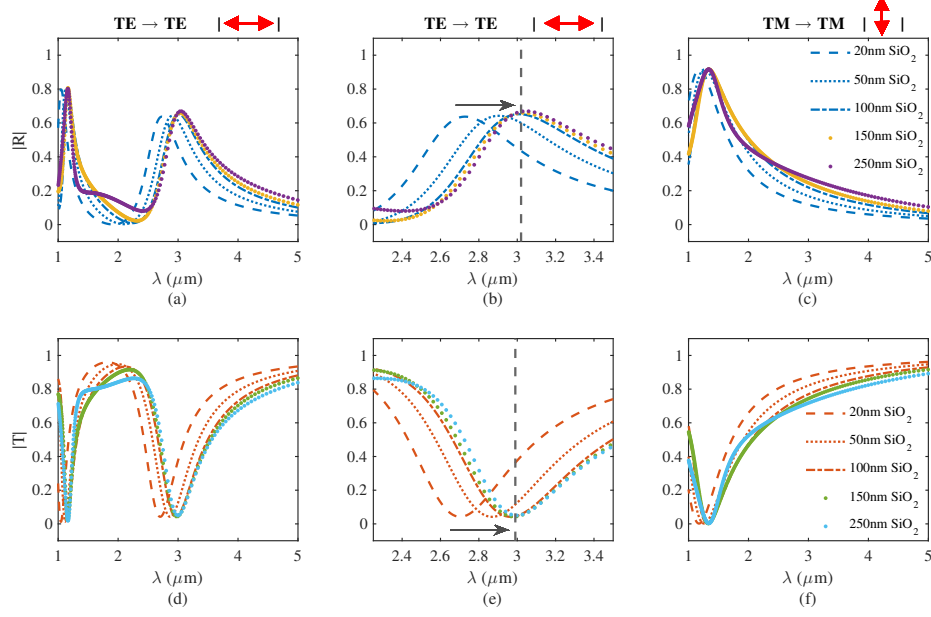


Figure 59. SRR Glass Depth Convergence, $\phi = 90^\circ$, $\theta = 10^\circ$. (b) and (c) show a zoomed in look at the resonance shift. Note that the resonance converges around $3 \mu\text{m}$ at 100 nm SiO_2 depth. Reflection curves in blue and transmission curves in red show no signs of Fabry-Pérot resonances. Red arrows indicate the $\vec{E}$ orientation to the capacitive plates (gap), depicted by black vertical bars.

that field penetration from the capacitive gap is no longer measurable at glass depths beyond 100 nm . Also note the existence of additional resonances between $1.5\text{--}2.5 \mu\text{m}$ on the 150 nm and 250 nm glass depth curves indicating that reflections from the back interface are contaminating the results. All simulations above $250 \mu\text{m}$ had no observable effect on the capacitive resonance but did show increasingly more of this Fabry-Pérot effect across the spectral region, contaminating the scattering. As such, they are not presented here.

Now that the certainty of the substrate requirement has been determined, a comparison of the reported scattering is made, shown in Figure 60. Note that even though the resonance from the simulations stopped around $3 \mu\text{m}$, shown in Figures 59b and c, this did not match the reported simulated nor measured results precisely. Ultimately, it is desired to match either the reported simulation or measured scattering in order

to compare the PPTE extractions to those reported.

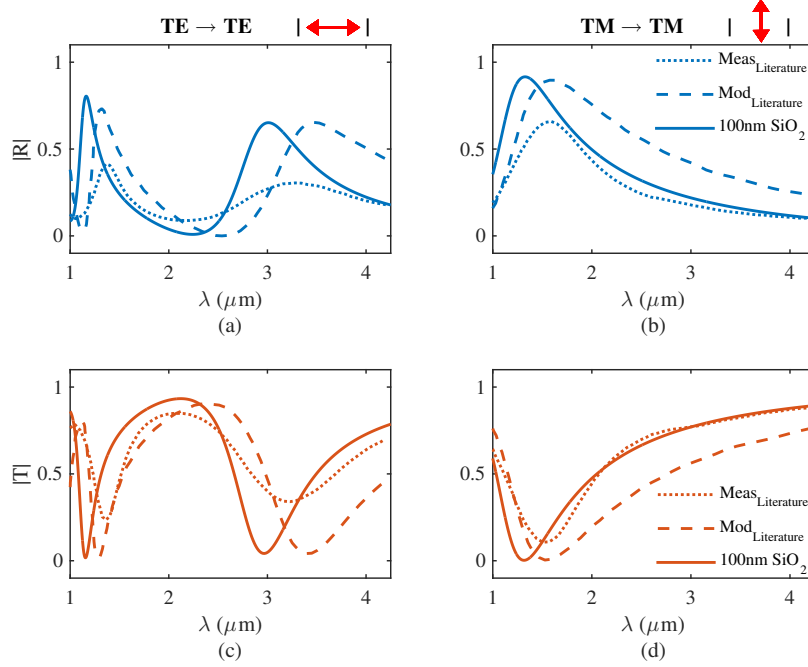


Figure 60. SRR Glass Depth 100 nm Compared to Literature Measured and Simulated Results. Note that the resonance from 100 nm SiO_2 is not aligned with reported values from Literature. Red arrows indicate the $\vec{E}$ orientation to the capacitive plates (gap), depicted by black vertical bars.

