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Beam Pattern Engineering of Metamaterial Terahertz Quantum-Cascade Devices

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Beam Pattern Engineering of Metamaterial Terahertz Quantum-Cascade Devices

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Electrical Engineering

by

Philip Wing-Chun Hon

2013
Abstract of the Dissertation

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Philip Wing-Chun Hon

Doctor of Philosophy in Electrical Engineering

University of California, Los Angeles, 2013

Professor Tatsuo Itoh, Co-chair

Professor Benjamin S. Williams, Co-chair

Generation and detection of microwave radiation is done with electronic systems where the underlying processes involve oscillating free charges (such as on an antenna or within a transistor or diode). On the higher energy side of the spectrum, generation and detection of near infrared and visible radiation is achieved via quantum transitions with emission wavelengths that are dictated by the material. Solutions moving up towards the THz regime using microwave based solutions are limited by carrier transit time and RC time-constant limitations. Techniques and solutions moving down toward the THz regime using photonic techniques have emission wavelengths naturally limited by the band gap of the material. However, THz quantum-cascade (QC) lasers, which are an extension of photonic concepts to lower energies, have artificially engineered energy levels and hence emission wavelengths. THz QC-lasers have been demonstrated to operate at frequencies between 1.2 and 5.0 THz and the best high-temperature operation is based upon the metal-metal (MM) waveguide configuration, in which the multiple-quantum-well active region is sandwiched between two metal cladding layers, typically separated by 2-10 μm. Soon after the demonstration of MM waveguide QC-lasers, it was recognized that the beam pattern from a conventional cleaved-facet Fabry-
Pérot (FP) ridge cavity produced a highly divergent beam pattern, characterized by concentric rings in the far field.

This thesis presents work on a new approach to tailor the beam pattern of THz MM waveguide QC-devices. Namely, dispersion engineering using metamaterials based on the composite right/left-handed (CRLH) transmission line formalism is adapted to the MM waveguide configuration to realize an entirely new class of devices. Dispersion, radiative loss, and radiation patterns are presented for many newly designed 1-D and 2-D THz QC transmission line metamaterial designs. The first ever active 1-D THz QC transmission line metamaterial is experimentally characterized and its radiation pattern and polarization closely match theoretical and full-wave finite element method (FEM) simulated predictions.

Proven microwave techniques such as circuit, antenna cavity modeling and array factor theory are used to understand the radiative properties of conventional THz QC-lasers. We predict far-field beam patterns and polarizations, approximate cavity quality factors, and associate these properties with individual surfaces or structures of the device. The analysis technique is also applied to the project’s 1-D and 2-D THz CRLH QC-devices yielding qualitative agreement with experiments.

The first THz design, analysis and experimental verification of a metasurface comprised of an array of passive THz QC transmission lines is presented. By using the cavity model, array factor, circuit and electromagnetic theory a surface impedance model is developed to characterize the metasurface. The surface impedance model reveals waveguide mode dependent radiative coupling with the light line and capacitive/inductive surface impedance. Polarization dependent angle-resolved Fourier transform infrared reflection spectroscopy measurements match the model and full-wave FEM predictions, further assisting the understanding of such devices.

To address the broader goal of a directive and scalable THz QC-device, the feasibility of a 2-D metamaterial inspired QC-laser and an active reflectarray is
considered. Finally, preliminary work on a technology enabling active metasurface reflector for a QC vertical external cavity surface emitting laser is discussed.
The proposal of Philip Wing-Chun Hon is approved.

Eric Pei-Yu Chiou

Yahya Rahmat-Samii

Benjamin S. Williams, Committee Co-chair

Tatsuo Itoh, Committee Co-chair

University of California, Los Angeles
2013
To my parents and all my other teachers.
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I would like to thank my advisors Professor Tatsuo Itoh and Professor Benjamin Williams for giving me the opportunity to conduct research under their guidance. An additional “thank you” to Professor Williams for his extra mentoring and enthusiastic discussions. I have both to thank for presenting me with such a great opportunity to learn and integrate concepts from the microwave and optics regime.

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Vita

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Publications


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During my Ph.D. studies, I had the pleasure of working with various groups and professors. There were two projects I focused on: a NSF funded project on terahertz transmission-line metamaterials for quantum cascade lasers and DARPA’s Electro-Magnetic Pulse Tolerant Microwave Receiver Front-End (EMPiRe) project. This thesis will focus primarily on the former, which is where I devoted most of my Ph.D. studies and the thesis will conclude with a section on the latter project.
The terahertz (THz) regime lies above the microwave and below the optical regime of the electromagnetic spectrum and is loosely defined as wavelengths ranging from 30-300 $\mu$m. Recently, the THz regime has been experiencing rapid development in sources [2] and applications [18–20]. Leveraging microwave technology, THz generation can be performed with frequency multiplier-based all solid-state electronic sources [21]. An alternative is THz generation via photonic methods such as with difference-frequency generation (DFG), where two optical beams interact in a medium with second-order nonlinear susceptibility $\chi^2$ [22]. However, until recently, there has been a lack of direct, compact, coherent THz sources [23]; a technological hurdle which now has an alternative solution, namely, quantum-cascade (QC) lasers [4].

The radio astronomy community was first to advocate the need for THz technology [23]. A very recent example of instrumentation capable of sensing THz radiation is the recently active (2009-2013) European Space Agency (ESA) headed Hershel Space Observatory, which had far-infrared sensing/imaging capabilities from three detectors: the photodetecting array camera and spectrometer (PACS), spectral and photometric imaging receiver (SPIRE), and the very high resolution heterodyne instrument for the far-infrared (HIFI). HIFI had a 1.9 THz GaAs Schottky diode frequency multiplier chain with more than 10 $\mu$W of output power [2]. The mission goal was to observe black body radiation from cool interstellar medium ranging in temperature from 5 K to 50 K and gases which
emit their brightest molecular and atomic emission lines between 10 K and a few hundred Kelvin (Fig. 1.1). Having such information could answer a few questions: formation and evolution of galaxies, information on the physical processes and energy production mechanisms in galaxies, how stars form out of molecular clouds in various environments, understanding the stellar/interstellar lifecycle and detailed high resolution spectroscopy of a number of comets, to name a few [20]. In recent years, other fields interested in using THz radiation have emerged such as medical imaging [24], surveillance of person borne hidden weapons and materials detection [19], just to name a few. Therefore, the THz portion of the electromagnetic spectrum offers unique benefits but also challenges, which will be discussed.

Figure 1.1: Example of an interstellar cloud’s spectral content with molecular rotation and atomic fine-structure line emissions. Taken from [1].

Generally, there are three methods to generate THz sources: frequency multiplication from the microwave regime, down converting from the optical regime, or directly. The first uses electronics technology such as high electron mobility transistors (HEMTs), metamorphic HEMTS (mHEMTs), heterojunction bipolar
transistors (HBTs), and GaAs Schottky barrier diodes, to name a few, where the power levels roll off at 6 dB/octave following the RC time constant of a typical first order filter (Fig. 1.2). The highest frequency multiplying source to date is a room temperature operating monolithically integrated circuit using GaN power amplifiers and Schottky diode multipliers which produces continuous wave output power ranging from 2-14 μW over the 2.49-2.72 THz range [25]. Using sources from the higher energy side of the EM spectrum, difference frequency generation sources with milliwatts of average power and a tuning bandwidth that covers the THz gap has been achieved under continuous wave operation [26], however, efficiency levels are low. For example, in the work presented in [26], the THz and the intracavity power were 2 mW and 500 W, respectively, giving a conversion efficiency much less than a percent. A hybrid of optical and microwave techniques include photomixing where it has the advantage of wide bandwidth and stability, but has only μWs of power in the THz regime [27]. Lastly, direct generation can be achieved by molecular gas lasers such as those used in single-detector heterodyne imaging systems [28], but are bulky in size. A more compact and direct (without upconverting or downconverting) alternative to generate THz radiation is with quantum-cascade (QC) lasers [4], which are an extension of photonic concepts to lower energies. By realizing artificially engineered energy levels, THz radiation is obtained via intraband radiative transitions in a 2-D coupled quantum-well heterostructure. The QC-laser concept was first demonstrated in 1994 in the mid infrared (4.2 μm) with an InGaAs/InAlAs material system lattice-matched to an InP substrate by Faist, et al. [29]. QC-lasers have since become the preferred mid-IR semiconductor laser source with room temperature (RT), continuous wave (CW) operation with as much as 5.1 W of power and a wall plug efficiency of 21% at 4.9μm [30] and have since reached commercial maturity levels [31]. In 2002, a QC-laser in the far IR at 4.4 THz was demonstrated in the GaAs/AlGaAs material system [32]. Great improvements in QC-laser performance followed such as
Figure 1.2: Shown output power levels for QC-lasers and III-V lasers are peak power levels. Majority of the power levels for other sources are CW. Figure taken from [2].

