Infrared Resonant-Coupled Metamaterial Sensing and Phonon-Polariton-Enhanced Infrared Interconnects

by

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Abstract

Title:
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Coupled-mode theory has been applied to various fields of endeavor from waveguide splitters/combiners and molecular sensing to light-matter interactions. Metamaterials, engineered periodic or aperiodic structures, are employed to sense molecular vibrational fingerprints in the mid to long infrared wavelengths. A metasurface, a 2D metamaterial, can be designed such that it has a resonance at a molecular vibrational frequency. Mode splitting results from the coupling of two electromagnetic field distributions, or modes, spatially and/or temporally. Metamaterial and molecular resonance coupling is a result of near field interaction. Fano resonances have an asymmetric line-shape that results from the coupling of a continuum and a discrete state in a quantum description or a bright and dark mode in a classical description. Analogous to the atomic system, a bright mode exhibits a broad resonance or short lifetime that couples strongly with incident far field radiation while, on the other hand, a dark mode provides a sharp quality factor, $Q$. 

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resonance or a long lifetime that couples weakly with an excitation far field. Polaronitons are quasiparticles that result from strong coupling of light and matter. Surface plasm polariton (SPPs) result from the coupling between plasmons, or free electrons in a noble metal, and electromagnetic waves. The SPP mode exists as a tightly bound transverse magnetic (TM) surface mode on a metal/dielectric interface. However, SPPs only exist in a spectrum from the ultraviolet to the near infrared (IR) for a noble metal. For polariton applications in the mid to long infrared range phonon polaritons are required. Surface phonon polariton (SPhPs), similar to SPPs, are a surface TM mode on a polar dielectric/dielectric interface. However, SPhPs only exist in a spectral region known as the reststrahlen band where the polar dielectric acts like a metal, i.e., negative real permittivity. Hexagonal boron nitride (hBN) is a van der Waals crystal with naturally occurring hyperbolic dispersion hat has been shown to support phonon polaritons in two distinct reststrahlen bands. The upper reststrahlen band, ranging from 1630 cm\(^{-1}\) (6.135 μm) to 1360 cm\(^{-1}\) (7.353 μm), provides highly volume-confined phonon polaritons. The lower reststrahlen band, ranging from 825 cm\(^{-1}\) (12.12 μm) to 760 cm\(^{-1}\) (13.16 μm), exhibits a negative index (or negative dispersion) and provides ultra-slow sub-diffraction volume-confined phonon polaritons. The subdiffraction confinement and ultra-slow nature of the type I hyperbolic phonon polaritons (HPhPs) are desirable properties for mid to long IR wavelength sensing.
In this dissertation, a carbonyl oxide bond vibrational resonance in poly(methyl methacrylate) (PMMA) will be used as an analyte. A wide-field-of-view perfectly absorbing metamaterial (PAMM) is then designed such that the metamaterial resonance couples to a molecular vibrational resonance in the analyte. Tuning the relationship between internal (absorption) and external (scattering) damping or loss in the PAMM results in both electromagnetically induced transparency (EIT) and electromagnetically induced absorption (EIA) response in the PAMM-analyte coupled system. Next, Fano resonance metamaterials (FRMM) coupled to the PMMA molecular resonance are investigated. FRMM’s asymmetric reflection spectrum is a result of hybridization of symmetric (bright) and asymmetric (dark) plasmon modes supported by the metamaterial’s geometry. The addition of the analyte results in multi-mode coupling between the FRMM’s modes and molecular resonance. Multi-mode coupling via a FRMM has advantages in selectivity and sensitivity by the tailoring of the metamaterial resonance prior to the introduction of the molecular resonance.

In addition to metamaterial-based sensing, different hybrid phononic waveguide geometries are investigated in this dissertation. The first geometry considered is a 4H-SiC (silicon carbide) substrate with a GaN spacer material and GaAs tracer. The results presented in this dissertation using a 4H-SiC substrate are the first practical analysis of a hybrid phononic waveguide in the mid to long IR. The 4H-SiC enhanced hybrid waveguide geometry is then used to create two fundamental
optical waveguiding devices: an optical directional coupler (ODC) and a Mach-Zehnder interferometer (MZI). The phonon polariton enhanced ODC and MZI in the mid to long IR presented in this dissertation are both original contributions. Hyperbolic phonon polariton enhance waveguides using hBN in the mid to long IR of similar confident of approximately $5 \times 10^{-2} (\lambda_0/2)^2$ have been shown to provide propagation lengths of $58 \lambda_0$ and $20 \lambda_0$ for type I and II HPhP enhanced waveguiding respectively. Unique and novel coupling between ultraslow negatively dispersive type I HPhP modes and positive dispersive high index waveguide modes are analyzed. The coupling between the type I HPhP modes and high index waveguide modes result in upper hybrid modes with forward and backward propagating modes that inherited the type I HPhP’s slow waves with group velocities ranging from $0.065c$ to $0.03c$. 
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Metasurface

Normal Mode Splitting

Metamaterial

Coupled Resonates

PMMA

Fano Resonates

Phonon Resonate

Surface-Enhanced Infrared Absorption

Vacuum Rabi Splitting

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\, nm]\) (d), \([d, h] = [2.75 \, \mu m, 10 \, nm]\) (e), \([d, h] = [4.0 \, \mu m, 10 \, nm]\) (f) as labeled in part 
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# List of Symbols

<table>
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<tr>
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<th>Description</th>
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<tr>
<td>$\hbar \Omega_r$ [meV, J]</td>
<td>Rabi energy</td>
</tr>
<tr>
<td>$2\Omega_r$ [rad/sec, Hz]</td>
<td>Rabi splitting</td>
</tr>
<tr>
<td>$d$ [μm]</td>
<td>Distance between two mirrors in a cavity</td>
</tr>
<tr>
<td>$k$ [rad/sec, Hz]</td>
<td>Coupling coefficient used in TCMT</td>
</tr>
<tr>
<td>$n$</td>
<td>Real part of the index of refraction</td>
</tr>
<tr>
<td>$R_n$</td>
<td>Power reflectivity from a mirror in a cavity</td>
</tr>
<tr>
<td>$t_{\text{rod}}$ [μm]</td>
<td>Distance between nano rod metasurface and PEC ground plane</td>
</tr>
<tr>
<td>$t_{\text{slot}}$ [μm]</td>
<td>Distance between nano slot metasurface and PEC ground plane</td>
</tr>
<tr>
<td>$V$ [rad/sec, Hz, meV]</td>
<td>Coupling coefficient used quantum state descriptions</td>
</tr>
<tr>
<td>$\beta$ [rad/m]</td>
<td>Phase constant</td>
</tr>
<tr>
<td>$\gamma$ [rad/sec, Hz]</td>
<td>Damping/Loss coefficient</td>
</tr>
<tr>
<td>$\gamma_e$ [rad/sec, Hz]</td>
<td>External or radiative loss</td>
</tr>
<tr>
<td>$\gamma_{0(1,2)}$ [rad/sec, Hz]</td>
<td>Internal or Ohmic loss</td>
</tr>
<tr>
<td>$k_0$ [rad/sec]</td>
<td>Free space wavevector</td>
</tr>
<tr>
<td>$\delta$ [rad/sec, Hz]</td>
<td>Detuning ($\omega_1-\omega_2$)</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Imaginary part of the index of refraction</td>
</tr>
<tr>
<td>$\lambda$ [nm, μm]</td>
<td>Wavelength</td>
</tr>
<tr>
<td>$\omega$ [rad/sec]</td>
<td>Radial frequency or radial eigenfrequency</td>
</tr>
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</table>
\( \omega_n [\text{rad/sec}] \) \quad n^{th} uncoupled normal mode

\( \omega_p [\text{rad/sec}] \) \quad Plasmon frequency

\( \omega_{sn} [\text{rad/sec}] \) \quad a delta shift (red or blue) in radial frequency to the \( n^{th} \) uncoupled mode

\( q \) \( [\text{eV, Hz}] \) \quad Asymmetry parameter of the Fano profile

\( \varepsilon_r \) \quad Relative Permittivity

\( L_m [\mu\text{m}] \) \quad Propagation Length/Distance

\( A_0 [\mu\text{m}^2] \) \quad Diffraction-limited Area in Free Space

\( A_m [\mu\text{m}^2] \) \quad Mode Area

\( |a|^2 \) \quad Mode Character

\( L_0 [\mu\text{m}] \) \quad Transfer Length
List of Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
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<tbody>
<tr>
<td>EIT</td>
<td>Electromagnetic Induced Transparency</td>
</tr>
<tr>
<td>EIA</td>
<td>Electromagnetic Induced Absorption</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Method</td>
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<tr>
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<td>Fano Resonance Asymmetric Metamaterial(s)</td>
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<td>FWHM</td>
<td>Full Width Half Maximum</td>
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<td>PAMM</td>
<td>Perfect Absorber Metamaterial(s)</td>
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<td>PMMA</td>
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<td>SEIRA</td>
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Dedication

To all the tree climbing fishes. May they find water.

“Everybody is a genius. But if you judge a fish by its ability to climb a tree, it will live its whole life believing that it is stupid.” – Albert Einstein
Chapter 1: Introduction

1.1 Motivation

The field of nanophotonics, the study of light interaction with nanoscale objects and control on the nanometer scale [1], has an array of applications including, but not limited to optical communication[2,3] and spectroscopy [4]. Two mechanisms for achieving the nanoscale control of light include using a metamaterial (formed from periodic or aperiodic building block elements known as meta-atoms [5,6]) or using metal optics [7]. Applications for metamaterials include cloaking, optical filters, optical antennas, lenses, photovoltaics, and sensors [8-14]. The contribution of each meta-atom results in exotic bulk material properties that are not found in nature that can be engineered or tailored. A metasurface is a special case of a metamaterial where the meta-atoms are arranged in a sheet or planar surface [6,15]. Metasurfaces are appealing to fabricate in comparison to a volumetric metamaterial when using conventional CMOS fabrication and thin-film techniques. Metamaterials and/or metasurfaces have been used in different forms of biological, molecular, and material sensing. In infrared (IR) spectroscopy, interaction between IR radiation and matter is used in the detection of biological markers or fingerprints in matter like DNA, proteins, and molecular vibrations. The introduction of a metallic surface can enhance the resonance signature of a molecule[10,16,17] as in
the case of surface enhanced Raman spectroscopy (SERS) [18-24] or surface enhanced IR spectroscopy (SEIRS) [11,25-28]. It has been reported that typical field enhancements of IR based nanoantenna for spectroscopy applications range from 1 to 4 orders of magnitude [29-32].

Metal optics allows for the nano-scale confinement of light, which has an appealing application in photonic integrated circuits (PIC) [33,34]. The perpetual need for minimization and reduction in SWAP (size, weight and power) has motivated the need for ultra-confined optical interconnects that can support several Gbps (gigabits per second) data links on silicon chips [2,35]. Surface plasmon polaritons (SPPs), quasiparticles that result from light-matter coupling, are tightly bound surface waves on metal-dielectric interfaces which lends SPPs to nano-scale confinement applications [7]. However for mid- to long-wave infrared application, SPPs in noble metals are no longer supported [4]. Therefore, other plasmonic materials or dielectric materials are required in place of SPP supporting noble metals. In the case of the latter, polar dielectrics with polar optical phonon interaction in the mid- to long-wave IR can support phonon polaritons in a band of frequencies between longitudinal (LO) and transverse optical (TO) phonon frequencies called the “reststrahlen” band [4]. In the reststrahlen band the relative permittivity of the polar dielectric is negative, and can be described with a Lorentz oscillator model [4]. The mid- to long-wave IR spectral region has applications in free space optics/remote sensing due to the atmospheric transmission window between 8 μm to 12 μm, and
in spectroscopy with the wealth of molecular fingerprints in that spectral region [4,30,36].

1.2 Method

1.2.1: ANSYS High Frequency Structural Simulator (HFSS)

ANSYS high frequency structural simulator (HFSS) is a commercially available full-wave finite element method (FEM) solver that is used to solve Maxwell’s equations [37,38]. The basic four steps in an FEM analysis are as follows [39]:

1. Divide the problem space in discrete elements. Discretization of the geometry is also known as meshing. An example of typical meshing elements used in HFSS is shown in Figure 1.

2. Determine the equations for the meshing elements.

3. Assemble the elements to be solved.

4. Use the system of equations determined to solve for the field at the given nodal points using the appropriate boundary conditions.

Figure 1. Four-node tetrahedron, node numbers labeled, by default is used as the meshing element in ANSYS HFSS.
In discretization of the geometry, HFSS has an automatic adaptive meshing process which starts with an initial mesh that is then iteratively refined in places with high field gradient [37,38]. The adaptive meshing process continues until a convergence criteria, S-parameters for driven model and resonant frequency delta for eigen mode, is met or the number of adaptive passes are met [37,38]. Also, HFSS provides “mesh operations” in which the user dictates the meshing element sizes directly, as opposed to the automatic adaptive meshing [37,38]. In general, FEM is more versatile, given its ability to solve in inhomogeneous media and irregular shaped structures [39]. Second, the system of equations that govern the meshing elements are determined. A relationship between the nodal field values and each meshing element is determined. Next, each element in the solution region is assembled, and a matrix relating the nodal fields to each other is obtained. Lastly, the assembled matrix is solved using boundary conditions to determine the nodal fields of the meshing elements. In HFSS, the resulting solution is checked against the convergence criteria inputted by the users. If the convergence criteria are not met then HFSS would refine the mesh and resolve for the nodal solutions.

Figure 2 shows the use of periodic boundaries in the setup of a metamaterial and waveguide structure in driven model in HFSS. The driven solution uses ports or incident field to excite the simulated structure which is used for determining S-parameters and field solutions. The slave boundary is linked to a master boundary
and a phase delay defining the phase shift between the boundaries. The master/slave ports shown in Figure 2.a define an infinite array in two directions. The Floquet port[40] is used to excite a plane wave of an infinite array where the phase delay in the slave port can be used to define the incidence angle of the excitation. The waveguide cross-section, shown in Figure 2.b with the master/slave boundaries, is used in an eigen model to define an infinite waveguide in the propagation direction. The eigenmode solution in HFSS is used to determine natural resonances of the structure, field solutions, and quality factor of the resonance. The phase delay in the slave port is used to calculate the propagation phase constant:

\[ p = n_{\text{eff}} k_0 l \]  

(1.1)

where \( p \) is the phase delay defined in the slave boundary, \( l \) is the thickness of the waveguide cross-section, \( k_0 \) is the free space phase constant, and \( n_{\text{eff}} \) is the effective index of the waveguide. For a given phase delay a complex resonance frequency is calculated using the eigenmode solver.
1.3 Dissertation Contribution

Mode coupling gives rise to normal mode splitting[26-28,41-45] as can be seen in Figure 3. In mode coupling two uncoupled modes (cyan and red dashed lines in Figure 3) interact with a coupling strength $\Omega$. The result is mode repulsion that forms hybrid modes (solid blue and black lines in Figure 3). In both metamaterial-molecular coupling and phonon-enhanced hybrid waveguiding, mode coupling is involved. In the following section resonant coupling between a PAMM[13,26,46-50] or FRMM[51-57] and molecular vibrational resonances will be discussed. Next, phonon-enhanced hybrid waveguiding and optical devices will be discussed [3,35]. Here, a practical surface phonon polariton (SPhP) enhanced waveguide architecture using 4H-SiC substrate in the mid to long IR is analyzed. Then, an optical directional coupler and Mach-Zehnder interferometer using the SPhP hybrid
waveguide is numerically analyzed [61,62]. Lastly, a hybrid waveguide geometry is explored with hyperbolic phonon polaritons (HPhPs) from hexagonal boron nitride (hBN).

Figure 3. An example of an anti-crossing dispersion diagram that describes level repulsion.

The contributions in this dissertation are as follows:

- A wide-field-of-view PAMM coupled to a molecular resonance is investigated to show mode coupling between the two resonances via the unique mode splitting signature. Temporal coupled mode theory was used
in analyzing the resulting coupling. Both reflective spectral signatures of electromagnetic induced transparency (EIT) and electromagnetic induced absorption (EIA) are shown to be related to the internal (absorption) and external (scattering) loss of the PAMM.