Three options were explored in an attempt to shift the resonance to the right: inclusion of the ITO wetting layer, using a higher index glass, and varying the height of the metal for the SRRs. While the previous glass simulations assume that the primary scattering mechanisms are controlled by the SRR and the glass substrate, some simulations were run with the ITO wetting layer to verify this. Although a small resonance shift was observed, it was very small, indicating that ITO is not one of the primary scattering mechanisms as the previous models assumed. Also, this layer displayed Fabry-Pérot resonances. This is due to the model making the layer of uniform thickness, when in actuality, the layer is far from uniform, especially at the 5 nm reported. However, it was also observed that the more lossy ITO extinction coefficient did cause the magnitudes to be much closer to those that were

measured. Nonetheless, the highly observable Fabry-Pérot resonances contaminating the scattering led to the exclusion of this layer from the model. To test the higher glass index approach, simulations were run with material parameters which were 1.2 times the original. Although, this did indeed push the resonance to the right, the literature reports that a “standard glass substrate” was used [31], so this approach was also abandoned. The last approach, varying the metal height did show promise. Although the simplified LC circuit model is independent of height, it will be shown in the following section that this is not the case in more rigorous or complete models.

4.2.2.9 Au Height Variance.

The metal height was reported to be and designed at 20 nm. While this is a very small metal deposition layer at 20 nm, it is within the realm of possibility that the metallic deposits might be varied slightly from the nominal 20-nm design. To test the effect of the varied metal height, several simulations were conducted varying the height of the deposited SRR from 13–30 nm. It was observed that metallic deposition greater than the previously simulated 20 nm had the effect of shifting the resonance to the left, the wrong direction. However, when the metallic height was between 13–15 nm, the resonances were observed to more closely match what was reported, shown in Figure 61. Figure 61 shows the results from FLO_K. Figure 61b and c zoom in closer to highlight the differences in scattering due to the metal height variance. The reported measured values are somewhat shifted from the reported modeled values from literature. It is observed that the metallic height of 15 nm more closely matches the measured results that were reported, while the metallic height of 13 nm matches more closely to the modeled values reported. With this in mind, the metallic height of 14 nm, which splits the difference, was chosen. Figure 62 clearly shows that when the results of the 14 nm metallic height are compared to both the

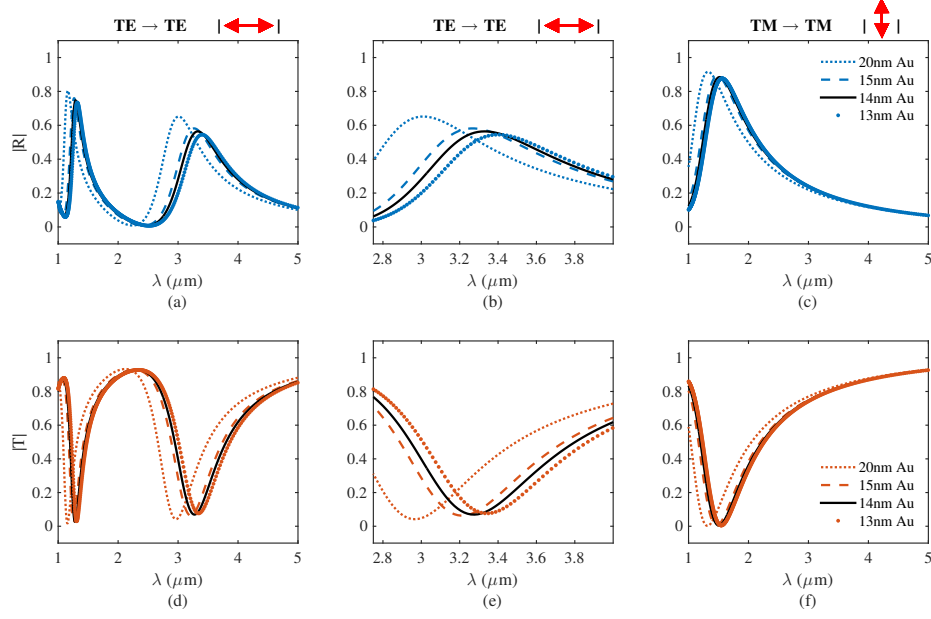


Figure 61. Au Height Variance Resonance Shift. Note that as the metal height decreases, the resonance shifts to the right, matching more closely the resonance that was reported in Literature. Red arrows indicate the $\vec{E}$ orientation to the capacitive plates (gap), depicted by black vertical bars.

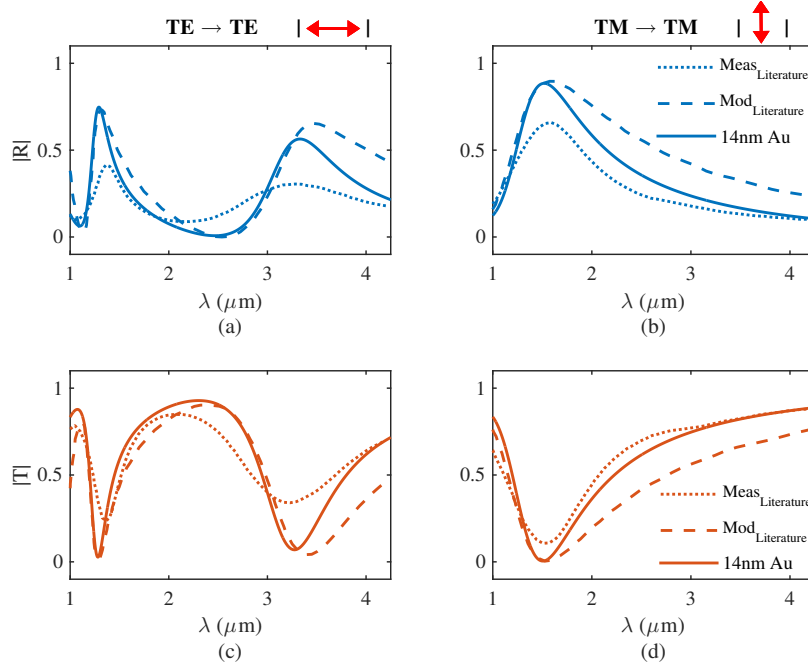


Figure 62. 14 nm Au Compared to Literature Measured and Simulated Results. Note that the resonance from the 14 nm Au curves lies between the reported values for measured and simulated that were reported in literature. Red arrows indicate the $\vec{E}$ orientation to the capacitive plates (gap), depicted by black vertical bars.