improved beam pattern, output power and operating tempertatures [4, 33]. THz QC-lasers have since become attractive candidates as sources for many applications in THz imaging, sensing, and spectroscopy, and have been demonstrated to operate at frequencies between 1.2 and 5.0 THz (without the assistance of a magnetic field) [4, 32, 34].

### 1.1 Quantum-Cascade Lasers

Unlike interband semiconductor lasers, which have an emission wavelength dependent on the materials bandgap (Fig. 1.3(a)) QC-lasers are unipolar semiconductor lasers that use intersubband transitions between quantized subband electronic states of a multiple quantum well (MQW) superlattice (Fig. 1.3(b)). The MQW superlattice or active region is made of a repeated stack of semiconductor MQW heterostructures such as GaAs/AlGaAs, where the electric field must be polar-
ized perpendicular to the growth direction to satisfy the selection rules and hence realize an optical transition (discussed in CH. 2).

In traditional interband semiconductor lasers, interband radiative transitions are bipolar processes involving the recombination of an electron hole pair, where the emission wavelength is dependent on the bandgap of the material. It is, therefore, not practical to use bipolar laser concepts in the far IR since semiconductors with bandgap energies $< 40$ meV are not readily available in nature. Although there are some materials with small bandgaps such as graphene or engineered type II heterostructures, they do, however, exhibit short recombination times, which reduces the feasibility of realizing a population inversion needed for lasing.

First proposed in 1971 [35], an intersubband laser is based on intersubband radiative transitions within the subbands of the conduction band or valence band itself and are unipolar processes involving only an electron or hole, respectively. The carrier relaxes from an upper subband to a lower subband and emits a photon in the process. Control of the subbands and hence emission wavelength lies in the active region design, where the active region consists of a semiconductor MQW heterostructure, which is a repetition of semiconductor material layers with different conduction band (CB) energies such as GaAs/AlGaAs (CB of Al $>$ CB of GaAs). A module consisting typically of a few of these layers is then repeated. Each semiconductor layer is on the order of a few monolayers thick. For a GaAs/AlGaAS material system, a monolayer thickness is defined as half the lattice constant of GaAs, $a_{\text{GaAs}} = 5.65 \, \text{Å}$. The resulting heterostructure provides quantum confinement of carriers, i.e. free carrier dispersion in the in-plane direction and quantization in the direction of growth generating subbands with different energies.
Figure 1.3: (a) Interband and (b) Intersubband (intraband) transitions. Figure taken from [3].
Consider a 3 level laser system, where carriers are pumped into upper lasing level \( u \) and radiatively transitions to the lower lasing level \( l \), where they quickly scatter to the ground state. Cascading of modules allows reuse of a single electron via the process of resonant tunneling and intersubband scattering, such that many photons can be generated for a single injected electron (Fig. 1.4). The shortest emission wavelength is limited by the heterostructure band-offset \( \Delta E_c \) in Fig.1.3(b)). Longer wavelength designs (below \(~1\text{ THz}) are not practical given the extremely small energy separation between the upper and lower lasing sub-band levels, making a selective current injection and population inversion difficult to realize.

The first THz QC-laser came almost a decade later after its first demonstration in the mid IR due to difficulties in realizing a population inversion for the small energy separation required between subbands \((\sim 4 \text{ to } 20 \text{ meV})\) and difficulties in developing a low-loss waveguide (absorption due to free carriers). The semi-insulating surface-plasmon and metal-metal (MM) waveguide are two waveguide configurations which have been used to address the latter. For reasons that will be mentioned later the MM waveguide configuration also resulted in the highest
device operating temperatures. The research in our group has, therefore, focused around the MM waveguide configuration.

1.2 THz Metal-Metal Waveguide QC-Lasers

The THz QC-lasers that exhibit the best high-temperature operation are based upon the so-called MM waveguide, in which the MQW active region is sandwiched between two metal cladding layers, typically separated 2-10 μm [36–38] (Fig. 1.5(a,b)). The resulting structure is a Fabry-Pérot (FP) cavity with highly reflective end facets. These provide the necessary boundary condition for mode reflection/confinement and power out coupling. The MM waveguide is character-
ized by low loss and a strong overlap of the mode with the active region, even when the transverse waveguide dimensions are scaled far below the wavelength (Fig. 1.5(c)). The reduction in dimension results in lower power dissipation [39], which is advantageous because thermally excited electrons reduce the population inversion and hence available material gain. Also, the increased mode overlap reduces the threshold gain required to meet the lasing criteria. Both topics will be further discussed in CH. 2.

1.2.1 THz MM-Waveguide QC-Laser Beam Pattern

Soon after the demonstration of MM waveguide QC-lasers, it was recognized that the beam pattern from a conventional cleaved-facet FP ridge cavity produced a highly divergent beam pattern, characterized by concentric rings in the far field [5] (Fig. 1.5(d)).
To address the poor beam quality from THz MM waveguide QC-lasers, research groups have proposed and demonstrated an array of different techniques. Using a hemispherical high resistivity silicon lens affixed to the facet of the MM waveguide QC-laser, Lee et al. [6] (Fig. 1.6(a)) demonstrated an increase in collection efficiency with a measured collection efficiency of 16 times more than a bare facet THz MM waveguide and an increase in peak power of 119 mW was reported. The measured FWHM of ~4.8 degrees in one of the principal planes (H plane) shows an improvement in the directivity. Another method involves a monolithic horn antenna integrated directly above the facet of the QC-laser that improves impedance matching from the guided wave within the waveguide to free space [7] (Fig. 1.6(b)). An improvement in directivity was noted with a 11° FWHM beamwidth in the E plane direction (plane that runs along the axis of the
laser) and 4° FWHM beamwidth in the H plane (in plane direction). A second order distributed feedback design, based on a Bragg grating, operating in a single mode gave greater output power with a small degradation in operating temperature relative to a standard MM waveguide. A single-lobed directive output beam along the waveguide axis direction (feedback direction) is achieved, however, the beam is less directive in the transverse direction [8] given the small aperture size in the transverse direction (Fig. 1.6(c)). A close relation of the 2nd order DFB is the 3rd order DFB, where the grating is designed such that the refractive index of the propagating mode is $\sim 3$ giving an endfire directed beam pattern with low divergence; approximately 30° in both principal planes [9] (Fig. 1.6(d)). Table 1.1 summarizes the beam divergence of each of these designs and includes other notable designs such as a graded photonic heterostructure. The design used absorbing boundaries to increase the antisymmetric mode loss and forced device operation in the symmetric mode, which is radiatively more efficient than the antisymmetric mode. Record-high peak-power surface emission greater than 100 mW and relatively low beam divergence (10°×30°) were achieved [40].
Table 1.1: Summary of different beam engineering results. The E and H cut columns, for the DFB and GPH devices, correspond to a cut along the axis of the ridge and a plane transverse to the ridge, respectively. * Designates cases where slope efficiency was not explicitly given, but absolute LI curves were given; the slope efficiency was taken close to threshold.