- Nanorod/nanoslot metamaterials with Fano asymmetric transmission/reflection spectra are numerically analyzed and shown to be the result of bright-dark mode coupling. Then an analyte, PMMA, with a molecular resonance at 52 THz is introduced and multimode coupling is observed. The resulting coupling, like in the case of the PAMM, provides a unique mode splitting signature, but unlike the PAMM the FRMM IR resonance that couples to the molecular resonance is the dark mode of the FRMM that has a higher Q factor resonance. This higher Q factor resonance allows for selectivity advantages as couple to the PAMM.

- The first practical mid- to long-wave IR hybrid waveguide enhanced by phonons in a polar dielectric 4H-SiC, silicon carbide, is numerically analyzed. It is shown that propagation length along the waveguide on the order of $7\lambda_0$ with confinement factors of less than $5\times10^{-2}(\lambda_0/2)^2$ are achievable where $\lambda_0 = 12.2 \, \text{μm}$. The results presented show a hybrid mode area in the mid- to long-wave IR that is more confined than the free space diffraction limited area and the high index dielectric waveguide mode area.
while maintaining a propagation distance that is several times bigger than the wavelength.

- Both an optical directional coupler (ODC) and Mach-Zehnder interferometer (MZI) were made using the 4H-SiC enhanced hybrid waveguide and are numerically analyzed. It is shown that the output port powers conform to coupled-mode theory as described in conventional dielectric waveguides. Thus, using the hybrid surface phonon polariton waveguide, fundamentally integral devices such as the ODC and the MZI were designed, which paves the way for future devices like modulators, optical filters and waveguide based sensors.

- Hexagonal boron nitride (hBN) has two reststrahlen bands: an upper (type II) and lower (type I). Both reststrahlen bands of the hBN, for the first time, are employed in hybrid waveguiding configurations and are compared. Type II HPhP hybrid waveguides are shown to maintain propagation lengths along the waveguide of $20\lambda_0$ with confinements of less than $5 \times 10^{-2} (\lambda_0/2)^2$ achievable where $\lambda_0 = 6.6 \, \mu\text{m}$. The type I HPhPs enhanced hybrid waveguide retains the ultra-slow group velocity property of the type I HPhPs while maintaining propagation length of $15\lambda_0$ with confinement factors of less than $2.25 \times 10^{-2} (\lambda_0/2)^2$ at $\lambda_0 = 13 \, \mu\text{m}$. 
Chapter 2: Perfect Absorbing Metamaterial

2.1 Introduction

PAMM, as the name implies, is a metamaterial that can be designed such that, in an ideal scenario, there is a frequency where there is 100% absorption of the incident radiation. In the case of a wide-field-of-view PAMM which is considered, the absorption of the incident radiation is independent of angle of incidence [48]. The resulting perfect absorption has been described as having an impedance match between free space and a resonant metamaterial in a transmission and nanocircuit model [13,49]. For a PAMM with a ground plane, there is not a fully defined S-matrix [48]. Therefore, the perfect absorption phenomenon is better described in terms of critical coupling where Ohmic (absorption) and radiative (scattering) losses of the PAMM are equal or “matched” [48]. Poly(methyl methacrylate) (PMMA) has been used as a stand-in analyte in several examples [26,29,47,63]. This is due to PMMA having an IR active carbon-oxygen molecular stretch vibration in the mid IR region at 52 THz (5.77 µm or 1733 cm⁻¹). PMMA is also a convenient material as it is a well-known commercially-available off-the-shelf photoresist in micro/nano fabrication. IR ellipsometry[64] was used to measure the complex optical properties of PMMA, as shown in Figure 4.
Figure 4. PMMA complex refractive index, imaginary (top) and real part (bottom), showing the C=O molecular bond resonance at 52 THz (1733 cm$^{-1}$).

### 2.2 Single Input Uncoupled System (SI-US)

Temporal coupled mode theory (TCMT) will be used to show the impedance matching condition between the Ohmic (internal) and radiative (external) losses, i.e. $\gamma_0 = \gamma_c$, in the metamaterial results in perfect absorption of incidence radiation. Figure 5 shows a circuit visualization for a PAMM as analogous to a single resonator coupled to a single input waveguide [47,48,58]. This single resonator coupled to a waveguide can be described by the following coupled mode equation [29,47,58,60]:

\[ 
\]
\[
\frac{da}{dt} = j\omega_0 a - (\gamma_0 + \gamma_e) a + \alpha S^+ \\
S^- = c S^+ + da
\]

where \(a\) is the normalized energy of the resonator, \(\omega_0\) is the resonant frequency where the PAMM is "perfectly" absorbing, \(\gamma_0\) is the internal loss of the resonator, \(\gamma_e\) is the external loss that describes the energy that does not "couple" into the resonator, \(S^+\) is the input field excitation onto the resonator, and \(S^-\) is the reflected field. The constants \(\alpha, d, \) and, \(c\) need to be determined.

![Circuit diagram](image)

Figure 5. Circuit description for a SI-US.

With the use of the principles of time reversal and energy conservation, it can be shown that [58]:

\[
|\alpha| = \sqrt{2\gamma_e} \\
d = \sqrt{2\gamma_e} \\
c = -\frac{|\alpha|}{d} = -1
\]

Therefore, Eq. 2.1 can be written as:
\[
\frac{da}{dt} = j\omega_0 a - (\gamma_0 + \gamma_e)a + \sqrt{2\gamma_e} S^+ \quad (2.3a)
\]
\[
S^- = -S^+ + \sqrt{2\gamma_e} a \quad (2.3b)
\]

Next, impedance matching results when the reflection coefficient, \( S_{11} \), is zero, where the scattering matrix in general is:

\[
S^- = S(\omega) S^+ \quad (2.4)
\]

Therefore, it can be seen that for a SI-US, there is only one element in the matrix:

\[
S^- = \left[ \frac{j(\gamma_e - \gamma_0) + (\omega - \omega_0)}{j(\gamma_e + \gamma_0) - (\omega - \omega_0)} \right] S^+ \quad (2.5)
\]

When at resonance, it can be seen that:

\[
S_{11}(\omega_0) = \frac{\gamma_e - \gamma_0}{\gamma_e + \gamma_0} \quad (2.6)
\]

It can be seen that when \( \gamma_e = \gamma_0 \), then \( S_{11}(\omega_0) = 0 \), which has been described as an impedance matched condition or critically coupled, where coupling is described in terms of the incident field coupling into the PAMM. Under- and over-coupled in terms of loss have been described as \( \gamma_e < \gamma_0 \) and \( \gamma_e > \gamma_0 \) respectively. Figure 6 provides a visual representation in the form of a Loci diagram in Figure 6.a[58] and a log curve that indicates the under- and over-coupled region with the ratio of \( \gamma_e/\gamma_0 \) at the resonated frequency \( \omega_0 \) in Figure 6.b [29,47]. The blue stars indicate the common point between the two representations.
Figure 6. a) Loci diagram of the reflection coefficient as seen in [58]. The critical circle is indicated in black. Increasing frequency is with clockwise rotation on the respective circle. Zero $\text{Im}(S_{11})$, indicated with a black line, is when the incident wave resonates with the resonator ("a"). Each dashed line circle on the Loci is a value to the ratio of $\gamma_c/\gamma_0$. b) Visualization of under- and over-coupling of the incident field at resonator resonance [29,47]. The blue stars in a) and b) indicate the same point for reference. As the Loci moves to PEC or PMC limits, the blue stars become indistinguishable from each other. The under- and over-coupled regions are indicated in orange and red respectively.

### 2.3 Resonant Coupling Between PAMM and Molecular Resonance

The TCMT description is expanded to include another equation that incorporates the introduction of a molecular resonance. In the framework of absorption, the intention of coupling a PAMM to a molecular resonance is to enhance the absorption signature of the bare molecular resonance. In comparison to the PAMM, the PMMA absorption is very small under excitation. If a dark mode (subradiant) is defined as a high Q-factor resonance that weakly couples to the incident
excitation[29,47], then a dark mode would be analogous to a molecular resonance. Conversely, the PAMM resonance that interacts strongly to the incident excitation would be defined as a bright mode (superradiant) [29,47]. The interference between a bright and dark mode results in a Fano resonance[51,52,54,65] and produces the typical asymmetrical line shape and scattering cross-section, $\sigma$, as shown in Figure 7 [66].

![Fano Resonance Scattering Cross Section](image_url)

Figure 7. The typical asymmetrical scattering cross section of Fano resonance is shown as a function of frequency for when the asymmetry parameter, $q$, is equals one (red solid line). The limiting cases of $q = 0$ and $q = \infty$ (solid blue and black respectively) are also shown for reference.
Using a TCMT description, Fano resonance[51,54,55], polaritonic systems[67-69], and electromagnetically induced transparency (EIT) or absorption (EIA)[70-73], phenomena can be described. The TCMT equations are as follows, where Figure 8 shows a circuit realization of the PAMM-PMMA coupled system [47, 54, 55, 58, 67]:

\[
\frac{da_1}{dt} = j\omega_1 a_1 - (\gamma_1 + \gamma_e) a_1 + jV a_2 + \alpha S^+_1
\]
\[
\frac{da_2}{dt} = j\omega_2 a_2 - \gamma_2 a_2 + jV a_1
\]
\[
S^- = cS^+ + da_1
\]

where \(a_1\) is the PAMM (bright) resonance, \(a_2\) is the molecular (dark) resonance, \(\omega_1\) is the PAMM resonant frequency, \(\gamma_1\) is the internal loss of the PAMM, \(\gamma_e\) is the external loss of the PAMM, \(\gamma_2\) is the absorptive losses of the molecular resonance, and \(V\) is the coupling strength between the PAMM and molecular resonance. \(S^+\) and \(S^-\) are the inputted field excitation and reflected field of the PAMM respectively.

Figure 8. Circuit visualization for a single input couple resonator system.
Using a matrix notation, the scattering matrix can be determined:

\[ S(\omega) = c + d\Omega^{-1}\alpha \]  

(2.8)

In the case of the single input coupled resonance system (SI-CS), then it can be seen that the scattering matrix is as follows [47,67]:

\[
\begin{bmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{bmatrix} = \begin{bmatrix}
c_1 & 0 \\
0 & 0
\end{bmatrix} + \frac{\alpha d_1 [j(\omega - \omega_2) + \gamma_2]}{\det[\Omega]} \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]  

(2.9)

The determination of the matrix \( \Omega \) provides the anti-crossing (level repulsion) dispersion relation that is plotted in Figure 4. Due to the single input, only the \( S_{11} \) parameter is of interest; therefore [47,67]:

\[
S_{11} = c_1 - \frac{\alpha d_1 [j(\omega - \omega_2) + \gamma_2]}{[(\omega - \omega_1) - j(\gamma_1 + \gamma_e)][(\omega - \omega_2) - j\gamma_2] - V^2}
\]  

(2.10)

where [47, 58, 67]:

\[
\omega_{\pm} = \frac{\omega_1 + \omega_2}{2} + \frac{j}{2}[(\gamma_1 + \gamma_e) + \gamma_2]
\]

(2.11)

\[
\pm \sqrt{\left(\frac{\omega_1 - \omega_2}{2}\right)^2 - \left(\frac{(\gamma_1 + \gamma_e) - \gamma_2}{2}\right)^2 + V^2 + \frac{j}{2}[\omega_1 - \omega_2][\gamma_2 - (\gamma_1 + \gamma_e)]}
\]

It can be seen from Figure 4 and Eq. 2.11 that under the condition \( \omega_1 = \omega_2 = \omega_0 \), the maximum splitting or repulsion is denoted by \( 2\Omega \); therefore, \( 2\Omega = |\omega_{-}(\omega_0) - \omega_{+}(\omega_0)| > 0 \), which leads to the result [74-76]:

\[
V > \left|\frac{(\gamma_1 + \gamma_e) - \gamma_2}{2}\right|
\]  

(2.12)
Due to the non-trivial nature of non-linear and non-orthogonal modes\cite{77,78}, the challenge becomes determining constants $c$, $d$, and $\alpha$; as such, primary results are derived. A similar process as in the case of SI-US, of applying energy conservation and time reversal, is used\cite{58} and it is assumed that the coupling strength '$V$' is a real constant with all frequencies. The power in each resonator is as follows\cite{58}:

\[
\begin{align*}
\frac{dW_1}{dt} &= a_1^* \frac{d a_1}{dt} + a_1 \frac{d a_1^*}{dt} = -2 \left[ (y_1 + y_e) + \frac{V^2 y_2}{y_2^2 + (\omega - \omega_2)^2} \right] W_1 \\
\frac{dW_2}{dt} &= a_2^* \frac{d a_2}{dt} + a_2 \frac{d a_2^*}{dt} = -2 \left[ y_2 + \frac{V^2 (y_1 + y_e)}{(y_1 + y_e)^2 + (\omega - \omega_1)^2} \right] W_2
\end{align*}
\]

(2.13)

Using time reversal, it can be seen that the energy that is scattered is a result of the energy in the bright resonator and the energy coupled from the dark resonator with $S^+$ turned off and no internal losses where hatted terms, for example, $\hat{\omega}$, denote time reversal terms.

\[
\frac{dW}{dt} = \frac{dW_1}{dt} + \frac{dW_2}{dt} = -2\gamma_e W_1 - \frac{2V^2 y_e}{(\gamma_e)^2 + (\hat{\omega} - \omega_1)^2} W_2 = -|S_1^+|^2
\]

(2.14)

From Eq. 2.7, the normalized bright and dark resonator amplitudes can be solved as:

\[
\begin{align*}
a_1 &= \frac{\alpha S_1^+ [j(\omega - \omega_2) + y_2]}{[j(\omega - \omega_2) + y_2][j(\omega - \omega_1) + (y_1 + y_e)] + V^2} \\
\alpha S_1^+ \\
a_2 &= \frac{jV\alpha S_1^+}{[j(\omega - \omega_2) + y_2][j(\omega - \omega_1) + (y_1 + y_e)] + V^2}
\end{align*}
\]

(2.15)

and assuming the detuning \cite{74}, $\delta \equiv |\omega_1 - \omega_2|$, is zero, the time reversed excitation is $\omega = \omega_1 - j\gamma_e$, and no internal loss; then:
\[ \tilde{a}_1 = \frac{\alpha \tilde{S}_1^+}{2\gamma_e \left( 1 + \frac{V^2}{2\gamma_e^2} \right)} \]
\[ \tilde{a}_2 = \frac{jV \alpha \tilde{S}_1^+}{2\gamma_e^2 \left( 1 + \frac{V^2}{2\gamma_e^2} \right)} \]  

(2.16)

Given at \( t = 0 \), \( |a_n| = |\tilde{a}_n| \) and \( |S_{\tilde{r}}| = |\tilde{S}_1^+| \) then:

\[ \left| S_1^+ \right|^2 = 2\gamma_e W_1 + \frac{2V^2\gamma_e}{(\gamma_e)^2 + (\omega - \omega_1)^2} W_2 = 2\gamma_e \bar{W}_1 + \frac{2V^2\gamma_e}{(\gamma_e)^2 + (\bar{\omega} - \omega_1)^2} \bar{W}_2 \]  

(2.17)

Combining the results of Eq. 2.16 and Eq. 2.17, and leaving \( \alpha \) as a function of \( \bar{\omega} \) results in:

\[ |\alpha| = \sqrt{2\gamma_e} \left( 1 + \frac{V^2}{2\gamma_e^2} \right) \left\{ \frac{\gamma_e^2 V^2}{2\gamma_e^2} \left[ V^2 + (\gamma - \omega_1)^2 \right] - \frac{V^4}{\gamma_e^2 (\omega_1)^2 + (\omega - \omega_1)^2} \right\}^{1/2} \]  

(2.18)

Next, solving for \( d_1 \) from Eq. 2.7 it can be seen that:

\[ |S_1^-| = d_1 a_1 \]  

(2.19)

when \( |S_1^+| = 0 \); therefore:

\[ |S_1^-|^2 = |d_1|^2 |a_1|^2 = 2\gamma_e |a_1|^2 + \frac{2\gamma_e V^2}{\gamma_e^2 + (\omega - \omega_1)^2} |a_2|^2 \]  