modeled and measured values, both the resonance and the amplitude seem to split the difference, implying that this is an ideal model with the given set of layers and material parameters. Indeed, this model matches even closer to the measured values than the simulated results presented by Linden [30]. The next step is to simulate over the same ϕ sweeps presented in the free space examples in order to utilize PPTE to extract the permittivity and permeability tensors.

4.2.2.10 SRR on SiO₂ PPTE.

Given that the reported permeabilities and permittivities were reported from 60-120 THz to show the effect over the SRR resonance, the following extraction was also made over the same range for comparison. As such, full extractions over the entire simulated spectral range are not included. Of note, higher errors were observed over the range not reported, specifically in the plasmonic resonance region.

Included within Benson's development of PPTE is the ability extract permittivity and permeability tensors from different layers, [7,8]. Although it was fully developed conceptually, it was never implemented within the code. This section employs this technique to isolate just the SRR layer from the SiO₂ layer in order to more specifically evaluate the SRR layer. Intuitively, it would be similar to what has been shown, except for resonances shifted as was observed in the scattering. However, this was not what was observed.

The development of PPTE includes T matrices for each layer. These T matrices represent a transfer matrix which is not at all unlike transfer functions that are used to describe linear systems. That is, there is some input to the system, the system does something to the input resulting in observable changes in the output. In this case, the material is the system, the input is the incident fields and the output is either the reflected or transmitted fields. The overall system T matrix is the matrix

product of all the layers of the material, e.g. $T_{system} = T_1 T_2 T_3 \dots T_n$ with T_1 being the top-most layer and T_n being the bottom-most layer. In this work, the system consists of only two layers, the SRR and an SiO_2 layer. In order to isolate the T_{SRR} layer, the T_{glass} layer must first be found. Simulations with the given material parameters and geometry of this layer were computed with FLO_K and then PPTE applied to determine the T_{glass} layer. After the T_{glass} layer is found, the T_{SRR} can easily be found by

$$T_{system} = T_{SRR} T_{Glass} \implies T_{SRR} = T_{system} T_{Glass}^{-1}.$$

Figures 63 and 64 show the extracted values from 60–120 THz. The most obvious difference observed is that in the previous examples, all the tensor elements in locations zx , zy , xz , and yx were zero while those presented here are clearly non-zero. The effect of coupling the glass layer to the SRR does not intuitively describe this as the glass is isotropic. All elements are also noted to have differing shapes as what was shown in the previous examples.

As before, the process was inverted to recover the scattered fields based on the extracted permittivity and permeability tensors, and to predict the fields at different sample rotations. Figures 65 and 66 are two examples of these predictions when compared to what was simulated with FLO_K. It is noted that the predictions match relatively well, especially in the non-cardinal angles. It is also observed that generally the errors are higher in reflection than what is observed for transmission.

The errors reported in Figure 67 are not quite as low as the 10° free space simulation for reflection, but are still remarkably low in the transmission and x-pol cases. The maximum error in the co-pol reflection cases was 10%, with an average shown to be much less than 5%. The x-pol reflection is the next highest with a maximum error of 4% and an average well below 2%. As with the free space 10° case, higher errors are shown at the cardinal angles in the x-pol for both reflection and transmission. The