<table>
<thead>
<tr>
<th>Design</th>
<th>FWHM (E cut) (deg)</th>
<th>FWHM (H cut) (deg)</th>
<th>Power</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hemispherical lens [6]</td>
<td>NA</td>
<td>4.8°</td>
<td>145 mW pulsed @ 5 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_{slope}=296 \text{ mW/A}$</td>
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<tr>
<td>Monolithic horn [7]</td>
<td>11°</td>
<td>4.0°</td>
<td>23 mW pulsed @ 10 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_{slope}=32 \text{ mW/A}$ *</td>
</tr>
<tr>
<td>2nd order DFB (array) [41]</td>
<td>5°</td>
<td>&gt;20°</td>
<td>6 mW cw @ 5 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_{slope}=43 \text{ mW/A}$ *</td>
</tr>
<tr>
<td>2D PhC [42]</td>
<td>12°</td>
<td>8°</td>
<td>1 mW pulsed @ 10 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_{slope}=3 \text{ mW/A}$ *</td>
</tr>
<tr>
<td>3rd order DFB [9]</td>
<td>10°</td>
<td>10°</td>
<td>13 mW pulsed, 11 mW CW @10K</td>
</tr>
<tr>
<td>3rd order DFB (5.6mm long) [43]</td>
<td>6°</td>
<td>11°</td>
<td>5 mW pulsed @ 10 K</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$\eta_{slope}=140 \text{ mW/A}$</td>
</tr>
<tr>
<td>Graded photonic heterostructure</td>
<td>10°</td>
<td>30°</td>
<td>50 mW @ 20 K</td>
</tr>
<tr>
<td>[40]</td>
<td></td>
<td></td>
<td>$\eta_{slope}=230 \text{ mW/A}$</td>
</tr>
<tr>
<td>Scanning Leakywave antenna</td>
<td>isotropic-like</td>
<td>10-15°</td>
<td>0.2 mW @ 4K,</td>
</tr>
<tr>
<td>(this work)</td>
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<td></td>
<td>$\eta_{slope}=20 \text{ mW/A}$</td>
</tr>
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</table>


1.3 Metamaterials

In general, electromagnetic metamaterials (MTMs) describe materials engineered to exhibit certain constitutive parameters, i.e. permittivity and permeability, which describe, on a macroscopic level, the material’s ability to polarize in response to an electric and magnetic field, respectively. Conventional materials found in nature exhibit either a positive or negative permittivity or permeability, but there has yet to be discovered a material, naturally occurring in nature, that exhibits both a negative permittivity and permeability. Fig. 1.7 shows the different material classifications. In the first quadrant, the permittivity and permeability are both positive. Most dielectrics fall under this category and are associated with propagating waves. Quadrant II and IV are associated with materials that exhibit a negative permittivity or permeability, respectively, and are associated with evanescent waves. Metals, ferroelectric materials and doped semiconductors
fall under quadrant II, while ferrite materials fall under quadrant IV. Materials exhibiting a negative permittivity and permeability simultaneously, which do not exist naturally in nature, falls under quadrant III and is associated with a propagating wave with antiparallel phase and group velocity [11]. Namely, from Maxwell’s equations we have the relation between the wavevector and the field components given as

\[ \mathbf{k} \times \mathbf{E} = \mu \omega \mathbf{H} \quad (1.1) \]
\[ \mathbf{k} \times \mathbf{H} = -\varepsilon \omega \mathbf{E}. \quad (1.2) \]

Instead of the usual right handed triad, the relation between the EM fields and wave vector is described by the left-handed triad, hence a left-handed propagation is expected, while power flow, related to the group velocity, is still in the right hand direction.

![Figure 1.8: Representative illustration of a (a) thin wire and (b) SRR array. Taken from [11]](image)

The concept of LH materials was first presented by Veselago [44] in 1964 when he predicted the fundamental phenomena that are possible with LH material such as the reversal of Vavilov-Cerenkov radiation, reversal of Snell’s law, plasmonic expressions of the constitutive parameters in resonant-type LH media, to a name a few. However, the first demonstration of LH material properties happened more
than 30 years later through the use of an engineered metamaterial by Smith, *et al.* [45], where a plasmonic-type negative permittivity and negative permeability structure was realized in the microwave with an array of thin metal wires and metal split-ring resonator (SRR) structures, respectively (Fig. 1.8). In general, the permittivity and permeability of a material are described by the Lorentz model

\[
\varepsilon_r(\omega) = 1 - \frac{\omega_{p,e}^2}{\omega^2 - \omega_{0,e}^2 + i\Gamma_e \omega} \tag{1.3}
\]

\[
\mu_r(\omega) = 1 - \frac{\omega_{p,m}^2}{\omega^2 - \omega_{0,m}^2 + i\Gamma_m \omega} \tag{1.4}
\]

where for noble metals \(\omega_{0,e}\) is zero assuming the free electron approximation [11], giving the electric Drude model. The plasma frequency is given by \(\omega_p\), resonant frequency by \(\omega_0\) and the damping factor, which accounts for material loss is given by \(\Gamma\). The effective relative permittivity of the array of thin wires can be determined one of two ways. Pendry [46] approached the solution quantum mechanically. He solved for the plasma frequency with an effective electron density, which was a function of the fill factor and he found the effective mass as a function of the vector potential \(A\) and canonical momentum [11, 46]. Both changes attributed to an effective plasma frequency orders of magnitude lower than the bulk metal. Alternatively, Marqués [47] used circuit theory to arrive at the same expression for the plasma frequency. For the SRR, Pendry [48, 49] considered an applied magnetic field, the resulting induced currents and calculated the effective relative permeability from the total magnetic field in the SRR [11].

Since the first demonstration in the microwave regime, SRR metamaterials have been demonstrated in the far-infrared, infrared and visible regime [50, 51]. Besides using the SRR/wire array and its variations, a negative index material can be realized with the so-called double fishnet structure [52, 53] which consists of 2-D hole arrays sandwiching a dielectric medium. The double fishnet structure exhibits a negative refractive index and extraordinary transmission attributed
to symmetric and antisymmetric combinations of surface modes, therefore, such structures could be used as filters. Some other practical applications for metamaterials in the THz include absorbers, quarter waveplates, switches and amplitude and phase modulators [51, 54]. For example a recent SRR/wire grid array, single layer metamaterial demonstration in the THz frequencies exhibited an absorptivity as high as 70\% [55] making it a possible candidate for a thin THz absorber for detector or stealth applications. Metamaterials have some promising applications, but they also have their challenges. In a step to realize a truly 3-D bulk lossless isotropic metamaterial (for example, needed for super-lensing [56]), researchers are actively exploring gain compensated metamaterials. Attempts, especially in the NIR and visible regimes where ohmic losses are significant, include a double fishnet structure in a background of rhodamine 800 dye doped epoxy which exhibited enhanced transmission [57]. In the THz, there has been a successful demonstration of coupling between metamaterial SRRs and intersubband transitions in semiconductor quantum wells [58], however, this was purely a passive configuration – no intersubband gain was involved.

In our effort to tailor THz MM waveguide QC device beam patterns, we adapted THz metamaterials based on the nonresonant composite right/left handed transmission line (CRLH) formalism to the MM waveguide configuration – the CRLH formalism was proposed by three different research groups almost at the same time [59–61]. Such a configuration, which will be discussed in detail in CH. 3, supports an optical mode that couples well with the intersubband transitions of the semiconductor quantum wells, therefore, rendering possible gain compensated devices.
1.4 Overview

The focus of this thesis is on the beam pattern engineering of THz QC-devices based on the MM waveguide configuration. An entirely new approach to tailor the beam pattern of THz MM waveguide QC-devices is achieved by adapting metamaterial concepts based on the CRLH formalism. The design, modeling, full-wave finite element method (FEM) simulations and testing details will be discussed.