(2.20)

where:

\[ |a_2|^2 = \frac{V^2 |a_1|^2}{\gamma_e^2 + (\omega - \omega_2)^2} \]  

(2.21)

which leads to:
\[ |d_1| = \sqrt{2\gamma_e \left[ 1 + \frac{V^4}{((\omega - \omega_2)^2 + \gamma_e^2)((\omega - \omega_1)^2 + \gamma_e^2)} \right]} \]  

(2.22)

Using conservation of energy to solve for \( c_1 \), the net power is then coupled into the resonator. One can be either be dissipated or coupled into the second resonator \((x_{12})\) adding to the energy rate of buildup:

\[ |S_1^+|^2 - |S_1^-|^2 = \frac{dW_1}{dt} + 2\gamma_1 W_1 + x_{12}W_1 + x_{DS} |S_1^+|^2 \]  

(2.23)

The nature of \( x_{DS} \) is revealed later. Solving for \( dW_1/dt \) similar to Eq. 2.13, it can be seen that:

\[ \frac{dW_1}{dt} = -2(\gamma_1 + \gamma_e)W_1 - \frac{2\gamma_2 V^2}{(\omega - \omega_2)^2 + \gamma_e^2} W_1 + |\alpha||S_1^+ a_1^* + S_1^+ a_1| \]  

(2.24)

and from squaring the last equation in Eq. 2.7:

\[ -|S_1^-|^2 = -|S_1^+|^2 - 2\gamma_e W_1 - \frac{2\gamma_2 V^2}{(\omega - \omega_2)^2 + \gamma_e^2} W_1 + x_{12} W_1 + x_{DS} |S_1^+|^2 + |\alpha||S_1^+ a_1^* + S_1^+ a_1| \]  

(2.25)

After combining the two equations in Eq. 2.25, it follows that:

\[ |S_1^+|^2 [|c|^2 + x_{DS} - 1] + W_1 \left[ |d_1|^2 - 2\gamma_e - \frac{2\gamma_2 V^2}{(\omega - \omega_2)^2 + \gamma_e^2} + x_{12} \right] \] 

\[ + |S_1^+ a_1^* + S_1^+ a_1| [|c_1||d_1| + |\alpha|] = 0 \]  

(2.26)

It can be seen from Eq. 2.26 that [58,67,68]:

\[ |c_1| = -\frac{|\alpha|}{|d_1|} \]  

(2.27)
The mathematical model is used similar to that in references [29,47,48] in parameter fitting the numerical results. Previous papers have reported work in PAMM, and resonated coupling has been reported in [75,79-81]. However, the silicon cavity thickness was on the order of the wavelength in the cavity, which leads to thick films of over 1 µm. From a private communication with collaborators at the Infrared Systems Lab at University of North Carolina at Charlotte, the cavity film thickness was too large to fabricate reliably. Therefore, a sub-wavelength cavity or spacer structure was investigated.

2.4 Numerical Modeling of PAMM and Resonated Coupling

2.4.1: Nano Patch Metasurface PAMM
A metallic nano patch metasurface with a sub-wavelength spacer of an ellipsometrically measured[64] amorphous Si (a-Si) spacer on a gold ground plane is seen in Figure 9. An overcoat of a dispersionless layer of PMMA was initially placed on the structure to remove any red or blue shifting of the PAMM’s resonance due to the dispersionless index on the PMMA as seen in Figure 9.
Figure 9. A dispersionless PMMA overcoated on top of a PAMM made of a gold patch metasurface separated from a ground plane by an amorphous silicon spacer. Both TE and TM at two orientations and various incidence angles are considered.

The SI-US mathematical analysis that was applied to the structure in Figure 9 is shown in Figure 10. Figure 10.a compares simulated results to the parametric fitting of Eq. 2.5, where the values are tabulated in Table 1. Figure 10.b confirms the over-, critically-, and under-coupled relationship in terms of a Loci diagram. Figure 10.c shows the linear relationship between the external ($\gamma_e$) and internal ($\gamma_0$) loss as a function of spacer thickness [29,47,48]. The patch length and unit cell were tuned so that the center resonance was approximately at the same frequency. Figure 11 is the spectral and angular resolution for the absorption for the CC case for both incident modes seen in Figure 9. It can be seen that the design patch metamaterial provides a polarization that is insensitive to transverse electrical (TE),
transverse magnetic (TM), or either mode orientation while providing a wide field-of-view [48].

Table 1. SI-US model fit parameters used in Eq. 2.5.

<table>
<thead>
<tr>
<th></th>
<th>(f_0) [THz]</th>
<th>(\gamma_e) [THz]</th>
<th>(\gamma_0) [THz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>OC</td>
<td>53.4</td>
<td>3.81</td>
<td>1.44</td>
</tr>
<tr>
<td>CC</td>
<td>53.5</td>
<td>2.07</td>
<td>2.07</td>
</tr>
<tr>
<td>UC</td>
<td>52.4</td>
<td>1.14</td>
<td>2.65</td>
</tr>
</tbody>
</table>

Using the numerical tool, the PAMM field enhancement can be extracted as a function of frequency of the over-, critically-, and under-coupled cases, as seen in Figure 12. The maximum field enhancement is at the frequency of maximum absorption, as to be expected. The maximum field enhancement is located on the edges on the gold nano-patch [47]. Similarly, from plotting the magnitude of the H field in Figure 13, a magnetic dipole can be seen located in the spacer, which agrees with the reports in [48]. The magnetic dipole is responsible for the perfect absorption nature of the PAMM [48]. Next, the PMMA molecular resonance is introduced to the over-, critically-, and under-coupled cases. The developed SI-CS mathematical model is used to analyze mode spitting.
Figure 10. a) Numerical, stars (*), and mathematical model, solid line, are shown for a case of over-, critically-, and under-coupled cases. b) The Loci diagram for these cases are shown. c) The linear relation between the external ($\gamma_e$) and internal ($\gamma_0$) loss is shown where the critically-coupled case is at 90 nm amorphous Si spacer thickness.
Figure 11. Normalized absorption spectra and angularly-resolved spectra for the critically-coupled cases as seen in Figure 9. Both TE (a, b) and TM (c, d) polarizations are shown for both mode orientations.
2.4.2: Resonant Coupling to a Nano Patch PAMM

The molecular resonance is then introduced to PAMM, which results in mode splitting or repulsion[45,47,73,82] and superscattering[47,83,71,72] in the over-coupled case. Figure 14.a shows the numerical and mathematical model parameter...
fitted for Eq. 2.10 for resonated coupling for the three cases of over-, critically-, and under-coupled. The parameters used for the mathematical model fit are tabulated in Table 2. For comparison, the Loci diagram generated from Eq. 2.10 for resonated coupling is shown in Figure 13.b. The loop in the Loci indicates the nonlinear nature of mode coupling that is occurring. It can also be seen that \( \lim_{f \to \pm \infty} Re[S_{11}(\omega)] < -1 \), which is out of bounds of the limit of \( Re[S_{11}(\omega)] \).

In the parametric fitting of Eq. 2.10, it is assumed that the coupling strength is a real constant for all frequencies [74-76]. However, if coupling strength is due to the near field, which in turn is related to storage field and field enhancement, then the frequency dependence of the coupling strength should mirror the field enhancement. However, it can be seen in Figure 13.a and in other references [51,54] that the mathematical model deviates from the simulation results in a similar fashion. For the CC and UC cases, mode splitting or EIT [55,73] is observed. On the other hand, the OC case superscattering or EIA[72,84] is observed as can be seen in Figure 14. Figure 14.b shows the avoidance crossing dispersion relation where the variation of only the A-Si spacer thickness results in changing the PAMM resonance or absorption maximum.
Figure 14. Absorption spectra for PAMM resonantly coupled to a molecular resonance at 52 THz (white dashed line) for OC (a) and UC (b) cases for various A-Si spacer thicknesses. c) Numerical, stars (*), and mathematical model, solid line, are shown for resonant coupled cases of over-, critically-, and under-coupled cases.

Table 2. SI-CS model fit parameters using Eq. 2.10.

<table>
<thead>
<tr>
<th></th>
<th>$f_1$ [THz]</th>
<th>$\gamma_e$ [THz]</th>
<th>$\gamma_1$ [THz]</th>
<th>$f_2$ [THz]</th>
<th>$\gamma_2$ [THz]</th>
<th>$V$ [THz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>OC</td>
<td>52.0</td>
<td>1.93</td>
<td>4.26</td>
<td>51.9</td>
<td>0.22</td>
<td>0.71</td>
</tr>
<tr>
<td>CC</td>
<td>52.1</td>
<td>2.34</td>
<td>2.12</td>
<td>51.8</td>
<td>0.20</td>
<td>0.70</td>
</tr>
<tr>
<td>UC</td>
<td>51.5</td>
<td>2.87</td>
<td>1.16</td>
<td>51.9</td>
<td>0.14</td>
<td>0.70</td>
</tr>
</tbody>
</table>

2.5 Conclusion

Mode coupling between the resonances of a wide-field-of-view PAMM and a vibration resonance in PMMA at 52 THz is observed. The PAMM is analyzed...
using TCMT, and the critical coupling condition where the internal and external losses are equal or impedance matched is shown. It is shown in Figure 14 how transition from undercoupled to overcoupled design of the PAMM results in transition from a transparency window centered at 52 THz to an absorption peak at 52 THz which provides evidence of mode coupling between the PAMM and vibrational resonances. Mode coupling based metamaterial devices provide benefits in selectivity as can be seen in Figure 14.a and 14.b. As the resonance of the metamaterial is tuned via the silicon spacer, the metamaterial molecular vibration coupled system decouples and the resonances return to their uncoupled states. In the case of a critically or undercoupled design, a unique mode splitting signature is produced and is used for identification purposes by increased absorption of metamaterial molecular vibration coupled system.
Chapter 3: Fano Resonance Metamaterial

(FRMM)

3.1 Introduction

Fano resonance[66] is evidenced by an asymmetric line shape, as seen in Figure 7. This line shape in a classical sense can be described as the interaction between a bright and dark mode. A Fano resonance metamaterial (FRMM)[51,55,85,86] is a metamaterial whose structure supports an asymmetric reflection or transmission spectrum. In the application of biosensing and/or molecular detection, FRMM provides a high Q-factor dark resonance, which can provide a relatively large field enhancement. In this section, TCMT and numerical analysis with HFSS are used on FRMM sensors. Then PMMA’s molecular resonance is introduced to observe mode coupling between the PMMA’s molecule resonance and the metamaterial resonance, and the effect of breaking the symmetry of the metasurfaces seen in Figure 16 is investigated with a discussion on the role of multi-coupled resonances. In the conclusion, there is a discussion of electromagnetic induced transparency (EIT) and absorption (EIA) and their relationship to FRMM design.
Figure 15. A FRMM as modeled in HFSS for a) a dual nano rod and b) a dual nano slot.

3.2 Reflection Spectrum

3.2.1 TCMT Mathematical Model for Fano Resonance

Given that in Figure 16 there is no ground plane, a new TCMT model needs to be developed with two ports. A single input single output coupled system (SISO-CS)[67,77,78] is as follows:

\[
\begin{align*}
\frac{d}{dt} \begin{bmatrix} a_1 \\ a_2 \\ \end{bmatrix} &= \begin{bmatrix} j\omega_1 - (\gamma_1 + \gamma_2) \\ jV_{12} \\ \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \end{bmatrix} + \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \\ \end{bmatrix} \begin{bmatrix} S_1^+ \\ S_2^+ \\ \end{bmatrix} \\
\begin{bmatrix} S_1^- \\ S_2^- \end{bmatrix} &= \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} S_1^+ \\ S_2^+ \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}
\end{align*}
\] (3.1)

where Eq. 3.1 can be written in general matrix form as:

\[
\begin{align*}
\Omega a &= \alpha S^+ \\
S^- &= cS^+ + da
\end{align*}
\] (3.2)
where \( \mathbf{\Omega} = \begin{bmatrix} j(\omega - \omega_1) + (\gamma_1 + \gamma_e) & j V_{12} \\ j V_{21} & j(\omega - \omega_2) + \gamma_2 \end{bmatrix} \). From the general scattering matrix in Eq. 2.8, it follows for \( S_{11} \) and \( S_{12} \) for a two-terminal coupled system that:

\[
S_{11}(\omega) = c_{11} + \frac{\alpha_{21} d_{12} [j(\omega - \omega_1) + (\gamma_1 + \gamma_e)] + \alpha_{11} d_{11} [j(\omega - \omega_2) + (\gamma_2)] - j [\alpha_{11} d_{12} V_{21} + \alpha_{21} d_{11} V_{12}]}{\det(\mathbf{\Omega})} \quad (3.3.a)
\]

\[
S_{21}(\omega) = c_{21} + \frac{\alpha_{21} d_{22} [j(\omega - \omega_1) + (\gamma_1 + \gamma_e)] + \alpha_{11} d_{21} [j(\omega - \omega_2) + (\gamma_2)] - j [\alpha_{11} d_{22} V_{21} + \alpha_{21} d_{21} V_{12}]}{\det(\mathbf{\Omega})} \quad (3.3.b)
\]

Exploiting the dark mode definition for \( a_2 \) (i.e. \( \alpha_{21} = \alpha_{22} = 0 \)) leads to:

\[
S_{11}(\omega) = c_{11} + \frac{\alpha_{11} d_{11} [j(\omega - \omega_2) + (\gamma_2)] - j \alpha_{11} d_{12} V_{21}}{\det(\mathbf{\Omega})} \quad (3.4.a)
\]

\[
S_{21}(\omega) = c_{21} + \frac{\alpha_{11} d_{21} [j(\omega - \omega_2) + (\gamma_2)] - j \alpha_{11} d_{22} V_{21}}{\det(\mathbf{\Omega})} \quad (3.4.b)
\]

It can be seen that Eq. 3.4 reduces to the SI-CS case, Eq. 2.9, when \( d_{12} = d_{21} = d_{22} = 0 \).

![Two-port coupled resonant circuit system that can use a Fano resonant metamaterial (FRMM).](image)

Figure 16. Two-port coupled resonant circuit system that can use a Fano resonant metamaterial (FRMM).
3.2.2: FRMM Simulated Results

Both unit cells shown in Figure 15 are simulated without and with PMMA's molecular vibrational resonance. Figure 17.e and 18.e show the dual nano rod and slot metasurface unit cell. Both unit cells were designed such that the transmission coefficient exhibits the Fano line shape, as seen in Figure 17.a and 18.a, as well as the phase distributions of the E-field and H-field for the nano rod and slot respectively, as seen in Figure 17.b-d and 18.b-d. The conclusion of this chapter explores the results of whether the reflection coefficient exhibits the Fano line shape.