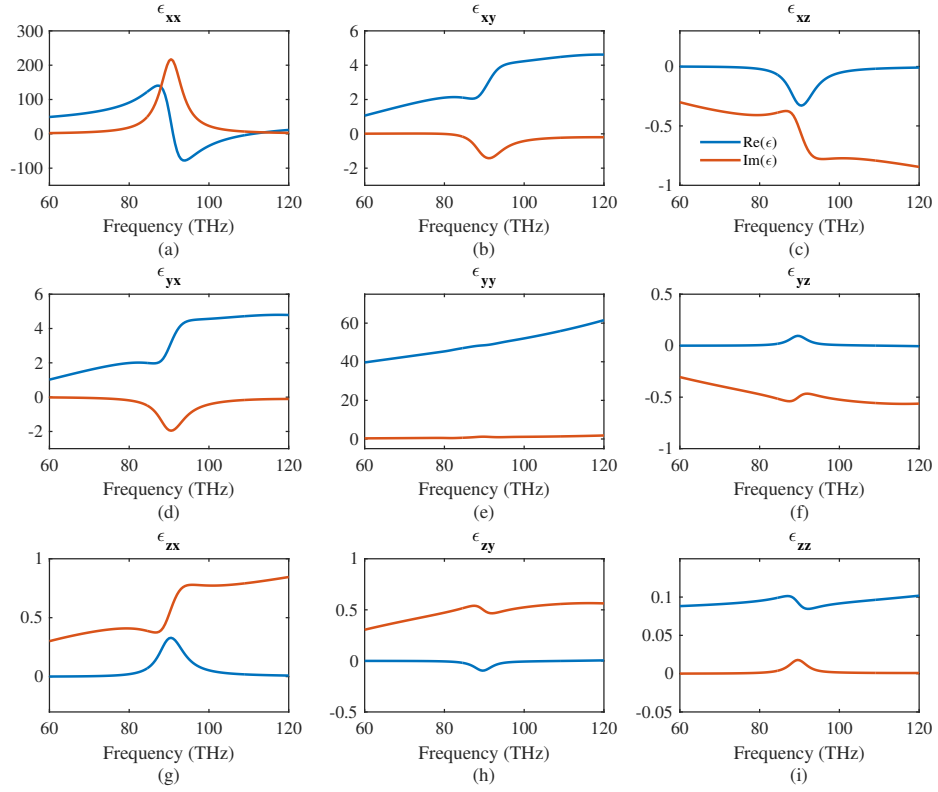


Figure 63. Extracted Permittivity Tensor from Literature SRR Coupled with SiO₂, $\theta = 10^\circ$.

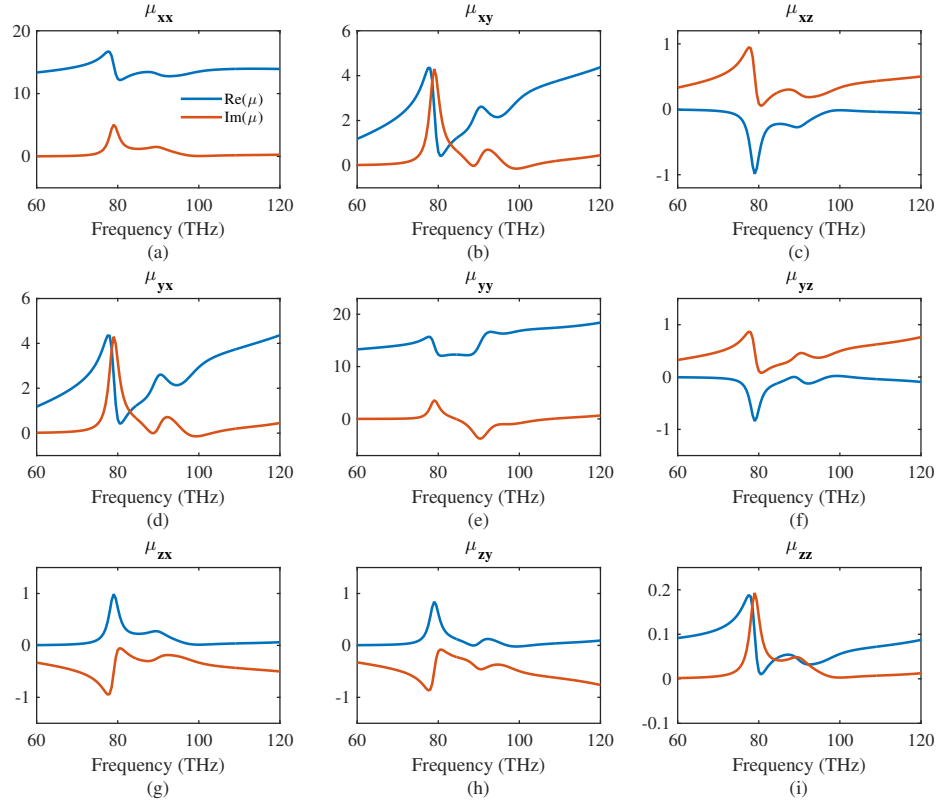


Figure 64. Extracted Permeability Tensor from Literature SRR Coupled with SiO_2 , $\theta = 10^\circ$.

same mechanism that were observed in the free space case remain evident. Specifically, remnants from bi-anisotropy coupling terms remain and do not completely go to zero. The x-pol transmission has the next highest errors reported with maximum of 3%. The lowest errors observed were for the transmission co-pol cases where the overall error is well below 0.5% with a maximum of 1%.

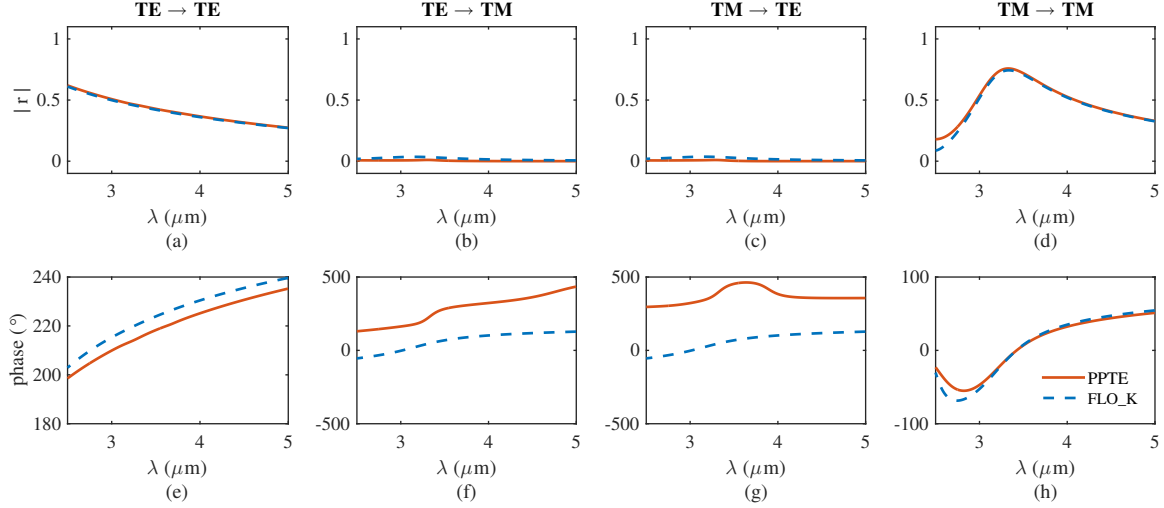


Figure 65. Literature SRR Coupled with SiO₂ Reflection Prediction vs FLO_K: $\phi = 0^\circ$, $\theta = 10^\circ$.