CH. 2 and CH. 3 outline the fundamental concepts behind THz QC-lasers and transmission line-based metamaterials to aid the discussion. CH. 4 discusses the modeling tool that combined antenna array theory and the antenna cavity model to predict radiation patterns, beam polarization and approximate radiative losses of conventional QC-lasers. Qualitative agreement between full-wave FEM simulations and model predictions for various heights and waveguide modes proved the model’s robustness.

Discussion of our first trial in realizing a 1-D THz QC transmission line metamaterial is covered in CH. 5 along with its application as a zeroth-order resonator and leaky-wave antenna (background of both discussed in CH. 3). Lessons learned helped guide the following generation of 1-D THz QC transmission line metamaterial designs. Additionally, a feasibility analysis for a scalable 2-D THz QC-laser is conducted.

A successful demonstration of an active right-handed only leaky-wave antenna and active metamaterial leaky-wave antenna capable of backward to forward scanning is presented in CH. 6. The cavity model is applied to these devices giving a quick and physically intuitive understanding of the radiation pattern, polarization and approximate cavity quality factor. Additionally, dominant radiating mechanisms, such as a surface or structure of the device, are revealed with the model. Many design variations aimed at controlling the radiative efficiency of the device,
for either a reduction in lasing threshold (lasing applications) or increase in power attenuation length (leaky-wave antenna), are analyzed and compared as well.

A parallel goal of proving the feasibility of passive THz CRLH transmission line metamaterials is covered in CH. 7. A metasurface comprised of an array of passive THz QC transmission lines is designed, analyzed and experimental verified for left and right handedness, a signature of a CRLH transmission line metamaterial. Using the cavity model, array factor, circuit and electromagnetic theory a surface impedance model is developed to characterize the metasurface. Namely, the surface impedance model reveals waveguide mode dependent radiative coupling with the light line and capacitive/inductive surface impedance. Polarization dependent angle-resolved Fourier transform infrared reflection spectroscopy measurements match the model and full-wave FEM predictions.

To address the broader goal of a directive and scalable THz QC-device, CH. 8 covers the feasibility of an active THz reflectarray, which eventually led to an active reflector design, which will be an enabling technology for an external cavity design.

Lastly, as mentioned in the preface, a dielectric field enhancer is discussed in the closing chapter.
CHAPTER 2

THz Quantum-Cascade Laser Theory

The following discussion is a brief review of the fundamental physics involved in the design and operation of QC-lasers. Of course, it is impossible to touch upon every detail. It is my goal to provide the reader with the required background on QC-laser operation to aid in the full comprehension and appreciation of the material to be presented in this thesis. The review here is adapted from various sources [3,12,62–64].

2.1 Engineering Optical Emission

In classical mechanics the velocity and location of a particle are described without uncertainty by Newtonian mechanics. On the other hand, in quantum mechanics (QM) the particle is described by its wave function $\Psi(x, t)$, where the magnitude of the wave function squared gives the statistical probability of finding the particle (electron) between some distance $a$ to $b$

$$\int_a^b |\Psi(x, t)|^2 dx = \left\{ \begin{array}{l}
\text{Probability of finding the particle} \\
\text{between a and b at time t}
\end{array} \right. \tag{2.1}$$

with the requirement that the particle must be somewhere within a range spanning from $-\infty \to +\infty$

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1. \tag{2.2}$$

20
The expectation value of an observable, when the particle is in some state \( \Psi \), gives the average of measurements performed on particles all in the same state. For example, the expectation value of \( x \) is given by

\[
\langle x \rangle = \int \Psi^*(x,t)x\Psi(x,t)dx = \langle \Psi(t)|x|\Psi(t) \rangle
\]

In order to calculate the particle’s wave function, one needs to solve Schrödinger’s equation

\[
i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi
\]

which has a time-independent form after applying separation of variables given by

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + V \psi = E \psi
\]

where \( \Psi = \psi(x) \phi(t) \). Some important points about the equation are noted below:

- the particle’s probability density function is determined by the magnitude of its stationary states \( \Psi(x,t) \) squared.
- the energy/Hamiltonian operator \( \hat{H} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \) is a linear operator and the time-independent Schrödinger equation can be represented as \( \hat{H} \psi = E \psi \).
- Schrödinger’s equation is an eigenvalue problem, where the eigenvector and eigenvalue are the particle’s wavefunction and corresponding energy.

One of the few quantum mechanical examples that can be solved exactly is the hydrogen atom, where its quantized energy states are found by solving Schrödinger’s equation with the potential \( V(r) \) given by the Coulombic potential.
between the hydrogen’s proton of charge $e$ and its electron with charge $-e$. But to understand the energy transitions made by the particle we must use time dependent perturbation theory which gives the transition probability of a particle which started out in a state $\Psi_a$ (with some corresponding energy $E_a$) to be in state $\Psi_b$ (with some corresponding energy $E_b$). There are three different processes of concern: absorption (non radiative), stimulated emission and spontaneous emission. In absorption, incident light loses a photon to the atom/quantum mechanical system due to the excitation of the particle from a lower energy level $E_a$ to a higher level $E_b$. In stimulated emission you get the opposite process where an incident photon results in an additional outputted photon due to the particle’s relaxation from the higher energy level to the lower one, which is also known as optical gain. Therefore, huge photonic gain is feasible if one can engineer a system with a majority of its electrons in the higher energy level to give a large number of photons for one incident photon. Known as a population inversion, this is one of the requirements to realize a laser.

The QM system could be an atomic system like the hydrogen atom, a semiconductor system, or engineered system. Solving Schrödinger’s equation for an interacting system reveals that a molecular system is comprised of linear combinations of the individual atomic orbitals consisting of antisymmetric and symmetric combinations. As more atoms are brought together, a continuum of energy levels will exist, but there will always exist bandgaps. The size of which dictates the material’s electrical properties. The material’s categorization as a metal, semiconductor or insulator depends on the occupancy of its valence and conduction band. Namely at $T = 0$, the last group of energy bands to be filled is considered the valence band and the first to be empty is the conduction band.

Let’s consider a semiconductor system, for example, gallium arsenide (GaAs), which has its energy bands described by Schrödinger’s equation with a modification to the mass ($m \rightarrow m^*$, only near the band extrema where one can make a
parabolic approximation). Namely, the effective mass \( m^* \) is used to account for the complex crystal potential and the resulting Schrödinger equation is

\[
-\frac{\hbar^2}{2m^*} \nabla^2 \psi + E_c \psi = E \psi
\]  

(2.6)

with corresponding energy solutions

\[
E = \frac{\hbar^2 k^2}{2m^*} + E_c
\]

(2.7)

where \( E_c \) is the conduction band offset energy. GaAs has a bandgap/radiative transition energy of 1.43 eV which corresponds to an emitted photon with \( \lambda = 867 \) nm. As previously mentioned, it is not practical to use bipolar laser concepts in the far IR since semiconductors with bandgap energies < 40 meV are needed. However, there are ways to engineer the energy levels of a QM system. Alloying is one method, but is not sufficient to generate THz wavelength radiation. Another method is to control the band structure via quantum confinement achieved by heterostructure quantum wells/barriers, which is realized by forming heterojunctions with two different band gap materials. Similar to the well with infinite barriers, where the wave functions (schematically shown in Fig. 2.1(a)) and corresponding energies are quantized, a heterostructure quantum well also has quantized energy levels. Alternating layers generate a conduction band which splits the conduction band into a series of subbands. Using the effective mass approximation and including a 1-D potential energy \( e\Phi(z) \) accounting for the band discontinuities at the heterojunction \( (z \) is the MQW growth direction), Schrödinger’s equation is modified to be

\[
-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*} \frac{\partial}{\partial z} \psi(z) + E_c(z) \psi(z) - e\Phi(z) \psi(z) = E \psi(z).
\]

(2.8)
where $m^*$ is the spatially dependent effective mass and $\psi$ is the slowly varying envelope function; the total wavefunction is a result of the slowly varying envelope function, $\psi$, modulating the Bloch wavefunction, $u(z)$, at the band minimum.