Figure 17. a) Transmission, reflection, and absorption of the dual nano rod metamaterial structure where the transmission exhibits typical asymmetric resonant response, which can be contributed to Fano-like resonant coupling; b-d) are E field phase distributions that show a parallel (bright) and anti-parallel (dark) field distribution; e) Top view of symmetric dual nano rod unit cell (meta-atom).
3.3 Normal Mode Splitting with an FRMM

With the use of the hybridization models for Fano resonance in nanostructures[54,87], the FRMM results from the coupling between two existing modes, a dark and a bright mode, which are both supported by the metamaterial. Therefore, with the introduction of the PMMA's photon resonance, multi-resonate coupling would occur. The phonon resonance of the PMMA is introduced to the FRMM. Then the asymmetry of the metasurface is tuned, as seen in the inset of Figure 19.a and 20.a. The percent of asymmetry is defined as:
\[ \alpha = 100\% \left(1 - \frac{\Delta L}{L}\right) \]  

where \(\Delta L\) and \(L\) are shown in the inset of Figures 19.a and 20.a. Figure 19.a shows the nano rod FRMM without PMMA and the effect of tuning the asymmetry of the metasurface where the black solid line is the symmetrical case for reference. With the FRMM with PMMA's molecular resonance, the typical mode splitting in the symmetrical case can be seen in Figure 19.b. It can be seen in Figure 19.b that by tuning the asymmetric parameter, there is an enhancement at both resulting hybrid mode resonances at around 51.4 THz and 52.6 THz, where enhancement is defined as a decrease in reflection. Similar results can be seen in Figure 20 at the hybrid modes frequency 51.4 THz in the case of the nanoslot FRMM where an enhancement can be seen when breaking the symmetry of the FRMM. The addition of breaking the symmetry of the FRMM adds an additional degree of freedom of tunability as can be seen in Figure 19.a and 20.a. The introduction of the PMMA’s vibrational resonance results in the mode splitting signature. The mode splitting signature reflectance can be further reduced or enhanced thus allowing better signal to noise ratio for reflection based spectrometry.
Figure 19. a) Nano rod metasurface without PMMA phonon resonance with varying asymmetry as depicted in the inset; b) The resulting mode splitting as a result of varying asymmetry of the metamaterial unit cell with the introduction of the PMMA molecular resonance.
3.4 Complementary Fano Resonated Metamaterial

As evident in Figures 17.a and 18.a, the transmission spectrum of both FRMMs, nanorod and nanoslot, have Fano resonance lineshapes. However, if a complementary metasurface i.e., metasurface where the metallization is inverted
(e.g. nanopatch metasurface complement would be a nanohole metasurface), is considered then the resulting transmission spectrum is inverted similar to that reported in [71,88-94]. Figure 21.a shows the results of a nano rod FRMM where the reflection coefficient exhibits the Fano resonated line shape as evident by the E-field phase distribution shown in Figure 21.c to 21.e. The results in Figure 21.b are the same as in Figure 17.a for comparison. Considering only the symmetric case, Figure 21.f shows the mode splitting results in the reflection spectrum. Figure 22 shows the transmission coefficient with the presence of the PMMA's molecular resonance. The results in the transmission have been explained in terms of electromagnetic induced transparency (EIT) and absorption (EIA)[71,72] where EIT and EIA are evident in the solid and dashed blue line respectively in Figure 22. Other work on this topic includes the nano slot EIT/EIA pair. Also, considering a field enhancement frame of mind with the use of the hybridization model, it can be predicted that the overall field enhancement of the uncoupled plasmonic dark mode increases with the coupling to the plasmonic bright mode.
Figure 21. a) Nano slot complement, i.e., nano rod metasurface with Fano-like resonance reflection coefficient; b) The result in Figure 17.a for comparison where a Fano-like resonance transmission coefficient exists; c-e) are $E$ field phase distributions that show a parallel (bright) and anti-parallel (dark) field distribution. f) The resulting mode splitting reflection coefficient when PMMA's phonon resonance is introduced.
Figure 22. The resulting mode splitting signature in the transmission coefficient for electromagnetic induced transparency (EIT) and absorption (EIA) in the solid and dashed blue lines respectively.

3.5 Conclusion

Nanorod and nanoslot metamaterials which exhibit asymmetric transmission spectra were explored for mode coupling with a molecular resonance of PMMA at 52 THz. The asymmetric transmission spectrum present is akin to a Fano resonance lineshape which results from the interaction of a broad spectral symmetric resonance (bright mode) and a high Q factor asymmetric resonance (dark mode). Both field distributions for a bright and dark mode are present as evidence in Figure 17.b-d and 18.b-d, and coupling arises due to temporal overlap brought on by the broad spectral wide of the bright mode. With the addition of the molecular
vibration, a third resonance is introduced to the coupling system. The stronger coupling between the dark mode and vibrational resonance results in the mode coupling signature. The high Q-factor nature of the FRMM’s dark mode with a spectral line with of less than 1 THz allows for advantages in selectivity as compare to the spectrally broad bright mode like in the case of the PAMM where the spectral width is approximately 8 THz. Symmetry breaking of the metasurface leads to an enhancement or reduction of the reflectance in the mode splitting signature which provides advantage to signal to noise ratios in reflective based sensing. Finally, a complementary metasurface to the nanoslot, i.e. nanorod metasurface with an inverted transmission and reflection spectrum, is investigated. In the case of the PAMM, an under and overcoupled metamaterial results in EIT and EIA respectively. A similar analogue is drawn between a metasurface and its complement coupled to a molecular resonance. Figure 22 compares the nanorod/nanoslot metasurface cases with inverted transmission/reflection spectrums. The “original” metasurface has a reduction in its transparency (EIA) at the resonance 52 THz as compared to the “complement” which has an increase in its transparency (EIT). The “complement” metasurface has an advantage when transmission-based spectroscopy is employed due to the increase in transparency in the coupled system.
Chapter 4: Phonon Polariton Enhanced

Hybrid Waveguide via 4H-SiC Substrate

4.1 Surface Phonon Polariton Theory

Surface plasmon polaritons (SPPs), see Figure 23.a, result from the coupling of electromagnetic radiation to free electrons in metal, which results in oscillation of electron charge density at the boundary of a metal and dielectric [7,95]. SPPs result in high field enhancement, which aids in spectroscopy and biosensing applications [7]. Typically, SPPs occur in a band of frequencies between near infrared (NIR) to ultraviolet (UV). For applications in molecular detection in the mid-IR (MIR) to long-IR (LIR), SPPs’ field enhancement becomes negligible. A solution to this is the use of surface phonon polaritons (SPhPs)[4,30,96] as seen in Figure 23.b. SPhPs are a result of coupling between transverse optical (TO) phonons in the IR and THz regime [30,97]. SPhPs have been demonstrated[4,98-100] and have applications ranging from long propagation length waveguiding in the IR to biosensing[3,4]. Large field enhancements of over $10^7$ due to localized hot spot in an IR dipole antenna feed gap using SPhP have been reported in [30].
Mathematically, SPPs and SPhPs are treated identically with Maxwell's equations and boundary conditions. It has been shown[7] that SPP and SPhP propagation supports only TM surface modes. As a starting point for determining the dispersion relation of a SPP (or SPhP), the single surface interface case of an SPP (or SPhP) is considered. Figure 24 shows the geometry of a single interface between a plasmon supporting noble metal (or a polar dielectric) and a dielectric with complex permittivity $\varepsilon_d$ and $\varepsilon_m$ respectively.
Figure 24. SPP and SPhP single interface propagation structure where $\varepsilon_d$ and $\varepsilon_m$ represent dielectric and metal(or polar dielectric) complex relative permittivity respectively of the two half spaces.

It has been shown[7], that TM solution field equations for $x > 0$ (dielectric half space) are:

$$
H_y(z) = A_2 e^{jk_{SPhP}z} e^{-k_d x}
$$
$$
E_z(z) = j \frac{A_2}{\omega \varepsilon_0 \varepsilon_d} k_d e^{jk_{SPhP}z} e^{-k_d x}
$$
$$
E_x(z) = \frac{-A_1}{\omega \varepsilon_0 \varepsilon_d} k_{SPhP} e^{jk_{SPhP}z} e^{-k_d x},
$$

and for $x < 0$ (metal or polar dielectric half space) are:

$$
H_y(z) = A_1 e^{jk_{SPhP}z} e^{-k_m x}
$$
$$
E_z(z) = -j \frac{A_1}{\omega \varepsilon_0 \varepsilon_m} k_m e^{jk_{SPhP}z} e^{-k_m x}
$$
$$
E_x(z) = -\frac{A_1}{\omega \varepsilon_0 \varepsilon_m} k_{SPhP} e^{jk_{SPhP}z} e^{-k_m x},
$$

where $k_{SPhP}$ is the complex propagation constant for the surface polariton mode, and $k_d/k_m$ are the wavevectors perpendicular to the material interfaces, and $A_1/A_2$ are complex constants determined from boundary conditions. From the continuity of
the boundary at \( x = 0 \), it can be seen from \( H_y(z) \) that \( A_1 = A_2 \), and therefore from \( E_\alpha(z) \), it can be seen that:

\[
\frac{k_m}{\varepsilon_m} + \frac{k_d}{\varepsilon_d} = 0.
\]  

(4.3)

From the formulation of the TM from Maxwell’s equation, it has been shown that the propagation constant, \( k_{sp} \), is in the two regions as the following [7]:

\[
\begin{align*}
 k_{sp}^2 + k_m^2 &= \varepsilon_m k_0^2 \\
 k_{sp}^2 + k_d^2 &= \varepsilon_d k_0^2.
\end{align*}
\]  

(4.4)

Solving for \( k_{sp} \) using Eqs. 4.3 and 4.4 gives the dispersion relationship for SPP or SPhP as follows [4,30]:

\[
k_{sp} = k_0 \sqrt{\frac{\varepsilon_m(\omega)\varepsilon_d}{\varepsilon_m(\omega)+\varepsilon_d}}.
\]  

(4.5)

The propagation distance, \( L_m \), of the TM mode in the \( z \) direction can be determined using Eq. 4.5 in terms of power or intensity as:

\[
L_m = \frac{1}{2Im(k_{sp})}.
\]  

(4.6)

The nature of the TM polariton mode is that of an exponentially decaying field in the transverse direction, \( x \) direction as shown in Figure 24, to the propagation into the metal (or polar dielectric) and dielectric regions, i.e., evanescent wave. The decaying exponential terms can be determined by substituting Eq. 4.5 into Eq. 4.4 resulting in:
\[ k_d = k_0 \sqrt{\frac{\varepsilon_d^2}{\varepsilon_m(\omega) + \varepsilon_d}} \]
\[ k_m = k_0 \sqrt{\frac{\varepsilon_m^2(\omega)}{\varepsilon_m(\omega) + \varepsilon_d}}. \] (4.7)

Similar to propagation distance, a skin depth concept can be applied to the TM surface modes; a penetration depth within the two regions is defined as:

\[ \delta_d = \frac{1}{2 \text{Im}\{k_d\}} \]
\[ \delta_m = \frac{1}{2 \text{Im}\{k_m\}}, \] (4.8)

where the total modal extent of the TM surface mode in the transverse direction can be defined as:

\[ \delta_{PD} = |\delta_d| + |\delta_m|. \] (4.9)

Using \( \delta_{PD} \) and \( L_m \), a figure of merit (FOM) can be established similar to the case of hybrid plasmonic waveguides \( (FOM = L_m/\sqrt{A_m}, \text{ where } A_m \text{ is the modal area}) \) which is:

\[ FOM = \frac{L_m}{\delta_{PD}}. \] (4.10)

The \( FOM \) in Eq. 4.10 is used to guide the design of the hybrid waveguide in the following section. The \( FOM \) in Eq. 4.10 provides away to compute an optimum trade-off between mode confinement and propagation distance as a function of frequency of the polariton mode. The optimum FOM will provide a frequency range in which to design the hybrid phonon polariton waveguide.
4.2 4H-SiC Phonon Polariton Hybrid Waveguide

Optical interconnects in the MIR to LIR can be achieved via a polar dielectric with a highly reflecting metallic-like material ($\varepsilon_{PD} < 0$), which is known as the reststrahlen band [4]. Silicon carbide (SiC) is a polar dielectric with a multitude of polytypes or crystalline structures [101-104]. The 4H-SiC polytype, seen in Figure 25, is commercially available as a substrate. 4H-SiC reststrahlen band and uniaxial complex permittivity tensor components[105] can be seen in the inset of Figure 26. 4H-SiC is difficult to pattern or etch into a tracer waveguide; however other polytypes such as 3C-SiC, aluminum nitride (AlN), and gallium nitride (GaN) thin films can be heteroepitaxially grown onto a 4H-SiC substrate [106].

![Figure 25](image)

Figure 25.(a) Simple 2D projection of the unit cell of the 4H-SiC with crystal ordination plane vector directions.(b) 4H-SiC 3D zigzag crystal plane with unit cell shown. [101]
Figure 26. 4H-SiC uniaxial anisotropic complex dielectric tensor components. The top shows the real part of the relative permittivity, and the bottom shows the dielectric loss tangent of 4H-SiC. The reststrahlen band is highlighting the inset of the real part of the permittivity[105].
The hybrid waveguide geometry that is considered is shown in Figure 27. GaN is a low-loss dielectric in the reststrahlen band of the 4H-SiC, as seen in Figure 28, in which a heteroepitaxial thin film can be grown on 4H-SiC. The hybrid waveguide shown in Figure 27, which is feasible to fabricate, provides a long propagating waveguide with highly confined modes in the mid- to long-wave IR bandwidth. The amorphous silicon (A-Si) tracer is a square with a width ‘d’ resting on a heteroepitaxial thin film of a GaN spacer of thickness ‘h,’ which is grown on a 4H-SiC substrate.

Figure 27. Geometry of the 4H-SiC enhanced hybrid phonon polariton hybrid waveguide. A square tracer of A-Si with dimensions d x d is separated a distance h from a 4H-SiC substrate by a GaN spacer. The principal axes anisotropic crystal of the 4H-SiC substrate is labeled with their respective relative permittivity.
Using the plasmon hybridization model[107] and coupled mode theory (CMT)[59,60], the waveguide hybrid mode can be analyzed from the interaction of two uncoupled modes, the waveguide or tracer mode and the polariton mode. The hybrid mode, using a first order approximation via CMT, is a superposition of the two uncoupled modes:

$$\psi_{\pm}(h, d) = a_{\pm}(h, d)\psi_{m1} + b_{\pm}(h, d)\psi_{m2}. \quad (4.11)$$

where $a_{\pm}(h, d)$ and $b_{\pm}(d, h) = \sqrt{1 - |a_{\pm}(h, d)|^2}$ are complex amplitude weights for the two uncoupled modes. Similar to that in coupled resonances, mode splitting occurs, resulting in an upper (‘symmetric’) and lower (‘antisymmetric’) hybrid polariton mode where the separation between the modes is related to a coupling strength ($\kappa$) [28,45,47,107].The coupled mode index equation can be written in a matrix form as follows:

$$\begin{bmatrix} n_{m1} \\ \kappa(h, d) n_{m2} \end{bmatrix} \begin{bmatrix} a_{\pm}(h, d) \\ b_{\pm}(h, d) \end{bmatrix} = n_{\pm}(d, h) \begin{bmatrix} a_{\pm}(h, d) \\ b_{\pm}(h, d) \end{bmatrix}, \quad (4.12)$$

where

$$\kappa^2(h, d) = (n_{\pm}(h, d) - n_{m1})(n_{\pm}(h, d) - n_{m2}), \quad (4.13)$$

where $n_{mi}$ are the index of the uncoupled modes, $n_{\pm}$ are the upper and lower hybrid modes respectively. It can be seen that for the lower hybrid mode, $n_{-}(h,d)$, does not exist or is ‘cut off,’ given the limiting factor for the hybrid mode is $n_{SPhP}$, i. e.,
\( n_-(h,d) < n \text{SPhP} \) [3]. Thus the only bound mode is the upper hybrid mode which is bound by tracer waveguide mode as \( d \to \infty \) and the SPhP as \( d \to 0 \).

![Complex permittivity for GaN](image_url)

**Figure 28.** Complex permittivity for GaN used for as a spacer in the hybrid waveguide. The top shows the real part of the relative permittivity, and the bottom shows the dielectric loss tangent of GaN.

The SPhP mode dispersion can be determined using Eq. 4.5 and is plotted in Figure 29 with the dielectric half space (\( \varepsilon_d \)) under consideration being air and both the 4H-SiCs being uniaxial dielectric components. Figure 30 plots the TM SPhP mode’s propagation length and penetration depth calculated from Eqs. 4.6 and 4.8 respectively. From the results in Figure 31, the FOM of Eq. 4.10 can be
determined, and thus guide the selection of an operation frequency for the hybrid waveguide.

Figure 29. SPhP dispersion relationship, Eq. 4.5, of the uniaxial 4H-SiC half space and air for both anisotropic components of the 4H-SiC.
Figure 30. (a) SPhP penetration depth, Eq. 4.8, and (b) propagation length, Eq. 4.6, for a uniaxial 4H-SiC and air half space.