Presented in Figure 68 is a comparison of the permittivities and permeabilities from PPTE and those from the literature [30]. Figures 68a and e show the orientation of the fields for the extractions reported by Linden [30], shown in Figures 68b and f. Figures 68c and g are the values reported from Figures 63 and 64.

Although not presented previously in this document, the layer depth, d , used in PPTE is effectively a scaling factor. All results presented previously used the specific physical dimensions of the geometry, e.g. $0.5 \mu\text{m}$ for the isotropic case and 14 nm for the SRR. As such, Figures 68c and g are found when the SRR layer was 14 nm and isolated from the glass. Figures 68d and h were from considering the entire depth of the material, 100 nm for the glass and 14 nm for the gold SRR. While this effectively makes the scale the same as those from literature, the magnitudes and shapes are not

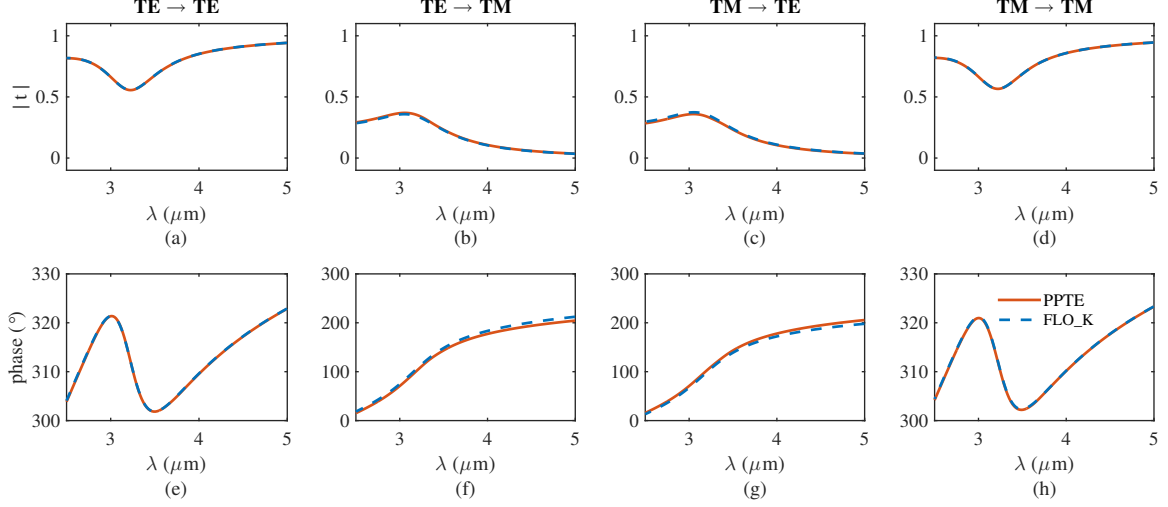


Figure 66. Literature SRR Coupled with SiO₂ Transmission Prediction vs FLO_K: $\phi = 45^\circ$, $\theta = 10^\circ$.

the same. It should be noted that this extraction still isolated the SRR layer from the glass, but applies the overall sample layer depth, an effect that does not physically represent the model.

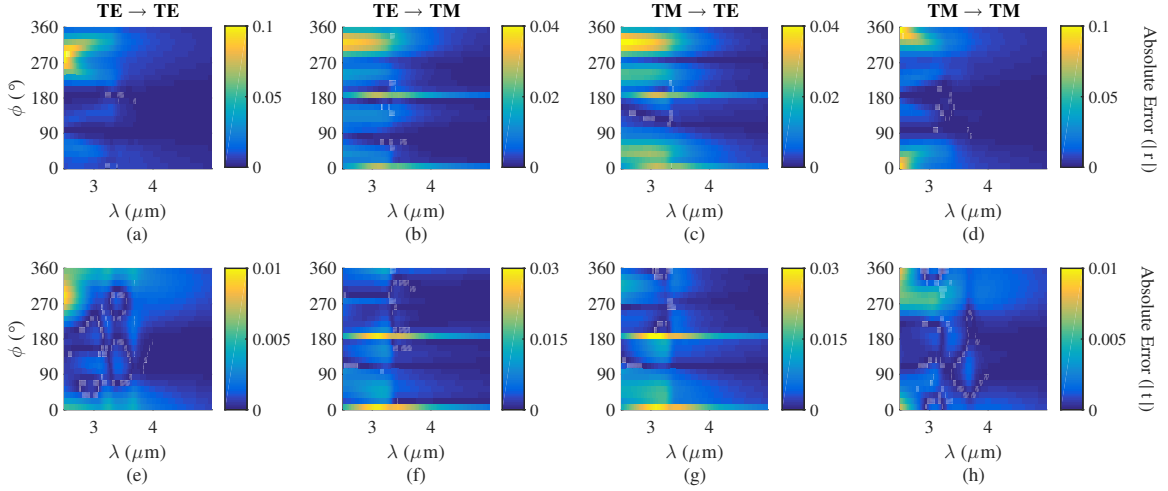


Figure 67. Literature SRR Coupled with SiO₂ Prediction vs FLO_K Error: $\phi = 0^\circ\text{--}360^\circ$, $\theta = 10^\circ$.

While the shape of the permittivity extracted for Figures 68c and d is similar to the what was found in literature, it is notably smoother and of different magnitudes.