The artificially engineered subbands within the conduction band and hence its emission wavelength are controlled via the well and barrier thicknesses. Fig. 2.1(b) is an illustrative example of a GaAs/GaAlAs system’s conduction band along with representative wave functions.

![Wave functions](image)

Figure 2.1: Wave functions for a hypothetical (a) well with infinite potential barriers and well length $\ell_w$ and (b) a heterostructure with GaAlAs barriers sandwiching a GaAs well.

### 2.2 Lasing

Next we revisit the necessary requirements for lasing. The first is the need for a population inversion as briefly mentioned above. Let us assume a two level system formed by the two lowest subbands of the conduction band of a heterostructure quantum well, where we have $N_1$ and $N_0$ electrons in energy levels 1 and 0, respectively, forming a total population $N_T = N_1 + N_0$. Assuming thermal equilibrium, the population of the states is given by Boltzmann's statistics, i.e. Boltzmann’s
distribution

\[ \frac{N_1}{N_0} = e^{-\frac{(E_1 - E_0)}{kT}}. \] (2.9)

assuming equal degeneracy. Assuming a transition in the optical regime \( E_{10} = h\nu_{10} = 500-800 \ \text{THz} = E_1 - E_0 \) and \( T = 295 \ \text{K} \), we see the ratio is \(~0 \ \text{(5.96e-22)}\) at thermal equilibrium suggesting that almost all electrons reside in the lower energy state. Even at increased temperatures the highest the ratio could theoretically be is unity, which corresponds to optical transparency; one incident photon results in one output photon.

Consider a three level laser with a total population of electrons \( N_T = N_0 + N_1 + N_2 \) (level 2 and 1 correspond to the upper \( u \) and lower \( l \) lasing level). An optical pump can be used to excite electrons from the ground state with energy \( E_0 \) to \( E_2 \), which is known as the \( E_{02} \) pump transition. Electrons in the upper lasing level with energy \( E_2 \) then radiatively relax to the lower lasing level with energy \( E_1 \) and much more quickly relax from \( E_1 \) to the ground state with energy \( E_0 \); \( E_{21} \) is assumed to be the radiative transition, although the system could be designed to have \( E_{10} \) be the radiating transition. Therefore, there is a relative population inversion between the upper lasing level \( E_2 \) and the lower lasing level \( E_1 \) giving optical gain.

The emitted photons coherently contribute to an optical mode that is sustained by a resonant cavity, which is the other integral part of a laser. Namely, the cavity provides optical mode confinement and feedback, essentially acting as a mode/frequency filter. To sustain lasing the optical gain must overcome the losses, which include the waveguide and mirror loss. Factoring in the confinement factor, which measures the optical mode overlap with the MQW gain medium,
the threshold bulk gain condition is given by

$$\gamma_{th} = \frac{\alpha_w + \alpha_m}{\Gamma}. \quad (2.10)$$

An ideal confinement factor of unity is desired to maximize the modal gain for a given population inversion. The expression is given by [65]

$$\Gamma = \frac{n_g \int_{act} \epsilon |E_{\perp}|^2}{n_{act} \int_{-\infty}^{\infty} \epsilon |E|^2 dv} \quad (2.11)$$

where $n_g$ and $n_{act}$ are the group index of the mode and the bulk refractive index of the active gain medium, respectively. $E_{\perp}$ is the EM field component that is along the growth direction, which satisfies the requirement for an optical transition to occur (a.k.a the intersubband polarization selection rule to be discussed shortly). The waveguide loss $\alpha_w$ is due to free carriers. The mirror loss is due to the mirrors’ finite reflectivities, which are necessary for power output coupling and is given as

$$\alpha_m = -\frac{\ln(R_1 R_2)}{2L} \quad (2.12)$$

where $L$ is the cavity length, $R_1$ and $R_2$ are the mirror reflectivities.

Considering a uniform medium with a propagating plane wave, the expression that relates the gain to the intensity of the plane wave is given as

$$\frac{dI_v}{dz} = \gamma(\nu) I_v = (\text{power/volume}) \quad (2.13)$$

which describes the change in the optical mode’s intensity as it traverses through the medium. Using Einstein’s coefficients $A_{21}$, $B_{12}$, $B_{21}$, which are related to the transition lifetimes for spontaneous emission, absorption, and stimulated emission, respectively, gain is intuitively given as the net power emitted per volume over the power per area traversing that volume. The power per volume is given by the
difference in the change in upper level population due to stimulated emission and absorption

\[ \frac{dL_v}{dz} = h\nu \left\{ \frac{dN_1}{dt} \bigg|_{\text{stim em}} - \frac{dN_1}{dt} \bigg|_{\text{absorption}} \right\}. \tag{2.14} \]

The gain is then given as [63, 64]

\[ \gamma(\nu) = \sigma(\nu) \Delta N \propto f_{if} \Delta Ng(\nu). \tag{2.15} \]

The stimulated emission cross section \( \sigma \) is a function of the transition line shape \( g(\nu) \) and oscillator strength \( f_{if} \). The transition line shape describes the transition frequency bandwidth/sharpness. For QC-lasers, it is homogeneously broadened due to impurity and interface roughness scattering at the heterojunction of the semiconductor layers and inhomogeneously broadened due to module-to-module non-uniformity. The oscillator strength is discussed shortly.

To maximize gain of the material, Eq. 2.15 suggests increasing the population inversion, which can be quantified by the rate equations. The rate equations for the upper and lower lasing level of a three level laser describe the rate of change in electron population and for an optically pumped system is given as

\[ \frac{dN_2}{dt} = R_2 - \frac{N_2}{\tau_2} - \frac{\sigma I_v}{h\nu} (N_2 - N_1) \tag{2.16} \]

\[ \frac{dN_1}{dt} = R_1 - \frac{N_2}{\tau_{21}} - \frac{N_1}{\tau_1} - \frac{\sigma I_v}{h\nu} (N_2 - N_1) \tag{2.17} \]

where \( R_2 \) is the pump rate from the ground energy level 0 to level 2, \( \tau_2 \) is the relaxation time from the upper lasing level that accounts for relaxation from 2\( \rightarrow \)1 and 2\( \rightarrow \)0 and the last term represents the rate of change due to net emitted power.
per unit volume. For an electrically pumped system like a QC-laser, if we assume unity injection efficiency then $R_2 = J/e$, where $J$ is the current density. At steady state, the population inversion is then given as

$$
\Delta N = N_2 - N_1 = \frac{R_2 \tau_2 (1 - \frac{\tau_1}{\tau_{21}}) - R_1 \tau_1}{1 + (\tau_1 + \tau_2 - \frac{\tau_1 \tau_2}{\tau_{21}})(\frac{Q}{k_B T})} \\
\approx R_2 \tau_2 (1 - \frac{\tau_1}{\tau_{21}})
$$

(2.18)

where, in the approximation made, it is assumed that there is negligible pumping to level 1 and a low intensity optical mode. Therefore to increase the population inversion, the relaxation lifetime $\tau_1$ of the lower lasing level must be as small as possible relative to the upper to lower level lifetime $\tau_{21}$ (one method is de-population via longitudinal optical phonon scattering [66]). Additionally, it is best to increase the lifetime of the upper lasing level $\tau_2$ (vertical vs horizontal transitions [37]).