Figure 31. The resulting FOM, Eq. 4.10, computed from the results shown in Figure 30 for a uniaxial 4H-SiC and air half space for both anisotropic components of the 4H-SiC.
It can be seen from Figure 31 that the maximum of the FOM in a bandwidth of wavelengths ranges from 12.0 to 12.4 μm. An operation wavelength in the middle of the band, 12.2 μm, is selected for the hybrid waveguide. In the case of the hybrid mode, the parameters of interest are the propagation length ($L_m$), mode area ($A_m$), and hybrid index. The propagation length is determined numerically with Ansys HFSS eigenmode solver via the quality factor, $Q$, as follows [108]:

$$L_m = \frac{1}{2a} = \frac{Q\lambda_0}{2\pi n_{hyb}}, \quad (4.14)$$

where $v_g$ and $v_p$ are the group and phase velocities respectively. The mode area of the hybrid can be determined via the stored electromagnetic energy as:

$$A_m = \frac{W_m}{\max\{W(r)\}} = \frac{\iint W(r) dx dy}{\max\{W(r)\}, \quad (4.15)$$

where $W_m$ and $W(r)$ are the electromagnetic energy and energy density, and for anisotropic media the energy density can be determined by [109]:

$$W(r) =\frac{1}{2} \left[ \frac{d(e'_{\perp}(\omega)\omega)}{d\omega} |E_x|^2 + \frac{d(e'_{\parallel}(\omega)\omega)}{d\omega} |E_y|^2 \right. + \left. \frac{d(Re[e'_{\perp}(\omega)\omega])}{d\omega} |E_z|^2 \right] + \mu_0 |H(r)|^2. \quad (4.16)$$

A more detailed discussion of determining the electromagnetic energy using Ansys HFSS field calculator is given in Appendix B. The parameters, tracer size, and spacer height are varied to characterize the tradeoff between propagation length ($L_m$) and the modal area ($A_m$). The modal area is normalized using the diffraction-
limited area, i.e., $A_0 = (\lambda_0/2)^2$, and the resulting normalized model, $A_m/A_0$, is plotted in Figure 32 along with the propagation length, $L_m$. The energy density of the hybrid modes for $[h,d] = [1.0, 2.0]$, [0.25, 2.0], and [0.25, 3.5] µm can be seen in Figure 33.c-e. It can be seen in Figure 32 that the mode is confined, ranging from $\lambda_0^2/10$ to $\lambda_0^2/50$ for a propagation length of 10 µm to 250 µm for a hybrid waveguide design that can be realistically fabricated.

Figure 32. The normalized mode area (a) and propagation length (b) for varying cases of GaN space thickness is shown with varying A-Si tracer heights/widths at a free space wavelength of operation at 12.2 µm. The inset of (a) shows the geometry for the ridge waveguide used in determining the normalized mode area for that ridge waveguide (dashed black line). The electromagnetic energy density distributions are shown in (c)-(e) for hybrid waveguide modes at $[h, d] = [1.0, 2.0]$ µm (c), $[h, d] = [0.25, 2.0]$ µm (d), and $[h, d] = [0.25, 3.5]$ µm (e).
The magnitude square of the complex amplitude, \( a_+(h,d) \), denotes the ‘character’ of the hybrid mode and is determined by:

\[
|a(h, d)|^2 = \frac{\kappa(h,d)^2}{(n_{hyb}(h,d) - n_{wg}(h,d))^2 + \kappa(h,d)^2},
\]

(4.17)

where the \( n_{wg} \) is the tracer embedded in an effective medium containing a weighted sum of air and spacer of GaN and thickness ‘\( h \)’. \( n_{wg}(h,d) \) used in Eq. 4.17 is depicted in Figure 33 by dashed color lines for various spacer thicknesses and ‘\( d \)’.

Figure 33. The effective index of the hybrid waveguide for varying tracer dimension, ‘\( d \)’, and space height, ‘\( h \)’. The dashed color line indicates the tracer mode embedded in an effective air-GaN spacer medium \( (n_{wg}) \), and the broken line indicates the SPhP mode in an effective air-GaN spacer medium \( (n_{SPhP}) \).
Figure 34. a) The mode character, Eq. 4.17, and coupling strength, Eq. 4.13, calculated for the tracer mode embedded in effective air-GaN media. $|a(h,d)|^2 > 0.5$ the hybrid mode is more cylinder-like and $|a(h,d)|^2 < 0.5$ the hybrid mode is more SPhP-like. $|a(h,d)|^2 = 0.5$ approximately when $d = 2.0 \, \mu m$, which is a slightly smaller tracer size than where the maximum coupling strength resides at around $2.5 \, \mu m$ or the range of $|a(h,d)|^2 \approx 0.55 - 0.60$.

4.3 Conclusion

The first practical mid- to long-wave IR waveguide is numerically analyzed at an operating wavelength of $12.2 \, \mu m$ in this dissertation. Sub-diffraction modal area of a factor less than $5 \times 10^{-2}$ times the free space diffraction-limited area with propagation length of 5 times greater than the free space wavelength are shown. Hybrid waveguides are limited by the propagation lengths of the pure polariton mode and therefore low-loss polar dielectrics are desirable. In addition, a multilayer system made from a thin film polar dielectric like aluminum nitride can be used to create coupled surface polariton modes which results in long-range propagation polariton modes. The mid- to long-wave IR spectrum hosts a multitude of IR
vibrational resonances which could be sensed using a hybrid waveguide based device like a Mach-Zehnder interferometer (MZI) that will be evaluated in the following chapter.
Chapter 5: Phonon Polariton Enhanced Optical Directional Coupler and Mach-Zehnder Interferometer via 4H-SiC Substrate

5.1 Ansys HFSS Driven Modal Surface Waves

Driven modal analysis in Ansys HFSS is used to calculate reflection and transmission coefficients (S-parameters) for passive high frequency structures like microstrips and waveguides \cite{37,38}. S-parameter analysis is needed when investigating and designing an optical directional coupler (ODC), and consequently, a Mach-Zehnder interferometer (MZI). The first fundamental question is: can an Ansys HFSS’ driven modal be used to excite TM surface polariton modes? To answer this question, a single interface of silver/SiO$_2$[110] is considered, where $\varepsilon_{\text{SiO}_2} = 2.25$, as seen in the inset of Figure 36. Figure 35 shows the magnitude and vector plots for the electrical and magnetic fields at 300 THz, simulated using Ansys HFSS driven modal analysis for a TM surface mode propagating on a SiO$_2$/Silver interface. The corresponding complex propagation constant is plotted in terms of $1/\lambda_{\text{SPP}}$ and $L_m$ (propagation length) in Figure 36.a and b respectively.
Figure 35. The driven modal results for a TM surface mode at 300 THz from a SiO$_2$/Silver interface. The $|E|$ and $|H|$ are shown in (a) and (b) respectively and the electrical and magnetic field vectors are shown in (c) and (d) respectively.

Figure 36. a) The driven model result for the TM surface mode is compared to the analytical expression in Eq. 4.5. b) The result for the propagation length of the numerical simulated TM surface mode is compared to the analytical expression in Eq. 4.6.

It can be seen that driven mode can indeed excite a TM surface mode. However, it can only be used to approximate a surface polariton mode in the transition region.
between surface polariton and Zenneck (or Uller-Zenneck) waves [7,111-113], i.e., \( Re(k_{SP}) \leq k_0(\varepsilon_d)^{1/2} \), as seen in the results of Figure 36. Therefore, in the designs of the ODC and MZI using the driven mode, wavelengths closer to the TO resonance inside the reststrahlen band are considered, and as such, the hybrid operation wavelength under consideration is 12.4 \( \mu m \) for the ODC and MZI designs.

5.2 Waveguide Isolation

Figure 37 shows the hybrid SPhP waveguide cross-section that is considered at a wavelength of 12.4 \( \mu m \). The tracer dimension is 2.5 \( \mu m \) on top of a 250 nm GaN spacer on an anisotropic 4H-SiC substrate. The numerical simulation results comparing eigen and driven modes of the hybrid geometry are shown in Figure 38 and tabulated in Table 3.
Figure 37. The hybrid SPhP enhanced waveguide geometry cross-section under consideration where the A-Si tracer is 2.5 μm square separated from a 4H-SiC substrate with a GaN spacer of 0.25 μm thickness. The separation, s, between A-Si tracers is shown.

Table 3. Hybrid SPhP waveguide results at wavelength 12.4 μm comparing eigen and driven mode results.

<table>
<thead>
<tr>
<th></th>
<th>Eigen Mode Results</th>
<th>Driven Mode Results</th>
</tr>
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<tbody>
<tr>
<td>n_{hyb}</td>
<td>L_m</td>
<td>A_m/A_0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.71</td>
<td>67.0 μm</td>
<td>1.60E-2 55%</td>
</tr>
</tbody>
</table>

In designing the ODC, the separation between the waveguide, s, is first quantified. Figure 38.a shows the coupling or transfer of power between the two waveguides as a function of separation distance ‘s’ as seen in Figure 37. It can be seen at s = 4 μm that, under 3% of the power is coupled from one waveguide to the other waveguide. Therefore, a separation distance of over 4 μm is considered to provide
sufficient isolation between the input ports. The $|E|^2$ on the 4H-SiC/GaN interfaces is shown in Figure 38.b-c for separation distances of 1.0μm, 2.0μm, and 3.5 μm.

![Graph showing $|A_n(L_0)|^2$ normalized for different separation distances (s).](image)

**Figure 38.** a) The normalized power for both output ports 3 and 4 as a function of waveguide separation “s” is shown. The $|E|^2$ on the 4H-SiC/GaN interfaces is shown for $s$ equal to 1 μm (b), 2 μm (c), and 3.5 μm (d).

### 5.3 Optical Directional Coupler

Using the isolation analysis between the two waveguides shown in Figure 38, the top view of the ODC with dimensions labeled is shown in Figure 39. The ODC device transverse dimension is currently 14.7 μm; however, with optimization, the ODC’s transverse direction footprint can be reduced to sub-wavelength either by
decreasing separation, reducing the tracer dimensions, or reducing the operational wavelength, i.e., a more SPhP-like design.

Figure 39. Top view of ODC geometry under consideration with dimensions labeled. The length $L$ where the two waveguides are in close proximity is shown.

The output power ports for a phase matched, symmetrical, ODC are computed [114-116]:

$$|A_1(z)|^2 = e^{-2\alpha L} \cos^2 \left( \frac{\pi}{2L_0} L \right),$$

$$|A_2(z)|^2 = e^{-2\alpha L} \sin^2 \left( \frac{\pi}{2L_0} L \right),$$

where two times the transfer length, $L_0$, is referred to as the beat length, $\alpha$ is the field attenuation as the wave propagates through the ODC, and $L$ is the coupled section length of the ODC. Figure 40.a and b show the normalized output port power and phase difference between the output ports, port 3 and 4, as a function of coupling section, $L$, respectively. The numerical results (*) of Figure 40.a take on
the exponentially decaying sinusoidal relationship described by Eq. 5.1. Figure 40.c shows the $|E|^2$ for a coupling section at the 3 dB coupling point. It can be seen that approximately both ports each have power and are $90^0$ out of phase with respect to each other.

![Diagram showing the normalized power and phase difference between the ports at various coupling lengths.](image)

Figure 40. The normalized power a) and phase difference between the ports b) of the output ports at various coupling lengths. c) The $|E|^2$ at the 4H-SiC/GaN interfaces is shown for when the ODC is a 3dB splitter.

In a power splitting application, port 2, seen in Figure 40.c, has negligible power outputted from the port. However, in a power combining application, i.e., input
power into port 1 and 2, the ODC can be used as a phase-to-amplitude transducer, as seen in Figure 41.b where the two input ports amplitudes are equal to each other. However, the relative phase is shifted by $\Delta \theta$ degrees. The power of the output ports is then coupled into a balance detector. In Figure 41.a, it can be seen that, as the relative phase difference between the two input ports changes the normalized output power amplitude level change with a similar sinusoidal relationship, as shown in Figure 40.a.

![Diagram](image)

Figure 41. a) The normalized output port power as a function of phase between the input ports ($\Delta \theta$) for an ODC. b) Diagram depicting the phase shift between the input ports of an ODC. The constructive and destructive output port signals of an ODC are detected with a balance detector.
5.4 Mach-Zehnder Interferometer

A Mach-Zehnder interferometer is formed by interconnecting two ODCs, as seen in Figure 42. The MZI that is considered is the two ODCs connected with a 5.0 μm section of waveguide. Similar to the case of the ODC, the normalized output power of the MZI is plotted as a function of the coupling section: $L$ in Figure 43.a. The normalized power takes on an exponentially decaying sinusoidal as described by Eq. 5.1. Figure 43.b shows the $|E|^2$ for the MZI where the coupling sections of the ODC are 3dB splitters. As can be seen in Figure 43.b, the MZI acts like an optical switch to transfer power into another guide.

![Figure 42. Top view of the MZI geometry with the port labeled.](image)

As in the case of the ODC, the MZI acts as a phase-to-amplitude transducer, as seen in Figure 44. The powers inputted into the ports are considered to have the same amplitude, with a relative phase difference between the inputs. The
normalized output port power as a function of phase between the input ports for both constructive and destructive ports can be seen in Figure 44.

Figure 43. a) The normalized output port power is shown as a function of the coupling length of the ODC. b) The $|E|^2$ at the 4H-SiC/GaN interfaces is shown for when the ODC coupling lengths are at 3dB splitter/combiner.
Figure 44. a) The normalized output port power as a function of phase between the input ports ($\Delta \theta$) for a MZI. b) Diagram depicting the phase shift between the input ports of the MZI. The constructive and destructive output port signals of the MZI are detected with a balance detector.

5.5 Conclusion

Numerical analysis for a mid to long IR ODC and MZI using a hybrid waveguide enhanced with 4H-SiC phonons is conducted. The normalized power output for both the ODC and MZI conform to CMT predictions. A MZI is a fundamental device that is used in interference based sensing where an unknown material is used to change the optical path length of a sensing arm of a MZI. The ultra-compactness and localized field enhancement brought on by polaritons play into both miniaturizing the device for SWaP and increasing field-analyte interaction which results in high sensor sensitivity in the mid- to long-wave IR spectrum. Also, the
relative phase-to-amplitude transducer capability of a mid- to long-wave IR polariton based ODC and MZI is analyzed. These results provide an incremental step forward in coherence detection in the mid- to long-wave IR wavelength for extracting phase information in IR antenna applications.
Chapter 6: Hyperbolic Phonon Polariton

Enhanced Optical Interconnects via

Hexagonal Boron Nitride

6.1 Hexagonal Boron Nitride

Hexagonal boron nitride (hBN) is a van der Waals material with naturally occurring hyperbolic dispersion that supports sub-diffractional volume-confined polaritons [96,117-122]. A thick film of hBN has been shown to provide interferenceless perfect electromagnetic absorption [123]. Hyperbolic materials are one path to negative index and sub-diffractional imaging [124,125]. Hyperbolic dispersion can lead to exotic behavior in which the wavevector $k$ is antiparallel to the Poynting vector $S$ which is normal to the hyperbolic $k$-surface, and thus negative dispersion or index [96,119]. Unlike 4H-SiC, hBN has two Reststrahlen bands: an upper (type II) and a lower (type I) as seen in Figure 45 [96]. At large $\vec{k}$, the hyperbolic dispersion can be approximated as a cone [96,118,119]:

$$\frac{k_z^2}{\varepsilon_r(\omega)} + \frac{k_t^2}{\varepsilon_z(\omega)} = 0,$$

where the complex permittivity tensor, $\varepsilon_{zt(\omega)}$, is shown in Figure 45. From Eq. 6.1, the HPhP $\vec{k}$ angles are restricted and the Poynting vector, orthogonal to $\vec{k}$, is given by the complex hBN permittivity as [96,119]:

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\[ \theta = \frac{\pi}{2} \pm \arctan \left( \frac{\sqrt{\varepsilon_x(\omega)}}{j\sqrt{\varepsilon_z(\omega)}} \right). \] (6.2)

The resulting propagation angle, \( \theta \), exists in both the upper and lower Reststrahlen bands, and is the key to the super-resolution or sub-diffraction imaging application in hBN [119,126].

![Diagram](image_url)

Figure 45. The real part (a) and dielectric loss tangent (b) of the complex permittivity tensor components of hBN [96,119]. The upper (type II) and lower (type I) Reststrahlen bands are shaded.