The permeability in this orientation does not match as closely in shape, but when considering the larger d , shows very similar magnitudes. Similarly for the other orientation, the permeability has a similar shape, shown in Figures 68f, g, and h, but the magnitudes do not match and are never observed to go negative as was reported by Linden [30]. The permittivity at this orientation follows the same overall trend when comparing Figures 68f and h, but the reported resonance from literature is not observed.

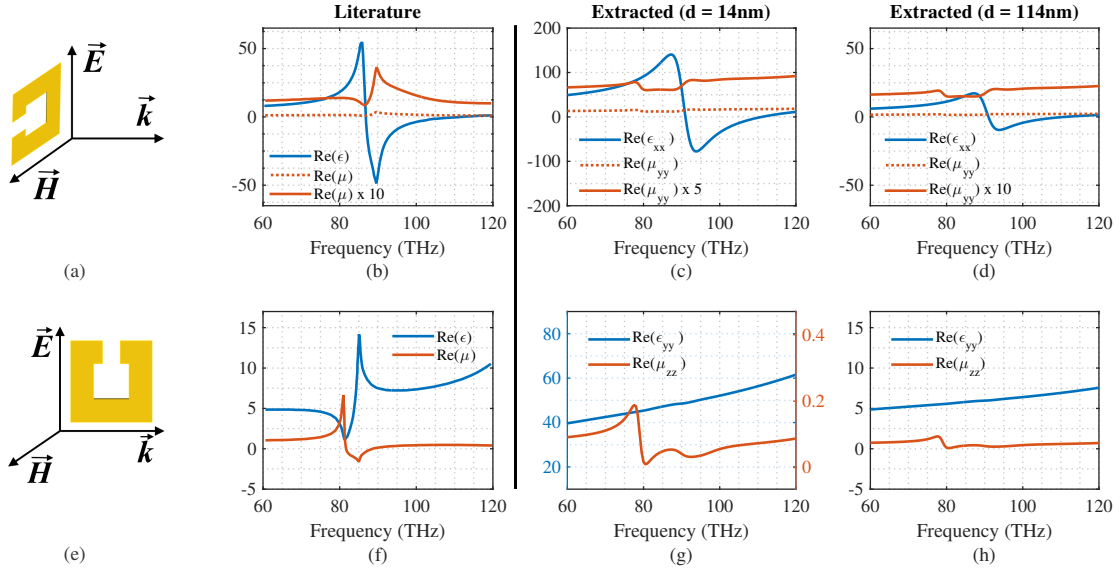


Figure 68. Extracted Permittivity and Permeability from Literature vs. PPTE. (a) and (e) show the orientation of the fields as they were reported in [30], while (b) and (f) show the reported permittivity and permeability at these orientation, [30]. (c) and (g) are the permittivity and permeability as they were reported here, shown in Figures 63 and 64. (d) and (h) use the entire layer depth, d , to place curves on the same scale (b) and (f), what was reported by Linden [30].

As it is presented here, it cannot be fully validated that either is correct or incorrect. Both are incomplete, as what was reported in literature only lists four elements [30] and PPTE reports on all 18 elements, but neither include the necessary $\bar{\zeta}$ and $\bar{\xi}$ field coupling terms. However, if PPTE can be ultimately proven correct for this type of structure, the completeness of extracting all tensor elements makes it a more useful extraction method.

4.3 Consideration of Application of PPTE to 3-D Cavity SRRs

To answer the question of PPTE's applicability to the 3-D cavity SRRs provided by Dr. Burckel, first consider a simpler, more constrained case, specifically the SRRs in free space. While there is nothing inherently bi-anisotropic from the Si resonant cavities, it is easier to conceptualize the problem when considering just the SRR. These SRRs are rotated out of the xy-plane and into the xz-plane, the yz-plane, or both. The development within this chapter shows that the SRRs do indeed exhibit bi-anisotropic activity when a significant component of the magnetic field lies parallel with the loop normal of the SRR. These SRRs when rotated out of the xy-plane will always have some significant component of the magnetic field parallel to the normal of the loop of the SRR. This violates the PPTE model assumptions implying PPTE cannot be applied.

To further explain this, consider the gap right SRR. At shallow angles of incidence, the only response observed would be driven by the magnetic field, which will be mostly horizontal, lying either parallel or perpendicular to the normal of the loop depending on the polarization. The capacitive gap will never be excited by a component of the electric field because there is never a large component of the electric field that is vertical. This case will have the bi-anisotropy maximized, not minimized, as was shown with those SRRs lying in the xy-plane. At higher incidence angles, responses will be driven by both, similar to those cases where the model did indeed break down when the SRRs were lying in the xy-plane. This implies that the best case scenario for these rotated SRRs is the worst case of what was presented in the in-plane SRR case.

Similar arguments can be made for the other two cases; gap up and both gap up and gap right. There is also the resonant cavity to consider which further complicates any responses that would be observed in the scattered fields. The evidence developed

in this chapter strongly supports that PPTE, in its current implementation, cannot be applied to these cases.