### 2.3 Light Matter Interaction

The rate of radiative transitions (lifetimes) is calculated by considering the transitions induced by a harmonic perturbation, i.e. light. To account for transitions, a time-dependent potential must be considered in the Hamiltonian, where a time-dependent perturbation can be used if the potential relative to the time-independent part is small. The unperturbing Hamiltonian is given by

$$
\hat{H}_0 = -\frac{\hbar^2}{2m^*} \hat{\nabla}^2 + E_c(z) - e\Phi(z).
$$

(2.19)

The radiative transition inducing perturbed Hamiltonian due to light-matter interaction according to the electric dipole approximation is

$$
\hat{H}' = -e\hat{\mathbf{E}} \cdot \hat{\mathbf{r}}
$$

(2.20)
giving a final Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}'$. The transition rate between two quantum-mechanical electronic states of $\hat{H}'$, from the initial state $i$ to the final state $f$, is described by Fermi’s Golden Rule [67]

$$W_{i\rightarrow f}(k_i, k_f) = \frac{2\pi}{\hbar} |\langle f|V'|i \rangle|^2 \delta(E_f(k_f) - E_i(k_i) \pm \hbar \omega). \quad (2.21)$$

It gives the rate for an optical transition between two electronic states and is a function of the optical matrix element ($\hat{H}' = \hat{V}'e^{i\omega t}$)

$$V'_{fi} = \langle f|\hat{V}'|i \rangle \quad (2.22)$$

which is a measure of the interaction between the final and initial electronic states with the perturbation.

Similar to the energy levels of a harmonic oscillator being described by lowering ($\hat{a}$) and raising operators ($\hat{a}^\dagger$), the electric field of a plane wave can be expressed as

$$\hat{E} = \sum_{\sigma} \sum_k u_\sigma \sqrt{\frac{\hbar \omega}{2V_{\text{cav}}}} (e^{ikr}\hat{a}_{k,\sigma} + e^{-ikr}\hat{a}_{k,\sigma}^\dagger) \quad (2.23)$$

where $u_\sigma$ is the unit vector and $\sigma = (1, 2)$ symbolizes one of the two orthogonal field polarizations, and $V_{\text{cav}}$ is the cavity volume. From Fermi’s Golden Rule Eq. 2.21, for a cavity mode with EM field wavevector $k$, polarization $\sigma$ and $n$ photons and an electronic state in the $i$-th subband with in-plane electronic wavevector $k_{||i}$, we find the transition rate to state $f$ to be given as
\[ W_{\text{abs/em}}^{\text{abs/em}}(n^i_{k^i,\sigma};i,k_{||,i}) \rightarrow (n^f_{k^f,\sigma};f,k_{||,f}) = |\mathbf{u}_\sigma \cdot \mathbf{z}|^2 \frac{2\pi}{\hbar} e^2 \frac{\hbar \omega_k}{2V_{\text{cav}} \epsilon_0} |z_{fi}|^2 \delta^{kr}(k_{||,f}, k_{||,i}) \]
\[
\times \{ \delta(E_f - E_i) n^i_{k^i,\sigma} \delta^{kr}(n^f_{k^f,\sigma}, n^i_{k^i,\sigma}) - 1) \\
+ \delta(E_f - E_i + \hbar \omega_k) (n^i_{k^i,\sigma} + 1) \delta^{kr}(n^f_{k^f,\sigma}, n^i_{k^i,\sigma} + 1) \} \\
\]

(2.24)

where the Kronecker delta function designates the necessity for conservation of in-plane momentum, and the scalar dipole matrix element \(z_{fi}\) describes the likelihood of an electronic transition from state \(i\) to \(f\) and is given by

\[ z_{fi} = \langle f|\hat{z}|i\rangle = \int_{-\infty}^{\infty} \psi_f^*(z) z \psi_i(z) \, dz \quad (m) \]

(2.25)

The intersubband polarization selection rule, which dictates whether a transition can occur, is clear from the scalar dipole matrix element calculation because only a time-harmonic EM field’s \(z\) component will couple the electronic states. The first term in expression Eq. 2.24 represents the absorption, and the second term represents the stimulated and spontaneous emission, where spontaneous emission into all cavity modes (for all wavevectors and polarization states) exist regardless of the photon count \(n\). The Dirac delta function is the assumed linewidth of the transition, which can be replaced by a Lorentzian to account for broadening. For stimulated emission, the net rate, while factoring in the quasi-Fermi distribution [68], is given by the summation of all rates for all in-plane wave vector.
values

\[ W_{i \rightarrow f, k, \sigma}^{\text{em}} = |\mathbf{u}_i \cdot \mathbf{z}|^2 \frac{2\pi}{\hbar} e^{i\frac{\hbar \omega_k}{2V_{\text{cav}}}} |z_{fi}|^2 \delta^{k\sigma} (E_i - E_f + \hbar \omega_k) n_i^{k, \sigma} \]

\[
\times \sum_{k_i} \sum_{k_f} \delta(k_{i||, f}, k_{i||, i}) f(E_i) (1 - f(E_f)) 
\]

\[
= \frac{N_i - N_f}{\tau_{i \rightarrow f, (k, \sigma)}^{\text{em}} (\hbar \omega_k)} 
\]

\[ = \frac{(N_i - N_f) n_i^{k, \sigma}}{\tau_{i \rightarrow f, (k, \sigma)}^{\text{em}} (\hbar \omega_k)} 
\]

\[ \equiv -W_{f \rightarrow i, k, \sigma}^{\text{sp abs}} 
\]

where \( N_i \) and \( N_f \) are the number of electrons in the initial and final subbands. Spontaneous emission occurs into all cavity modes, therefore a similar calculation for the net rate requires an additional summation over all cavity modes. Using Eq. 2.24, assuming no photons \((n_i^{k, \sigma} = 0)\) we have

\[ W_{i \rightarrow f, k, \sigma}^{\text{em}} \approx \frac{2\pi}{\hbar} e^{i\frac{\hbar \omega_f}{2\epsilon}} |z_{fi}|^2 N_i \rho_{\text{cav}} (\hbar \omega_{if}) \]

\[ = \frac{N_i}{\tau_{i \rightarrow f}^{\text{sp}}} \]

(2.27)

where the last approximation is the assumption that there is no variation in energy with momentum (not considering nonparabolicity). The spontaneous lifetime \( \tau_{i \rightarrow f}^{\text{sp}} \) is independent of the level population and dependent on cavity modal properties, namely, energy density. For THz QC-lasers, \( \tau_{21} \sim 1 \text{ ps} \) and \( \tau_1 \sim < 1 \text{ ps} \) are typical lifetimes.

By definition oscillator strength

\[ f_{fi} = \frac{2m^* (E_i - E_f)}{\hbar^2} |z_{fi}|^2. \] (2.28)

is a relative comparison in strength of an atomic transition to a single electron’s theoretical transition strength using the classical harmonic oscillator model. It is
an important dimensionless parameter detailing the probability of transition from
an initial to final energy state, where the strength of the transition is dictated by
the selection rules, initial and final state wave functions and how strongly light
interacts with them.