Interest in boron nitride can be traced back to the development of boron nitride nanotubes (BNNT) in the mid-1990s[127], slightly after the development of carbon
nanotubes [128]. Only in the last few years have mid-IR phonon polaritons have been measured in hBN [118,129]. Phonon polariton excitation in 1D, BNNTs, has been reported in [129-131]. In the case of BNNTs, the supported phonon polariton has been referred to as “surface” phonon polaritons where Eq. 4.5 applies in describing the BNNT dispersion [129-130]. A metal slab (or insulator-metal-insulator, IMI, heterostructures) analogy has been applied to thick hBN in a discussion of BNNT [130]. In an IMI structure two modes are supported: a symmetric and asymmetric mode with fields on both insulator/metal interfaces. When the metal slab thickness increases, the symmetric and asymmetric modes become degenerate, and the dispersion of the two modes converges onto that of a surface polariton mode (Eq. 4.5) [7,130]. However, using the cone approximation from Eq. 6.1, a thin hBN slab where $\lambda_{\text{HPhP}} \ll \lambda_0$, the dispersion for the hyperbolic phonon polaritons in the hBN is [118]:

$$k_{\text{HPhP}} = -\frac{\psi}{d} \left[ \arctan \left( \frac{\varepsilon_{\text{oc}}}{\varepsilon_t(\omega)} \psi \right) + \arctan \left( \frac{\varepsilon_s}{\varepsilon_t(\omega)} \psi \right) + \pi l \right],$$

$$\psi = -j \sqrt{\frac{\varepsilon_s(\omega)}{\varepsilon_t(\omega)}},$$

(6.3)

where $\varepsilon_{\text{oc}}$ and $\varepsilon_s$ are the permittivities of the over-coated and the substrate materials respectively, $l$ is the modal number where type II: $l = 0, 1, 2, \ldots$ and type I: $l = -1, -2, -3, \ldots$ as can be seen in the solid color lines in Figure 47. Figure 46 compares eigen mode numerical results for the type II HPhP index of a $1 \mu$m thick hBN slab as a function of frequency to the approximations of Eq. 4.5 and Eq. 6.3 for the
cases of with and without a SiO$_2$ substrate. For Eq. 4.5, the first order approximation of $(\varepsilon_{\text{air}} + \varepsilon_{\text{SiO2}})/2$ were used for $\varepsilon_d$. It can be seen that they hold fairly well in their respective regimes; however, it is important to stress that Eq. 4.5 is an approximation, and the HPhP mode is not a pure surface mode as in the case of 4H-SiC nor is it an IMI mode with field only on the insulator-metal boundaries. The mode field, strictly speaking, not only resides on the interfaces, but also resides in the hBN slab volume itself due to the anisotropic material, i.e., $\varepsilon_z > 0$, and the TM mode nature. Also, the SPhP approximation does not speak to the HPhP’s multimodal nature, the hBN thickness dependence, and is not valid for type I HPhP. The SPhP approximation is only valid for the type II fundamental asymmetric (Asym-$M_0$) and symmetric (Sym-$M_0$) modes, which are degenerate as seen in Figure 47.a.

In the following sections, hybrid geometries are considered with a coupling mode description for both type I and type II HPhPs. First, a slab waveguide is considered, then a cylinder waveguide. The frequency-dependent direction, Eq. 62, can be seen with a cylinder waveguide coupled to the hBN slab [119].

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Figure 46. The HPhP index as a function of frequency for a 1 μm hBN slab embedded in air (a) and with air overcoat and SiO₂ substrate (b) is compared to the SPhP approximation (solid red line), Eq. 4.5,[130] and hyperbolic cone approximation (dashed blue line), Eq. 6.3,[118]. The first order approximation, i.e., \((\varepsilon_{\text{air}} + \varepsilon_{\text{SiO₂}})/2\), was used for \(\varepsilon_d\) in Eq. 4.5 in (b).

Figure 47. a) Type II HPhP effective index at 6.6 μm wavelength for the first three modes. The SPhP approximation, Eq. 4.5, is shown as the dashed blue line in (a). b) Type I HPhP effective index at 12.6 μm wavelength for the first three modes. Solid color lines are from Eq. 6.3 in (a) and (b). The inset shows the normalized \(|E_t|\) along the c-axis or optical axis of the hBN slab.
6.2 Hybrid hBN Slab Waveguide

The hybrid slab geometry that is considered is shown in the inset of Figure 48.a. The dispersion of the type II hybrid is similar to that of an SPP or SPhP hybrid waveguide [132]. Using coupled mode theory, a system of coupled equations, Eq. 4.12, can be used to establish it. The type II \( n_\pm \) mode can be analyzed in a similar ways as reported in [3] as well as similar to the hybrid waveguide enhanced with 4H-SiC SPhPs in Chapter 4. Given that the upper hybrid mode, \( n_+ \), is limited to the slab waveguide mode, as the slab thickness, \( d \), becomes large. Conversely, when \( d \) becomes small, the slab dispersion tends to the index of the surrounding media, i.e., air; therefore, given \( n_{\text{HPhP}} > n_{\text{air}} \) the lower limit of the \( n_+ \) mode is that of the type II HPhP. Qualitatively, the lower mode is “HPhP-like” at lower frequencies then becomes “waveguide-like” at high frequencies, which is converse to the upper mode. Therefore, the maximum index of the lower hybrid mode is that of the HPhP, and it is limited by the waveguide index on the lower extreme. It follows that in the case of type II, the lower mode is unbounded or “cut-off” as reported in [3], given that the field is, for the most part, in the surrounding media.

As can be seen in Figure 48.a and 48.b, the \( m_0 \) type I mode’s dispersion curve decreases with increasing frequency, which results in the group velocity being anti-parallel to the phase velocity, i.e., the type I HPhP mode is backward propagating or in effect the HPhP has a negative index [133]. Mode coupling between forward and backward propagating waveguides was reported over a decade ago [134,135].
With ongoing interest in polaritons in 2D van der Waals crystals [117], coupling between phonons and plasmons of hBN and graphene to form a hybrid material in both reststrahlen bands is currently being investigated [136-138].

Unlike reported in [3], the numerical results in Figure 48.a and 48.b show the presence of both an upper and lower hybrid mode. The presence of a backward propagating upper hybrid mode can also be seen in Figure 48.b. If only the forward propagating hybrid modes are considered, it can be seen that the hybrid dispersion is bound by the same limits as the slab waveguide, i.e., air index when \( d \to 0 \) and slab waveguide index when \( d \to \infty \); therefore, in Eq.4.12 \( n_{m1} = n_{wg} \) and \( n_{m2} = 1 \).

The \( n_+ \) is more interesting given that the mode has two distinct regions: a forward and backward propagating region [135,137]. In the upper hybrid mode, \( n_+ \), forward propagation regime, similar to the type II case, is bounded by the slab waveguide mode as \( d \to \infty \), but is limited by the air index (or surrounding media), like the \( n_- \) mode, as \( d \to 0 \). Therefore, it is later shown that the \( n_+ \) forward propagation regime in the type I case can provide mode repulsion benefits without the HPhP impressing its full penalties. Also, it can be seen from the dispersion curve for \( n_+ \) in Figure 48.b that as \( |k_t| \) increases, the mode transitions from a forward to a backward propagating mode. Therefore, in a small neighborhood of the said transition point, the black vertical dashed line in Figure 48.b, slow[133] hybrid forward or backward propagating modes are possible.
Figure 48. a) The hybrid mode dispersion curve that results from coupling the type II HPhP with a slab waveguide of thicknesses $d = 3.0 \, \mu m$, $1.5 \, \mu m$, $1.0 \, \mu m$. b) The upper and lower hybrid modes are shown for slab waveguide of thicknesses $d = 5.0 \, \mu m$, $3 \, \mu m$, $2.5 \, \mu m$ for the type I case. $m_0$ calculated from Eq.3 and numerically determined are shown for type II (a) and type I (b). The hybrid waveguide geometry is shown in the inset of (a).

### 6.3 Hybrid hBN Cylinder Waveguide

The hybrid geometry that is under consideration is depicted in Figure 49. A high index cylinder waveguide of diameter of ‘$d$’ is suspended from an hBN slab of thickness of 1 $\mu m$ a distance of ‘$h$’ and embedded in air. The dielectric tensor components are shown in Figure 45, where the c-axis, optical axis, is oriented parallel to the normal of the hBN slab. The hybrid mode is characterized by varying the cylinder diameter ($d$) and height, ($h$) to study the propagation length, $L_{m_0}$, modal
area, $A_m$, and the energy density of the hybrid mode at a wavelength 6.6 $\mu$m, which is in the middle of the upper reststrahlen band.

![Figure 49](image)

Figure 49. The hybrid waveguide geometry consisting of a 1 $\mu$m thick hBN slab with a cylinder trace of $\varepsilon_d = 12.25$ (GaAs) elevated a distance $h$ above the hBN slab and suspended in air of $\varepsilon_{air} = 1$.

### 6.3.1: hBN Type II Hybrid Waveguide

The type II hybrid results for normalized modal area, $A_m/A_0$, where $A_0$ is the diffraction-limited area in free space ($\lambda_0^2/4$), propagation length, and energy density, are shown in Figure 50. As already indicated, in the type II hybrid case the only hybrid mode is the upper mode whose index is constricted by $n_{cly}$ for large $d$ and $n_{HPH}$ as $d$ approaches zero, as can be seen in the effective hybrid index shown in Figure 51. Therefore, coupled waveguide equations, Eq. 4.12, can be rewritten where $n_{m1} = n_{cly}$ and $n_{m2} = n_{HPH}$. Thus the amplitude $|a(h,d)|^2$ describes how much the hybrid mode is like a cylinder waveguide mode, and is referred to as the modal character.
The modal area, Eq. 4.15, as a function of cylinder diameters for various gap heights $h$. The cylinder modal area, solid black line, is shown for reference. b) The propagation length for the hybrid type II HPhP mode is shown for a range of cylinder diameters over different gap widths $h$. The propagation length for the pure hBN type II HPhP mode suspended in air is indicated by the dashed black line. c-f, The electromagnetic energy density, Eq. 4.16, for $[d,h] = [2.25 \text{ \mu m}, 100 \text{ nm}]$ (c), $[d,h] = [1.25 \text{ \mu m}, 100 \text{ nm}]$ (d), $[d,h] = [1.25 \text{ \mu m}, 10 \text{ nm}]$ (e), $[d,h] = [2.25 \text{ \mu m}, 10 \text{ nm}]$ (f) as labeled in part a.

The resulting modal character and coupling strength, Eq. 4.13, are plotted in Figure 52. From Figure 52.a, it can be seen when $|a(h,d)|^2 > 0.5$, the hybrid mode is more “cylinder-like”. The converse is true when $|a(h,d)|^2 < 0.5$; the hybrid mode is more type HPhP like, which can be seen by the energy density plot where there is an increase in energy inside the hBN slab rather than in the cylinder waveguide. The transition point, $|a(h,d)|^2 = 0.5$, occurs when $n_{\text{cly}} \equiv n_{\text{HPhP}}$ at $d \approx 1.25 \text{ \mu m}$[3].
Similarly, the maximum coupling strength occurs at a $d$ value greater than where the $|a(h, d)|^2 = 0.5$ transition point occurs, as is shown in Figure 52.b [139,140]. Given the strong anisotropy that leads to the hyperbolic dispersion in hBN, the frequency dependent angular propagation, Eq. 6.2, in the hBN is present in the hybrid mode, shown in Figure 53.

![Image](image_url)

Figure 51. The hybrid effective index values for different cases of gap widths $h$ range from the HPhP index of the type II, dashed black line, as $d$ approaches zero to the cylinder index, solid black line, as $d$ increases. The intersection point of the cylinder and HPhP mode is approximately when the cylinder’s diameter is 1.25 $\mu$m.
Figure 52. The modal character, Eq. 4.17, depicts two regions where when $|a|^2 > 0.5$ the hybrid mode is more “cylinder-like;” conversely, when $|a|^2 < 0.5$ regime the mode is more “HPhP-like.” The transition between points as well as the maximum coupling strength is in the vicinity of when the cylinder diameter is 1.25 μm.

Figure 53. a) The type II angle propagation within the hBN for the hybrid geometry $[d, h] = [1.5 \mu m, 100 \text{ nm}]$. The hybrid geometry’s (red circles) critical angle, $\theta$, is compared to the analytical Eq. 6.2 (solid black line). b-g) The electric-field distribution ($|E_z|$) in the c-axis is shown for wavelength values in the upper reststrahlen band. The angular propagation of the hybrid waveguide in the hBN is determined, and are plotted as red circles in part a.
6.3.2: hBN Type I Hybrid Waveguide

The type I hybrid geometry is the same as the type II shown in Figure 49. As previously discussed, the type I hybridization results in an upper and lower hybrid mode. The upper hybrid mode has a forward and backward propagation region due to bending of the upper hybrid mode. The upper-forward hybrid mode at a wavelength of 13.0 μm is under consideration and is simply named type I hybrid mode. As in the case of the type II hybrid mode, the propagation length, normalized mode area, and energy density is studied and presented in Figure 54. In the limit of \( d \to 0 \), the propagation length is not bound by the HPhP mode as in the case of the type II hybrid mode, as seen in Figure 50.b. This is a result of the lower limiting conversion to the index of air rather than the HPhP in the type II case. Therefore, in the coupled waveguide matrix in Eq. 4.12 \( n_{m1} = n_{cly} \), similar to the type II case, and \( n_{m2} = n_{air} = 1 \) results from the limiting results as explained previously. When \( n_{cly} \approx 1 \) at \( d = 2.0 \) μm, it can be seen in Figure 56.a that the mode character is approximately 0.5, as to be expected using coupled mode analysis. Similarly, for the coupling strength, the maximum occurs at a diameter greater than \( d = 2.0 \) μm.
Figure 54. a) The modal area, Eq. 4.15, as a function of cylinder diameters for various gap heights $h$. The cylinder modal area, solid black line, is shown for reference. b) The propagation length for the hybrid HPhP mode is shown for a range of cylinder diameters over different gap widths $h$. c-f) The electromagnetic energy density, Eq. 4.16, for $[d,h] = [4.0 \, \mu\text{m}, 100 \, \text{nm}]$ (c), $[d,h] = [2.75 \, \mu\text{m}, 100 \, \text{nm}]$ (d), $[d,h] = [2.75 \, \mu\text{m}, 10 \, \text{nm}]$ (e), $[d,h] = [4.0 \, \mu\text{m}, 10 \, \text{nm}]$ (f) as labeled in part a.
Figure 55. The hybrid effective index values for different cases of gap heights $h$. The cylinder mode becomes one approximately when the cylinder diameter is 2.0 μm.

Figure 56. The modal character, Eq. 4.17, depicts two regions where when $|a|^2 > 0.5$, the hybrid mode is more “cylinder-like”. The transition between points as well as the maximum coupling strength is in the vicinity of when the cylinder diameter is 2.0 μm.
The slow forward wave propagation can be seen as a function of $d$ at three different wavelengths when $h = 100$ nm. The group velocity decreases into the regime of $v_g \ll c$, i.e., an order of magnitude smaller, when $d < 3 \, \mu m$ or when the coupling strength increases, as seen in Figure 52.b and 57. It can be seen for $12.8 \, \mu m$ ($781$ cm$^{-1}$) and $13.0 \, \mu m$ ($770$ cm$^{-1}$) that the group velocities are $\sim 0.03c$ and $\sim 0.065c$ at $d = 2.25 \, \mu m$ respectively. Highly confined and slowly propagating hybrid waveguides are useful in sensing applications [133]. The frequency dependent propagation angle, $\theta$, in Eq. 6.2 also exists in the lower reststrahlen band, which results in the type I hybrid exhibiting this property inside the hBN slab. Figure 58 shows the hybrid angle as compared to Eq. 6.2. The nanofocusing of the hBN slab can be seen in the $|E_z|$ plot of Figure 58.b-g.

Figure 57. The phase and group velocities of the type I hybrid mode are plotted as a function of cylinder diameter ‘$d$’ for $\lambda_0 = 13.0$, 12.9, and 12.8 $\mu m$. Ultra-slow forward propagating waveguide modes are shown for $d$ approaching the maximum couple point.
Figure 58. a) The type I angle propagation within the hBN for the hybrid geometry $[d, h] = [3.0 \, \mu m, 100 \, nm]$. The hybrid geometry’s (red circles) critical angle, $\theta$, is compared to the analytical Eq. 6.2 (solid black line). b-g) The electric-field distribution ($|E_z|$) in the c-axis is shown for wavelength values in the lower reststrahlen band. The angular propagation of the hybrid waveguide in the hBN is determined and is plotted as red circles in part a.