4.4 Conclusion

This research initially set out to answer if PPTE could extract permeabilities from magnetic materials and if so, can it be applied to an in-plane SRR structure. PPTE has been shown to extract the intrinsic permeability of isotropic magnetic materials with great accuracy. To answer the second question, first the bi-anisotropic nature of the split ring needed to be considered. It was shown that of the θ angles tested, 10° showed the most promise due to the minimization of magnetic field interaction observed in the scattering. When PPTE was applied to this case, the predictions from the extracted permittivities and permeabilities support that the model's assumptions were not substantially violated. When higher incident angles were considered, magnetic field interaction with the structure proved to be more troublesome when PPTE was applied, showing that the underlying assumptions of PPTE were violated. The degree of this error is observed in the deviation in the recovered fields from the material parameter extractions. This implies that PPTE cannot be used to gain insight on the material parameters of these planar SRRs at the higher incident angles which are required for ellipsometric extractions

Recovering the fields from the extracted material parameters is, in effect, inverting the process that PPTE applies. While this is necessary to show that the underlying assumptions were not violated, it does not sufficiently prove that the extracted effective parameters correctly describe the material. To do this, the extracted parameters need to be compared to extractions used from other methods. The problem is that other methods only extract these effective parameters in certain orientations and not as complete tensors. Linden reports parameter extractions in two orientations [30]

and when compared to those extracted using PPTE did have some agreement, but not the same level of agreement found in the biaxial anisotropic permittivity shown in the development of PPTE as seen in Benson's work [7,8]. The evidence presented within this chapter does not conclusively prove that the effective permeability tensor is indeed correct and it should continue to be tested. CST, another CEM tool, allows for full tensors to be input as material parameters where a slab could be examined for comparison of the scattered fields and could be used to provide a validation of the extracted material parameters from PPTE, but was not accomplished during the course of this research.

The third question of whether or not PPTE can be applied to the 3-D cavity SRRs was addressed conceptually. It is expected that PPTE cannot be applied to these structures in its current implementation. Further development of PPTE extending it to include the $\bar{\zeta}$ and $\bar{\xi}$ terms for bi-anisotropy will need to occur before these materials can be examined in the methods outlined here. Again, this implies that insight cannot be gained to effectively guide the ellipsometric extraction process.

V. Conclusion

This chapter summarizes the research that was presented throughout this document, which sought to answer if Permittivity and Permeability Tensor Extraction (PPTE) could be applied to magnetic materials, with the end goal of gaining insight into the material parameters prior to ellipsometric extractions on realized media. Given that PPTE is developed based on computational simulations, a mesh study of resonant structures was conducted on the tool chosen, FLO_K. After this, PPTE was applied to an isotropic, intrinsic magnetic material and then to several versions of split ring resonators (SRRs). Conclusions are made as to whether or not PPTE can be used on the given geometries. This chapter concludes with recommendations for future research.

5.1 Conclusions

This thesis sought to determine whether PPTE could be applied to inherently magnetic, anisotropic materials, specifically SRRs both in the xy-plane, and rotated into the xz-plane and/or the yz-plane. PPTE was developed based on the information that cannot be determined in measurement, but can be determined through simulations. Because of this, an extensive study on the mesh requirements needed for accurate and converged solutions of periodic resonant structures from FLO_K was conducted. Various localized meshing refinement techniques were used to determine the sensitivities of three different periodic resonant structures. It was determined that these geometries require a global mesh with at least ~ 50 cells per wavelength ratios, much higher than what is required for non-resonant materials. It was discovered that some standoff was required in the floquet apertures to not contaminate the far-field results. The standoff required was a very small fraction of the incident wavelengths,

indicating that while the apertures are not impervious to near field contamination, they are certainly very resilient. These lessons learned were applied to SRRs to ensure the sources of any errors were isolated from PPTE.

After the mesh study was concluded, the research then moved to application of PPTE to magnetic materials. First, it was applied to an isotropic, intrinsically magnetic material and was shown to be highly accurate. Errors, though small, were determined to be caused by mesh inadequacy at the higher index of refraction, which controls the compression of the wavelengths within the material. This work provides conclusive evidence that PPTE can extract an intrinsic permeability from a simple media. This however, does not prove that when the tensor elements are uniquely different are still accurate.

To determine if PPTE could retrieve an effective permeability from an anisotropic medium, an SRR from literature was chosen for study. However, the SRR is inherently bi-anisotropic, which led to an exploration of the scattering at different incident angles to determine if any conditions existed where the bi-anisotropic effects could be minimized. It was determined that at shallow incidence angles, the bi-anisotropy was indeed minimized, but not zero. Using this information PPTE was then tested against SRRs in free space at 10° , 40° , and 70° incident angles. The 10° case was the most constrained and had the least bi-anisotropic effects observed in the scattering. While 70° relaxes this constraint, it also showed the highest bi-anisotropic effects. When PPTE was applied to these cases, it was clearly observed that at 10° , the accuracy of recovering the fields and predicting at different sample rotations showed that the underlying assumptions on which PPTE was developed were not heavily violated. The same could not be said for the other two cases, the error of which provides a measure for how much of the underlying assumptions were broken. This was due to PPTE assigning values which should be associated to the field coupling

terms, $\bar{\zeta}$ and $\bar{\xi}$, to the permittivity and permeability terms, $\bar{\epsilon}$ and $\bar{\mu}$. These results imply that PPTE cannot be used at the higher incident angles ellipsometry requires, and can therefore not be used to gain insight into the material parameters prior to ellipsometric extractions.

After the free space SRRs were studied, the substrate layer was then considered. First, many iterations of varied glass depth were simulated to determine the field depth penetration which affects the capacitance, and subsequently the resonance, of the SRR. It was shown that a depth of 100 nm of glass was needed to fully capture the field depth and depths any greater showed Fabry-Pérot resonances which contaminated the scattered fields. However, the resonance shift due to coupling the glass layer did not shift the resonance as far as what was reported in literature. To achieve this, the metal height was varied and determined that 14-nm metal height showed the best match between the model presented in this research and what Linden reported for measured and modeled results for 20 nm [30]. At this point, the scattering matched very well and PPTE was applied for direct comparison of the reported permittivity and permeability from this structure.