2.4 FL86Q QC-Laser Design

![Conduction band of MQW active region with a LO-phonon depopulation scheme. Figure adapted from [4,12]](image)

To maximize material gain, Eq. 2.18 suggest engineering a relatively quick relaxation time from the lower lasing level to the ground state ($\tau_1$ small). The devices used in our research are based on the resonant phonon depopulation scheme which relies on longitudinal optical phonon scattering for quick depopulation from the lower lasing level to the ground state ($E_{LO}=36.25$ meV for GaAs). The MQW design used in our research, the FL86Q, is based on the FL series presented by Williams et al. [66], where the FL designates a device module designed with four wells and a LO-phonon depopulation scheme (Fig. 2.2). The FL86Q design consists of 86 modules adding up to a 5 $\mu$m thick MQW active region. Fig. 2.3(a)
Figure 2.3: FL86Q design’s (a) conduction band at design bias of 53.6 mV/mod and (b) anticrossing plots. Figure taken from [12].

is the conduction band diagram at the design bias and was obtained using Semiconductor Electrostatics by QUantum AnaLysis (SEQUAL) [69], which is a 1-D Schrödinger equation solver. Levels 1 and 2 represent the injector/depopulation energy levels. In this SEQUAL simulation, levels 1 and 2 are more accurately described by level 1’ and 2’ because the 2 module simulation in SEQUAL will assume an infinitely thick barrier to the left and right of the two module simulation. Level 1’ is more distributed into the next module relative to 2’, therefore it is the injector level.

Level 1’ is anticrossed with level 5 within the injector barrier (10 monolayers thick), which leads to resonant tunneling of an electron from the injection level 1’ to the upper lasing level 5 of the next module at the design bias of 52.3 mV/mod; its anticrossing gap corresponds to a minimum energy difference (Fig. 2.3(b)). The level 5 to 4 radiative transition frequency is $\nu=2.5$ THz ($E_{54} = 9.7$ meV) and depopulation via LO-phonon scattering between level 3 and level 2 with an energy difference of $E_{32}=35.2$ meV selectively and quickly (relative to the upper state lifetime $\tau_2$) depopulates the lower radiative level, where the process continues with the next cascaded module.
2.5 Metal-Metal Waveguide Configuration

The MM waveguide configuration bears great resemblance to a microwave microstrip transmission line (Fig. 2.4), where it consist of two metal layers sandwiching the MQW active region. The waveguide’s fundamental TM$_{00}$ mode satisfies the polarization of the intersubband transitions and has close-to unity mode confinement factor $\Gamma$. The high confinement factor and low metallic loss contribute to lower waveguide loss $\alpha_w$ and higher modal gain $\gamma_{\text{mod}}$ ($\gamma_{\text{mod}} = \Gamma \gamma_{\text{bulk}}$) [13, 36]. An increase in device operating temperature reduces the population inversion due to various mechanisms such as thermally activated phonon scattering which was prohibited at lower temperatures [64]. But because there is less waveguide loss and greater modal gain due to a high mode confinement, MM waveguides have demonstrated the highest operating temperatures (200 K pulsed [70]). Fig. 2.5 shows the MM waveguide losses along with its mode confinement for various geometries. Loss due to free-carrier losses attributed to the two gold metallization layers were accounted for using the Drude model as detailed in Appendix A.4 and the active region was assumed to be lossless.

Figure 2.4: MM waveguide operating in its (a) fundamental TM$_{00}$ and (b) higher-order lateral TM$_{01}$ mode.
2.6 Summary

In summary, starting from the fundamentals of quantum mechanics, the physical building block of a QC-laser, the heterostructure quantum well, is explained. The electronic states, discretized energies and the perturbation theory-derived light matter interaction Hamiltonian were discussed for the heterostructure. Radiative and nonradiative lifetimes were derived, which are used to calculate the population inversion using the rate equation. The material gain is shown to be strongly dependent on the oscillator strength, population inversion and the transition line shape. Detailed in [3], from density matrix formalism, calculated peak material gain can range from 50-100 cm\(^{-1}\). Lastly, the electromagnetic wave confinement and modeling is presented for the metal-metal waveguide configuration. Fig. 2.6 details the flow of the topics discussed.
Figure 2.6: QC-laser topics and their relationship.
Metamaterials and Transmission Line Theory

Electromagnetic metamaterials describe materials engineered to exhibit certain constitutive parameters and can be achieved with either resonant or non-resonant approaches. As mentioned in CH. 1.3, the resonant approach has a restrictive design tradeoff between loss and bandwidth. In our work, we focused on metamaterials realized using the formalism of composite right/left-handed transmission-line theory. The CRLH transmission line metamaterial concept, originally explored in the microwave regime, has been used to implement a wide variety of guided-wave devices (e.g. multi-band and enhanced bandwidth components, power combiners/splitters, compact resonators, phase shifters, and phased array feed lines), as well as radiated-wave devices (e.g. 1D and 2D resonant and leaky-wave antennas) [10, 71, 72].

3.1 Composite Right Left Handed Transmission Line Meta-materials

The following background is extracted from various sources [10, 71]. From conventional transmission line circuit theory, a waveguide supporting a transverse electromagnetic propagating mode can be modeled as distributed series inductance and shunt capacitance and is also known as a right-handed (RH) transmission line; the transmission line is modeled as a periodic array of unit cells with size $p$ satisfying the rule for homogeneity. The RH transmission line has a dispersion
that lies below the light line and is associated with a bound propagating mode, where the phase velocity and group velocity exhibit the same sign. The dual of the RH transmission line is the left-handed (LH) transmission line which is modeled with distributed series capacitance and shunt inductance. The hypothetical LH transmission line has a purely LH dispersion where the phase and group velocity are anti-parallel, i.e. phase is progressing in the backward direction, while power, which is associated with the group velocity is propagating in the forward direction. Unlike the the RH only dispersion, the LH dispersion exhibits a range of operation in both the bound and radiated regime, a.k.a. the leaky-wave regime and is the portion of the dispersion that traverses through the light cone (discussed in detail in CH. 3.3). A transmission line with series capacitance and inductance, as well as shunt capacitance and inductance will have a dispersion with a LH and RH portion (Fig. 3.1). Commonly referred to as a composite right/left-handed (CRLH) transmission line, its dispersion exhibits a finite bandwidth that cuts through the light cone, where operation within the light cone is associated with radiation via the leaky-wave mechanism. In general, the “unbalanced” dispersion has a bandgap at the $\Gamma$ point ($\beta p = 0$) where the band edge frequencies correspond
to either the shunt or series LC resonant tank given by the following expressions.

\[ \omega_{sh} = \frac{1}{\sqrt{L \cdot C}} \]  

(3.1)

\[ \omega_{sh} = \frac{1}{\sqrt{L \cdot C}}. \]  

(3.2)

By judiciously choosing the equivalent shunt and series component values, a “balanced” dispersion can be realized and a seamless transition from the LH branch to the RH branch can be obtained with a transition frequency given by

\[ \omega_0 = \omega_{sh} = \omega_{se}. \]  

(3.3)

The cutoff frequencies \( \omega_{cR} = 2\omega_R \) and \( \omega_{cL} = 2\omega_L \) originate from the purely RH low pass transmission line and purely LH high pass transmission line, respectively. The balanced design is important because power flow is allowed at the transition frequency due to the nonzero group velocity. A CRLH waveguide operating within the leaky-wave region (i.e. where the propagation constant \( |\beta| < \omega/c \)), will function as a leaky-wave antenna.