### 6.4 Conclusion

A hybrid waveguide enhanced with type I and type II volumetric phonon polaritons in hBN was numerically analyzed. The type I HPhP hybrid waveguide inherits the ultra-slow wave nature for the HPhP mode. Also, a novel positive-negative dispersive mode coupling in hybrid waveguide architecture has been presented. This novel positive-negative mode splitting numerical results presents the existence of a lower hybrid mode in contrast to the claims made in reference [3]. The positive-negative mode coupling shows the resulting upper hybrid mode inherits backward propagation characterized from the type I HPhP mode. A slow light waveguide like what is numerically shown has application in slow light applications, IR imaging, and sensing [133].
Chapter 7: Conclusion

7.1 Summary of Results

This dissertation presents results for mode coupling between a metamaterial and C=O molecular resonance in PMMA for two different types of metamaterial: a perfect absorbing metamaterial and a metamaterial with a Fano resonance linewidth. Temporal coupled mode theory is applied to describe mode splitting that results from the coupling between the metamaterial and molecular resonance. Superscattering (or EIA and EIT) are observed in the overcoupled and undercoupled cases, respectively for the PAMM. A FRMM that supports dark mode quadrupoles and bright mode dipoles results in a metamaterial response that exhibits an asymmetrical Fano line shape. That FRMM is then coupled to the PMMA’s molecular resonance resulting in mode splitting. IR FRMM coupled sensing is used to improve the sensitive and selectivity for the detection of molecular fingerprints in the mid- to long-wave IR. A phonon polariton enhanced waveguide in the mid- to long-wave IR through 4H-SiC was analyzed using coupled mode theory, and the tradeoffs between modal confinement and propagation length were studied. IR hybrid waveguide modes with modal areas smaller then the free space diffraction area and propagation length that are a few times greater than the free space wavelength are numerically shown. Then that
SPhP waveguide was used for optical directional coupler and Mach-Zehnder interferometers. The ODC and MZI output ports’ sinusoidal relationship in power was investigated, and the use of an ODC and MZI as a phase-to-amplitude transducer was shown. ODC and MZI numerically shown is the first step to an IR modulator, waveguide IR sensing, and IR lab-on-chip. Slow propagating waves for a hybrid waveguide enhanced via type I HPhP in a slab of hBN was demonstrated and compared to a type II HPhP hybrid waveguide. The HPhP hybrid waveguides were analyzed using the coupled mode theory description. The resulting coupling between type I HPhP and dielectric waveguide results in both a lower and upper hybrid mode that is counter to reference [3]. The CMT analyzed shows that type I HPhP hybrid waveguide inherited both negative dispersion and ultra-slow light characteristics in addition to subwavelength field confinement [133]. It is possible that hybrid modes could inherit other properties like electro-optical effects in graphene or in a graphene/hBN hybrid material [136].

7.2 Future Work

7.2.1: Graphene

Geim and Novoselov received the 2010 Nobel Prize in Physics for their groundbreaking experiments on graphene [141]. Graphene, like hBN, is a hexagonal monolayer of carbon atoms that results in a van der Waals material that
supports plasmon polaritons in mid- to long-wave IR [117,142]. The energy vs. momentum, $E-k$, the diagram describes the electron transport for graphene and topological insulators[143] as Dirac cones. The energy states of graphene fill as a function of bias and result in graphene having electro-optic properties [144]. The complex conductive of graphene can be determined using the Kubo formulation as follows [142,145]:

$$\sigma = \sigma_{\text{intra}} + \sigma_{\text{inter}},$$

(7.1)

where[146,147]

$$\sigma_{\text{intra}} = \frac{q^2 k_B T}{2\pi \hbar} \left[ \frac{\mu_c}{k_B T} + 2 \ln(e^{\frac{-\mu_c}{k_B T}} + 1) \right],$$

(7.2)

$$\sigma_{\text{inter}} \approx \frac{jq^2}{4\pi \hbar} \ln \left[ \frac{2|\mu_c| - 2\pi \hbar(f - j\Gamma)}{2|\mu_c| + 2\pi \hbar(f - j\Gamma)} \right],$$

where $q$ is the elementary charge, 1.602e-19 c, $k_B$ is Boltzmann constant, 8.617e-5 eVK$^{-1}$, $f + j\Gamma$ is the complex frequency, $\hbar$ is Planck’s constant, 4.136e-15 eVs, and $\mu_c$ is the chemical potential, and $E_f$ is the Fermi Energy, which can be approximated as [145,147]:

$$E_f \approx \mu_c \approx \hbar v_f \sqrt{\frac{\pi \epsilon_0 \epsilon_{r \text{gate}} V_{Bias}}{q t_{\text{gate}}}},$$

(7.4)

$$v_f = 10^8 \left[ \frac{cm}{s} \right]$$

for when $\mu_c \gg k_B T$ [146], and $v_f$ is the Fermi velocity, $\epsilon_{r \text{gate}}$ and $\epsilon_{r \text{gate}}$ are the thickness and relative permittivity of the dielectric gate used for biasing, and $V_{Bias}$
is the DC bias voltage applied to the biasing gate. Figure 59 plots the Fermi energy as a function of DC bias voltage assuming a gate permittivity of 3.9 and thickness of 1 μm. The complex permittivity of graphene, shown in Figure 60 for $E_f = 0.25 \, eV$, can be determined in terms of the complex conductivity in Eqs. 7.1 and 7.2 as follows:

$$\varepsilon_r^g = 1 + j \frac{\lambda_0 \eta_0 \sigma}{2\pi d},$$  \hspace{1cm} (7.3)

where $\eta_0$ is the intrinsic impedance of free space: 377 Ω, and d are the thickness of the graphene layer (3.3 Å for a graphene monolayer). The plasmon polariton dispersion for a graphene monolayer is defined as the following [136,142,146]:

$$k_{spp}^g = j \varepsilon_0 (\varepsilon_r^{sub} + 1) \frac{2\pi f}{\sigma},$$  \hspace{1cm} (7.5)

where $\varepsilon_r^{sub}$ is the permittivity of the embedding media. Figure 61 plots the graphene plasmon polariton dispersion as a function of Fermi energy with $\varepsilon_r^{sub}$ being air. The penetration depth for the evanescent field of the plasmon polariton into the surrounding dielectric is [146]:

$$k_z = \frac{1}{2Re \left\{ \sqrt{k_{spp}^g - k_0^2} \right\}^{-1}},$$  \hspace{1cm} (7.6)

Using Ansys HFSS driven and eigen modes, a graphene monolayer is defined as a layer impedance boundary on a 2D sheet. The thickness is the monolayer thickness of 3.3Å. The HFSS numerically determined plasmon polariton dispersion, using
both driven and eigen modes, is compared to the analytically determined dispersion of Eq. 7.5, and the results are shown in Figure 62.

![Fermi energy as a function of DC bias voltage (Eq. 7.4) assuming gate permittivity of 3.9 and thickness of 1 μm.](image)

Figure 59. Fermi energy as a function of DC bias voltage (Eq. 7.4) assuming gate permittivity of 3.9 and thickness of 1 μm.
Figure 60. Complex permittivity of graphene, Eq. 7.3, for a graphene monolayer: 3.3 Å and Fermi energy 0.25 eV.

Figure 61. Graphene plasmon polariton dispersion, Eq. 7.5, at different Fermi energies: 0.75, 0.50, 0.37, 0.25 eV.
Figure 62. Ansys HFSS numerical results for eigen mode and driven mode compared to the analytical equation: Eq. 7.5.

7.2.2: Hybrid Material

With the discovery of phonon polaritons in hBN [118], an interest developed in graphene-hBN heterostructures, which supports tunable plasmon-phonon polaritons in a hybrid material [136,138,148-151]. The hybridization process, like the hybrid polariton waveguide, trades off properties of the uncoupled contributors. The plasmon polaritons in graphene provide highly confined sub-diffractional modes. However, graphene plasmon polaritons have limited propagation lengths on the order of 1 μm [152]. On the other hand, phonon polaritons have long propagation lengths compared to plasmon polaritons, but they only have a small band in which
they excite in. It has been shown that phonon-plasmon polaritons also retain the graphene electro-optical properties with DC bias [136-138].

Ultra-compact absorption-based graphene polariton modulators for photonic integrated circuits have been reported [147,153,154]. A mid- to long-wave IR polariton Mach-Zehnder modulator[155] could be realized by expanding on the MZI presented in this dissertation and optical switching [156]. Hybrid graphene-hBN material has other applications, such as tunable polariton antennas[157-160] and metamaterials [161-163].

7.2.3: $\varepsilon$ and $\mu$-Near-Zero Material and Hybrid Waveguiding and Sensing

Polar dielectrics, like 4H-SiC, have a transition region in which the dielectric relative permittivity transitions from positive to negative near the longitudinal optical phonon resonance [4,164]. In the transition region, right before the longitudinal optical phonon resonance, the polar dielectric has a relative epsilon between values of one and zero. A material with $0 < \varepsilon_r < 1$ is referred to as a $\varepsilon$-near-zero (ENZ) material. Similarly, a $\mu$-near-zero material (MNZ) is a material with relative permeability within the range: $0 < \mu_r < 1$. MNZ can be achieved through the design of a metamaterial [165].

ENZ has three main applications which are: matched zero-index media (ZIM), radiation pattern shaping, and supercoupling effects (a similar application holds for
MNZ). ZIMs are, in general, not found in nature and thus metamaterials with ZIM properties have to be designed. It has been shown [166] that a ZIM can be designed with an ENZ host material with regular dielectric with periodic or aperiodic inclusion. ZIMs have applications as delay lines, increasing the directivity of antennas, reducing bend losses in waveguide bends, and manipulating curved wavefronts into planar ones [167]. An antenna application of ENZ involves wavefront manipulation, where the incident wavefront can be contorted via the wave passing through ENZ media [167,168]. Also, ENZ has been shown to modify the resonance frequency and directionality behavior of antennas using an ENZ substrate [164].

The theory of supercoupling effect in ENZ material was described in [169] and the term was coined in [170]. Supercoupling itself describes a counterintuitive phenomenon in which near perfect matching of two waveguides can be achieved with an arbitrarily shaped ENZ interconnect [170-172]. Furthermore, low loss ENZ can provide energy squeezing by reducing the ENZ filled waveguide dimensions. The energy squeezing effect is a result of the electric field, being several times larger in the ENZ region, i.e., $k \rightarrow 0$, than in free space, and thus the ENZ can be arbitrarily shaped. Therefore, with a strategic design, the ENZ region can be designed to reduce the overall volume and thus squeeze the energy within that volume. Supercoupling effects have also been demonstrated for MNZ materials with TM surface waves [173].
The energy squeezing concept of supercoupling can be employed in reducing the mode area in a hybrid waveguide. However, a metamaterial would be required to achieve MNZ material, given the TM nature of SPPs or SPhPs. With a high index layer, an artificial transverse electric (TE) surface mode can be achieved that mimics its TM counterpart [174]. With the use of a polar dielectric, a supercoupled enhanced hybrid waveguide can be studied. Recently, magnetic hyperbolic metamaterial has been reported [175]. Expanding on the artificial TE mode idea, a high index layer on top of hBN can be investigated in the support of artificial TE hyperbolic polaritons in both the lower and upper reststrahlen band. Similarly, supercoupling of ENZ material can be employed with artificial TE HPhP enhanced hybrid waveguides.
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Appendix
Appendix A: Mode Area for HFSS Field Calculator

The modal area calculation is based on Ansoft HFSS Field Calculator Cookbook section: “Calculating the Peak Electrical Energy in a Volume” [176]. Figure A.1 depicts the geometry of a hybrid waveguide cross-section that is considered to calculate the modal area. It is assumed that the materials of a step profile exist as a constant over a given an area, i.e., that the material is linear; otherwise, an effective mode area or effective index method would need to be applied [177].

Figure A.1. Cross-section geometry of a hybrid waveguide with relative permittivity is shown with geometry dimensions labeled.
The step profile over an area can be defined using the rectangle function defined as follows:

\[
\text{rect} \left( \frac{x}{Δx}, \frac{y}{Δy} \right) = \begin{cases} 
1, & \quad -\frac{Δx}{2} < x < \frac{Δx}{2} \text{ and } -\frac{Δy}{2} < y < \frac{Δy}{2}, \\
0, & \quad \text{otherwise}
\end{cases}
\]  

(A.1)

where \( Δx \) is the horizontal dimension of the box that contains the hybrid waveguide, \( Δy \) is the vertical dimension of the air and 4H-SiC substrate. The dielectric permittivity, as seen in the geometry shown in Figure B.1, as a function of position can be written as follows:

\[
ε(x,y) = ε_{A-Si} \text{rect} \left( \frac{x}{Δx}, \frac{y}{Δy} \right) + ε_{air} \left[ \text{rect} \left( \frac{x}{Δx}, \frac{y - \left( \frac{Δy}{2} - \frac{d}{2} \right)}{Δy} \right) - \text{rect} \left( \frac{x}{Δx}, \frac{y + \left( \frac{Δy}{2} + \frac{d}{2} \right)}{Δy} \right) \right] + ε_{GaN} \text{rect} \left( \frac{x}{Δx }, \frac{y + \left( \frac{h}{2} + \frac{d}{2} \right)}{h} \right) + ε_{4H-SiC} \text{rect} \left( \frac{x}{Δx }, \frac{y + \left( \frac{Δy}{2} - \frac{d}{2} - \frac{h}{2} \right)}{Δy} \right)
\]  

(A.2)

The modal area is defined in terms of the storage of electromagnetic energy; therefore, only the real part of the dispersive dielectric permittivity is required. The imaginary part of the dispersive permittivity is related to dissipated electromagnetic energy \([5,178]\). Given the linearity of differentiation and multiplication, it can be shown that Eq. B.2 becomes:
\[ \frac{d(\varepsilon_0 \varepsilon'(x,y) \omega)}{d\omega} \bigg|_{\omega_0} = \varepsilon_0 \varepsilon^*(x,y) \bigg|_{\omega_0} \]

\[ = \varepsilon_0 \varepsilon_{A-Si} \mathbf{rect} \left( \frac{x}{d}, \frac{y}{d} \right) \]

\[ + \varepsilon_0 \varepsilon_{air}^* \mathbf{rect} \left( \frac{x}{\Delta x}, \frac{y - \left( \frac{\Delta y}{2} - \frac{d}{2} \right)}{\Delta y} - \mathbf{rect} \left( \frac{x}{d}, \frac{y}{d} \right) \right) \]

\[ + \varepsilon_0 \varepsilon_{GaN}^{*} \mathbf{rect} \left( \frac{x}{\Delta x}, \frac{y + \left( \frac{h}{2} + \frac{d}{2} \right)}{h} \right) \]

\[ + \varepsilon_0 \varepsilon_{4H-SiC}^{*} \mathbf{rect} \left( \frac{x}{\Delta x}, \frac{y + \left( \frac{\Delta y}{2} - \frac{d}{2} - h \right)}{\Delta y} \right) \]

(A.3)

The electromagnetic energy can be broken into electrical and magnetic energy as follows:

\[ W_m = \iint_{-\infty}^{\infty} W(x,y) dx dy = \iint_{-\infty}^{\infty} W_e(x,y) dx dy + \iint_{-\infty}^{\infty} W_h(x,y) dx dy \quad (A.4) \]

where,

\[ W_h(x,y) = \frac{1}{2} \frac{d(\mu(x,y) \omega)}{d\omega} \mu_0 \left| H(x,y) \right|^2 = \frac{1}{2} \mu_0 \left| H(x,y) \right|^2 \quad (A.5) \]

and,

\[ W_e(x,y) = \frac{1}{2} \varepsilon_0 \varepsilon^*(x,y) \bigg|_{\omega_0} \left| E(x,y) \right|^2 \]. \quad (A.6)

Via the linearity of integration, the electrical energy can be written as a sum of integrals:
\[ \int_{-\infty}^{\infty} W_e(x, y) \, dx \, dy = \frac{1}{2} \varepsilon_0 \varepsilon_{A-Si}^* \int_{\rho_{A-Si}} |E(x, y)|^2 \, dx \, dy \]

\[ + \frac{1}{2} \varepsilon_0 \varepsilon_{air}^* \int_{\rho_{air}} |E(x, y)|^2 \, dx \, dy \]

\[ + \frac{1}{2} \varepsilon_0 \varepsilon_{GaN}^* \int_{\rho_{GaN}} |E(x, y)|^2 \, dx \, dy \]

\[ + \frac{1}{2} \varepsilon_0 \varepsilon_{4H-SiC}^* \int_{\rho_{4H-SiC}} |E(x, y)|^2 \, dx \, dy. \]

(A.7)

where \( \rho_i \) indicates the limits of integration over the area defined by the rectangle function.
Appendix B: Coupled Mode Theory for Hybrid Waveguiding

It is shown that the hybrid index \( n_\pm(d, h) \), mode character \(|a_\pm(h, d)|^2\), and coupling strength \( \kappa(h, d) \) can be determined from the coupled system of equation:

\[
\begin{bmatrix}
 n_{m1} & \kappa^*(h, d) \\
\kappa(h, d) & n_{m2}
\end{bmatrix}
\begin{bmatrix}
 a_\pm(h, d) \\
b_\pm(h, d)
\end{bmatrix}
= n_\pm(d, h)
\begin{bmatrix}
 a_\pm(h, d) \\
b_\pm(h, d)
\end{bmatrix},
\]  \quad (B.1)

where \( a_\pm \) and \( b_\pm \) are the amplitudes of the uncoupled modes. It is assumed that weakly coupling holds and energy/momentum is conserved [60]. These assumptions allow the simplification of the coupling parameter where: \( \kappa_{12}(h, d) = \kappa_{21}^*(h, d) = \kappa(h, d) \).