In order to determine the specific effects attributed to the SRR, this layer was isolated using the method outlined by Benson [7,8]. By inverting the process, predictions were made, effectively recovering the scattered fields and predicting the responses observed at various sample rotations. The overall error shown indicates that the model's assumptions were not heavily violated for this case. As such, the permittivity and permeability matching the orientations reported in the literature were compared to determine the accuracy of PPTE. Although, similar shapes and magnitudes were reported, it did not conclusively show the accuracy of PPTE.

More than 400,000 hours of simulation was accomplished using the HPC during the course of the work presented here. This can roughly be translated to more than

two years and ten months of simulation on a robust workstation consisting of 16 cores and 32 GB of RAM. Without the use of the HPC, this work would not have been completed within the strict timelines AFIT requires. While not everything that was simulated has provided plots within this document, it was all incredibly useful in learning the tools and in furthering my understanding of the many problem sets that were studied.

5.2 Future Work

5.2.1 IR-VASE Material Parameter Extraction Measurements.

Dr. Burckel provided samples of 3-D cavity SRRs. While it was hoped that these could be modeled and have PPTE applied, it was shown that this was not possible with the current implementation of PPTE. However, future research should include full ellipsometric characterization of the material parameters of the samples provided by Dr. Burckel. Although these samples have been studied extensively over the last few years, they have never been studied with the infrared variable angle spectroscopic ellipsometer (IR-VASE). If PPTE is further developed to include the coupling terms for bi-anisotropy, the results from IR-VASE measurements as compared to PPTE could provide another level verification.

5.2.2 PPTE Development for Generalized Bi-anisotropy.

Dr. Benson developed PPTE for a specific problem, one that was anisotropic with metallic inclusions that were unaligned. Its utility, when used within the constraints of its development, has far reaching implications in the study of complex materials. The problem of extracting full permittivity and permeability tensors is non-trivial, solving unambiguously for 18 unknowns. The problem of bi-anisotropy is at least twice as difficult, solving for 36 unknowns. However, there is a need for this development,

specifically to continue the study of these types of materials, whose application is of great interest to the USAF.

Dr. Benson proposed that two areas of further study lied in incident angle, θ , and the bi-anisotropic coupling terms, $\bar{\zeta}$ and $\bar{\xi}$, [8]. These were proposed as separate areas of study. However, I propose that there is a relationship which could be exploited, at least in the planar SRR – those lying in the xy-plane. If the bi-anisotropy can be sufficiently small, ideally zero, then the extracted permittivity and permeability should not be contaminated by the bi-anisotropic coupling terms. This assumes that the extracted tensors are correct – Benson showed that the permittivity was valid, while the validation of the permeability was inconclusive as it was developed herein. If they can be assumed to be correct, though, then these tensors should be able to rotated with a rotation matrix in y , which would have the effect of changing the incident angle (θ) in the same way a rotation about z had the effect of rotating the sample (ϕ angle). Then a comparison could be made to these rotated tensors to those extracted at that incident angle and any difference should be associated with $\bar{\xi}\vec{H}$ and $\bar{\zeta}\vec{E}$. If the fields are either known ($\vec{E}$) or can be determined ($\vec{H}$), then $\bar{\xi}$ and $\bar{\zeta}$ should be able to be found at that angle of incidence. It should be noted that this would only apply to the planar SRRs and could not be used on the out-of-plane SRRs because the bi-anisotropy can never be minimized, allowing for unambiguous extractions of the permittivity and permeability, which this method would need. It is unknown if this would sufficiently characterize these bi-anisotropic coupling terms, but further research in this area might expand the current set of cases to which PPTE can be applied.

5.2.3 PPTE within a Lab Setting.

Although Dr. Benson notes in his dissertation that PPTE might have potential utility within the microwave regime where magnitude and phase values can be measured, he also notes that it is not currently possible to use PPTE within a lab setting [8]. I propose that there may exist an opportunity to utilize PPTE on microwaves within a lab setting. During my time at AFIT, I was taken on two tours of the GE Aviation facilities at Cincinnati, OH. It was at their electromagnetics lab, where a not-dissimilar method to ellipsometry was observed being used to measure fields in the microwaves. The instrument, although proprietary in nature, is indeed very congruent with the way the FLO_K experiments were set-up, save for one difference – only the reflections were measured.

I propose that collaborative work can be done between an AFIT student and GE, as has happened many times in the past, to alter this instrument to also account for transmission in an attempt to apply PPTE to measured field values from both reflection and transmission. There may need to be some alterations to PPTE in its current implementation as well, leading to the possibility for further research within the microwave regime.

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14. ABSTRACT Recent developments in material parameter extraction techniques have been made, allowing for full tensor extractions of the effective permittivity and permeability of anisotropic materials. This technique, PPTE, requires the use of simulated scattered fields, specifically from FLO_K. A rigorous study of the FLO_K meshing requirements for resonant structures was conducted, determining that mesh convergence alone was insufficient for accurate solutions, a small floquet aperture standoff was required. PPTE has been validated to extract effective permittivity tensors, but has yet to be validated on magnetic materials, retrieving an effective permeability. Here, the technique was applied to an isotropic medium with defined material parameters and was shown to extract the intrinsic material parameters with a high level of agreement. Next, PPTE was applied to SRRs. Careful consideration of the bi-anisotropic nature of SRRs was considered. PPTE yielded the best results when incident angle was small, thus minimizing any bi-anisotropic effects. However, a comparison of results from PPTE with literature proved inconclusive.						
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