\textbf{B.1 Hybrid Index}

The hybrid index can be determined by the eigen values as follows:

\[
det\begin{bmatrix}
 n_{m1} - n_\pm(d, h) & \kappa^*(h, d) \\
\kappa(h, d) & n_{m2} - n_\pm(d, h)
\end{bmatrix}
= \left(n_{m1} - n_\pm(d, h)\right)\left(n_{m2} - n_\pm(d, h)\right) - |\kappa(h, d)|^2
\]
\[
= n_\pm(d, h)^2 - n_\pm(d, h)(n_{m1} + n_{m2}) + n_{m1}n_{m2} - |\kappa(h, d)|^2
= 0,
\]  \quad (B.2)

then,
\[ n_{\pm}(d, h) = \frac{n_{m1} + n_{m2}}{2} \pm \sqrt{\left(\frac{n_{m1} + n_{m2}}{2}\right)^2 - n_{m1}n_{m2} + |\kappa(h, d)|^2}, \quad (B.3) \]

Simplifying leads to the results of reference [3]:

\[ n_{\pm}(d, h) = \frac{n_{m1} + n_{m2}}{2} \pm \sqrt{\left(\frac{n_{m1} - n_{m2}}{2}\right)^2 + |\kappa(h, d)|^2}. \quad (B.3) \]

**B.2 Mode Character**

Next, the mode character is determined from Eq. B.1. Taking the first row of Eq. B1:

\[ a_{\pm}(h, d)n_{m1} + \kappa(h, d)b_{\pm}(h, d) = n_{\pm}(d, h)a_{\pm}(h, d), \quad (B.4) \]

and simplifying,

\[ a_{\pm}(h, d)(n_{\pm}(d, h) - n_{m1}) = \kappa(h, d)b_{\pm}(h, d) \quad (B.5) \]

where,

\[ |b_{\pm}(d, h)|^2 = 1 - |a_{\pm}(d, h)|^2, \quad (B.6) \]

then squaring both sides of B.5 and substituting Eq. B.6 into B.5 results in:

\[ |a_{\pm}(h, d)|^2(n_{\pm}(d, h) - n_{m1})^2 = |\kappa(h, d)|^2 \left(1 - |a_{\pm}(d, h)|^2\right) \quad (B.7) \]

solving for \(|a_{\pm}(h, d)|^2 \) leads to the result in reference [3]:

\[ |a_{\pm}(h, d)|^2 = \frac{|\kappa(h, d)|^2}{(n_{\pm}(d, h) - n_{m1})^2 + |\kappa(h, d)|^2} \quad (B.8) \]
B.3 Coupling Strength

With the assumption of weakly coupled and conservation, it can be seen that:

$$|\kappa(h,d)|^2 > 0. \quad (B.9)$$

The coupling strength in terms of the hybrid and the uncoupled index can be determined by first rearranging the first row of Eq. B1 to the following:

$$b_\pm(d,h) = \frac{a_\pm(d,h)(n_\pm - n_{m1})}{\kappa^*(h,d)}. \quad (B.10)$$

The second row of Eq. B1 is the following:

$$a_\pm(d,h)\kappa(h,d) + b_\pm(d,h)n_{m2} = n_\pm b_\pm(d,h), \quad (B.11)$$

and substituting Eq. B.10 into Eq. B11 yields:

$$a_\pm(d,h)\kappa(h,d) + \frac{a_\pm(d,h)(n_\pm - n_{m1})}{\kappa^*(h,d)}n_{m2} = n_\pm \frac{a_\pm(d,h)(n_\pm - n_{m1})}{\kappa^*(h,d)} \quad (B.12)$$

The term $$a_\pm(d,h)$$ can be eliminated, and multiplying by $$\kappa^*(h,d)$$ yields:

$$|\kappa(h,d)|^2 + (n_\pm - n_{m1})n_{m2} = n_\pm(n_\pm - n_{m1}). \quad (B.13)$$

Rearranging B.13 and the results reported in [140] are shown:

$$|\kappa(h,d)|^2 = (n_\pm - n_{m1})(n_\pm - n_{m2}) \quad (B.14)$$
Appendix C: Mode Area in Lossy Media

The dispersion of a polar dielectric takes the form of a Lorentz oscillator [4]:

\[
\varepsilon_1(\omega) = \varepsilon_\infty \left(1 - \frac{\omega_{\text{LO}}^2 - \omega_{\text{TO}}^2}{\omega_{\text{TO}}^2 - \omega^2 + j\gamma\omega}\right)
\]  

(C.1)

where \(\omega_{\text{TO}}\) and \(\omega_{\text{LO}}\) are the longitudinal, LO, and transverse, TO, phonon resonance frequencies, respectively. \(\varepsilon_\infty\) is the high-frequency component of relative permittivity, and \(\gamma\) is the damping constant of the polar dielectric. The polarization vector is related to the electric field vector by susceptibility tensor.

\[\vec{P} = \varepsilon_0 \chi \vec{E}\]  

(C.2)

Susceptibility component for anisotropic polar dielectric crystal is related by the permittivity as follows:

\[\chi_i = \frac{\varepsilon_i}{\varepsilon_0} - 1 = \varepsilon_{\infty} + \varepsilon_{\alpha,i} \frac{\omega_{\text{LOi}}^2 - \omega_{\text{TOi}}^2}{\omega_{\text{TOi}}^2 - \omega^2 + j\gamma_i\omega} - 1.\]  

(C.3)

The polarization vector components are a linear combination of electric field components. The principal axis coordinate system is used for crystal ordination then from eq. C.2 and C.3 the polarization vector can be written as:
\[ \sum_{i=x,y,z} \ddot{\vec{P}}_i = \sum_{i=x,y,z} \varepsilon_0 \left( \varepsilon_{\infty} + \varepsilon_{\infty} \frac{\omega_{LO i}^2 - \omega_{TO i}^2}{\omega_{TO i}^2 - \omega^2 + j\gamma_i \omega} - 1 \right) \ddot{E}_i \]

\[ \Rightarrow \sum_{i=x,y,z} \ddot{\vec{P}}_i \left( \omega_{TO i}^2 - \omega^2 + j\gamma_i \omega \right) \]

\[ = \sum_{i=x,y,z} \varepsilon_0 \left( \varepsilon_{\infty} - 1 \right) \left( \omega_{TO i}^2 - \omega^2 + j\gamma_i \omega \right) \]

\[ + \varepsilon_0 \varepsilon_{\infty} \left( \omega_{LO i}^2 - \omega_{TO i}^2 \right) \ddot{E}_i, \]

and rewriting eq. C.4 in time differential form:

\[ \sum_{i=x,y,z} \frac{d^2 \ddot{P}_i}{dt^2} + \gamma_i \frac{d\ddot{P}_i}{dt} + \omega_{TO i}^2 \ddot{P}_i = \]

\[ \sum_{i=x,y,z} \varepsilon_0 \left( \varepsilon_{\infty} - 1 \right) \frac{d^2 \ddot{E}_i}{dt^2} + \varepsilon_0 \left( \varepsilon_{\infty} - 1 \right) \gamma_i \frac{d\ddot{E}_i}{dt} + \]

\[ [\varepsilon_0 \varepsilon_{\infty} \left( \omega_{LO i}^2 - \omega_{TO i}^2 \right) + \varepsilon_0 \left( \varepsilon_{\infty} - 1 \right) \omega_{TO i}^2] \ddot{E}_i \]

From Maxwell’s equations it can be shown [179,180]:

\[ \iint_s \vec{E} \times \vec{H} \, d\vec{s} = - \iiint_V \left[ \varepsilon_0 \frac{d\vec{E}}{dt} \vec{E} \cdot d\vec{P} + \vec{E} \cdot \frac{d\vec{P}}{dt} \vec{E} \cdot \frac{d\vec{H}}{dt} + \mu_0 \vec{H} \cdot \frac{d\vec{M}}{dt} \right] dV \]  

(C.6)

Term \( \vec{E} \cdot \frac{d\vec{P}}{dt} \) from the right hand side (RHS) of eq. C.6 is first considered:
\[ \sum_{i=x,y,z} \vec{E}_i \cdot \frac{d\vec{P}_i}{dt} = \sum_{i=x,y,z} T_{\infty i} \left( \frac{d^2\vec{P}_i}{dt^2} + \gamma_i \frac{d\vec{P}_i}{dt} + \omega_{R0i}^2 \vec{P}_i \right) \cdot \frac{d\vec{P}_i}{dt} \]

\[ = \sum_{i=x,y,z} T_{\infty i} \frac{d}{dt} \left( \frac{d\vec{P}_i^2}{dt} + \gamma_i \frac{d\vec{P}_i^2}{dt} + \omega_{R0i}^2 \vec{P}_i \right) + T_{\infty i} \gamma_i \frac{d\vec{P}_i^2}{dt} \]

where

\[ T_{\infty i} = \left[ \epsilon_0 (\epsilon_{\infty} - 1)(\omega_{R0i}^2 - \omega^2 + j\gamma_i \omega) + \epsilon_0 \epsilon_{\infty} (\omega_{R0i}^2 - \omega^2) \right]^{-1} \]

as can be seen from eq. C.5. The RHS of eq. C.6 can be rewritten as:

\[ \iint_V \left[ \epsilon_0 \vec{E} \cdot \frac{d\vec{E}}{dt} + \vec{E} \cdot \frac{d\vec{P}}{dt} + \mu_0 \vec{H} \cdot \frac{d\vec{H}}{dt} + \mu_0 \vec{H} \cdot \frac{d\vec{M}}{dt} \right] dV \]

\[ = j2\omega \iint_V \sum_{i=x,y,z} [\vec{W}_{ei} + \vec{W}_{mi}] dV + \iint_V \sum_{i=x,y,z} \left[ T_{\infty i} \gamma_i \frac{d\vec{P}_i^2}{dt} \right] dV \]

where \( \vec{W}_e \) and \( \vec{W}_m \) are the stored time-average electrical and magnetic energy densities. The term \( T_{\infty i} \gamma_i \frac{d\vec{P}_i^2}{dt} \) is the dissipated or lost electrical energy density in the crystal. The polar dielectric’s relative permeability is simply \( \mu_r = 1 \) therefore, the time-average magnetic energy density for time harmonic dependence in the \( i^{th} \) direction is:

\[ \vec{W}_{mi} = \frac{\mu_0}{4} |\vec{H}_i|^2. \]
The time harmonic dependent time-average electrical energy density in the $i^{th}$ direction is:

$$\bar{W}_{el} = \frac{\varepsilon_0}{4} |\vec{E}_i|^2 + \frac{|T_{\infty i}|}{4} \left( \omega^2 + \omega^2_T \right) |\vec{P}_i|^2 \tag{C.11}$$

where,

$$|\vec{P}_i|^2 = \varepsilon_0^2 |\chi_i|^2 |\vec{E}_i|^2. \tag{C.12}$$

Substituting in eq. C.12 into eq. C.11 yields:

$$\bar{W}_{el} = \varepsilon_0 \frac{|\vec{E}_i|^2}{4} \left[ 1 + \varepsilon_0 |T_{\infty i}| |\chi_i|^2 \left( \omega^2 + \omega^2_T \right) \right] \tag{C.13}$$

So, for time harmonic dependence the energy density is:

$$W(r) = \frac{\varepsilon_0}{2} \sum_{i=x,y,z} |E_i(r)|^2 \left[ 1 + \varepsilon_0 |T_{\infty i}| |\chi_i|^2 \left( \omega^2 + \omega^2_T \right) \right] + \frac{\mu_0 |H(r)|^2}{2} \tag{C.14}$$

This is a general form lossy anisotropic dispersive polar dielectric crystal with relative permittivity describe by eq. C.1.

In the case that $\varepsilon_{\infty i} = 1$ in eq. C.1 then:

$$T_{\infty i} = \frac{1}{\varepsilon_0 (\omega^2_{LOi} - \omega^2_{TOi})} \tag{C.15}$$

and

$$\chi_i = \frac{\omega^2_{LOi} - \omega^2_{TOi}}{\omega^2_{TOi} - \omega^2 + j\gamma_i \omega} \tag{C.16}$$
so,
\[
W_{ei} = \varepsilon_0 \frac{|\bar{E}_i|^2}{4} \left[ 1 + \frac{(\omega_{L,0i}^2 - \omega_{T,0i}^2)(\omega^2 + \omega_{T,0i}^2)}{(\omega_{T,0i}^2 - \omega^2)^2 + (\gamma_i \omega)^2} \right]
\]  \hspace{1cm} (C.17)

Given \( \varepsilon_{ri} = \chi_i + 1 \) and using the definition in eq. C.16, eq. C.17 can be rewritten as [179,180]:
\[
\bar{W}_{ei} = \varepsilon_0 \frac{|\bar{E}_i|^2}{4} \left[ \varepsilon_i' + \frac{2 \omega \varepsilon_i''}{\gamma_i} \right].
\]  \hspace{1cm} (C.18)

In the limited of \( \gamma \rightarrow 0 \) then:
\[
\frac{2 \omega \varepsilon_i''}{\gamma_i} \rightarrow \frac{2 \omega^2 (\omega_{L,0i}^2 - \omega_{T,0i}^2)}{(\omega_{T,0i}^2 - \omega^2)^2},
\]  \hspace{1cm} (C.19)

and
\[
\lim_{\gamma \rightarrow 0} \frac{d \varepsilon_i'}{d \omega} = \frac{2 \omega (\omega_{L,0i}^2 - \omega_{T,0i}^2)}{(\omega_{T,0i}^2 - \omega^2)^2}.
\]  \hspace{1cm} (C.20)

So,
\[
\lim_{\gamma \rightarrow 0} \frac{2 \omega \varepsilon_i''}{\gamma_i} \approx \omega \frac{d \varepsilon_i'}{d \omega},
\]  \hspace{1cm} (C.21)

and Eq. C.18 can then be rewritten in the form for the energy density of a near lossless anisotropic materials [3,179,180]:
\[
\bar{W}_{ei} = \varepsilon_0 \frac{|\bar{E}_i|^2}{4} \left[ \varepsilon_i' + \omega \frac{d \varepsilon_i'}{d \omega} \right] = \frac{|\bar{E}_i|^2}{4} \frac{d \omega \varepsilon_i'}{d \omega}.
\]  \hspace{1cm} (C.22)

The time harmonic dependence energy density for near lossless anisotropic material is [3,109]:

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\[ W(r) = \frac{\varepsilon_0}{2} \sum_{i=x, y, z} |\bar{E}_i(r)|^2 \frac{d\omega\varepsilon_i'}{d\omega} + \frac{\mu_0|\bar{H}(r)|^2}{2}. \]