Practical implementation of a CRLH transmission line involves loading a conventional RH transmission line, for example a microstrip line, periodically with distributed series capacitance \( C_L \) and shunt inductance \( L_L \); the loaded transmission line becomes highly dispersive and exhibits regions of left-handed (backward wave) and right-handed (forward wave) propagation. The resulting dispersion is obtained by applying transmission line theory to the circuit model given in Fig. 3.1, which gives the following Telegrapher’s equations.

\[ \frac{dV}{dz} = -Z' I = -j\omega(L'_{R} - \frac{1}{\omega^2 C'_L})I \]  

(3.4)

\[ \frac{dI}{dz} = -Y' V = -j\omega(C'_{R} - \frac{1}{\omega^2 L'_L})V \]  

(3.5)
\[
\frac{d^2 V}{dz^2} - \gamma^2 = 0 \tag{3.6}
\]

\[
\frac{d^2 I}{dz^2} - \gamma^2 = 0. \tag{3.7}
\]

The complex propagation constant \( \gamma \) is given by

\[
\gamma = \alpha + j\beta = \sqrt{Z'Y'} \tag{3.8}
\]

and the per-unit length impedance and admittance are given by

\[
Z'(\omega) = j(\omega L'_R - 1/\omega C'_L) \tag{3.9}
\]

\[
Y'(\omega) = j(\omega C'_R - 1/\omega L'_L). \tag{3.10}
\]

The dispersion is then finally given by

\[
\beta(\omega) = s(\omega) \sqrt{\omega^2 L'_R C'_R + \frac{1}{\omega^2 L'_L C'_L} - \frac{L'_R}{L'_L} - \frac{C'_R}{C'_L}} \tag{3.11}
\]

\[
|x| = \begin{cases} 
-1 & \text{if } \omega < \omega_{T_1} = \min\left(\frac{1}{\sqrt{L'_R C'_R}}, \frac{1}{\sqrt{L'_L C'_L}}\right) \\
+1 & \text{if } \omega > \omega_{T_2} = \max\left(\frac{1}{\sqrt{L'_R C'_R}}, \frac{1}{\sqrt{L'_L C'_L}}\right).
\end{cases}
\]

To obtain the expression for the complex permittivity and permeability, we use the expression for the propagation constant, characteristic impedance of the line which is given by \( Z_0 = \sqrt{Z'/Y'} \) and the wave impedance.

\[
j\beta = \sqrt{Z'Y'} \tag{3.12}
\]

\[
\beta = \omega\sqrt{\mu\epsilon} \tag{3.13}
\]

\[
Z_0 = \sqrt{Z'/Y'} = \eta = \sqrt{\frac{\mu}{\epsilon}}. \tag{3.14}
\]

Finally from using Telegrapher’s and Maxwell’s equation we can obtain the effec-
The resulting permittivity and permeability exhibit the same electric Drude and magnetic Lorentz response (Eq. 1.3), where the electric plasma frequency $\omega_{p,e} = 1/\sqrt{L_L C_R}$ and magnetic plasma frequency $\omega_{p,m} = 1/\sqrt{L_R C_L}$ are the same band edge frequencies previously mentioned (Eq. 3.1, Eq. 3.2). The damping factors in Eq. 1.3, for a first order approximation, are considered negligible given the non-resonant nature of the CRLH transmission line [73] and $\mu$ is non-resonant ($\omega_{rm} = 0$). The CRLH transmission line’s dispersive relation and its similarity to the wire and SRR array is not coincidental and is shown by Caloz [73] to be the limit of a strongly capacitively coupled array of wires and inductively coupled array of SRRs.

3.2 CRLH MTM Resonators

If we consider a traditional RH only transmission line with open boundary conditions, the fundamental (no variation in the transverse direction) resonant modes of the structure are governed by the transmission line’s dispersion and the integer number $m$ of half guided wavelengths that can fit within the transmission line (the electrical length $\theta = \beta \ell = m\pi$). For a RH only transmission line, $m$ can only be positive and nonzero integer multiples, but this restriction does not apply for the CRLH transmission line (Fig. 3.2(a)), which has negative, zero and positive integer values. Of particular interest is the zeroth order resonance (ZOR), $m = 0$, which has a non-varying field distribution across the length of the structure; it still has an angular frequency oscillation of $\omega_0$. The ZOR is impor-
Figure 3.2: CRLH transmission line (a) dispersion with resonances \( \omega_m \) for a CRLH transmission line resonator, where \( m \) is one less the number of unit cell \( N \). In this illustration \( N = 4 \). (b) Open-ended CRLH transmission line voltage standing wave with an infinite wavelength \( (m = 0 \) mode). Figure taken from [10].

important because its operation is independent of the CRLH transmission line’s physical length, which allows for arbitrary length resonators. At the \( \Gamma \) point for a generally unbalanced case, the structure will resonant in one of two of the available band edge frequencies depending on the applied boundary condition. Namely, applying open boundary conditions result in a shunt ZOR and shorted boundary conditions result in a series ZOR. For the shunt ZOR, the fields are polarized out of plane since it is associated with the shunt elements \( (L_L, C_R) \), and for the series ZOR, the fields are polarized in-plane (parallel to the ground plane) since it is associated with the series elements \( (L_R, C_L) \).

3.3 CRLH MTM Leaky-Wave Antennas

As previously mentioned, operation within the light cone (the leaky-wave regime) is associated with radiation. A conventional purely RH transmission line operating in its fundamental mode is associated with a bound mode and operates in the slow-wave regime. In contrast, the fast-wave regime is associated with radiation.
Figure 3.3: (a) The leaky-wave regime (fast-wave), at a particular frequency, corresponds to wavenumbers (momentum) smaller than points along the perimeter of the light cone (the light line) and the bound regime (slow-wave) corresponds to wavenumbers outside the light cone. (b) Within the leaky-wave regime, operation along the left-handed branch results in frequency scanned beams in the backwards direction, while forward scanned beams are obtained when operating along the right-handed branch. Figure taken from [10].

The differentiation between the slow-wave and fast-wave regime is made by the light cone, which is defined by $|\beta| = \omega/c$ (Fig. 3.3). Analytically, the origin of the leakage radiation can be explained via the general wave form for a wave propagating along a leaky-wave antenna (LWA)

$$
\psi(x, z) = \psi_0 e^{-\gamma z} e^{-jk_x x} = (e^{-\alpha z} e^{-j\beta z})e^{-jk_x x}
$$

(3.17)

where $\beta$ is the in-plane propagation constant and $k_x$ is the out-of-plane propagation constant given by the dispersion relation

$$
k_x = \sqrt{k_0^2 - \beta^2}.
$$

(3.18)

When operating in the fast-wave regime, the phase velocity $\nu_p > c$, which has a corresponding in-plane wavenumber $\beta < k_0$ that gives a real out-of-plane wavenumber $k_x$ and hence a non attenuated component, i.e. radiation. An alternative
explanation is that there is coupling to free space due to momentum matching between the waveguide’s mode and the in-plane component of a TEM, free space propagating mode. For operation in the slow-wave regime, the out-of-plane wavenumber $k_x$ is imaginary leading to an evanescent wave in the out-of-plane direction. Again, an alternative explanation is that momentum is not matched in this case and hence there is no coupling to the TEM, free space propagating mode.

3.4 Summary

CRLH transmission line theory is a physically intuitive tool for realizing metamaterials, which exhibit EM responses not naturally found in available materials. In comparison to the resonant type metamaterials in CH. 1.3, CRLH metamaterial transmission lines are more easily integrated, have greater bandwidth and are less lossy. In the following chapters, we adapt CRLH transmission line concepts to the MM waveguide configuration used for THz QC-lasers to realize novel THz devices.
CHAPTER 4

Radiation Modeling

Given the similarity to the microstrip transmission line, we proposed the use of the cavity antenna model to capture the radiative mechanisms of THz devices based on the MM waveguide configuration. The model is a proven microwave technique that provides a quantitative estimate of the radiative loss, as well as the far-field beam pattern and polarization from MM waveguide cavities and antennas [74]. Here, we use the cavity antenna model along with transmission line theory to predict radiative losses and beam patterns for different QC-devices. Additionally, the model provides physical insight and speed to the analysis of different THz MM waveguide based-device designs.

4.1 Cavity Model and Array Factor Theory

The cavity antenna model is based upon the use of Huygen’s principle to formulate a simplified equivalent problem. The principle states, for a closed surface around the structure of interest, the fields at a given observation point outside of the closed surface can be found by considering radiation from equivalent sources represented by the surface electric and magnetic surface current densities, $J_s$ and $M_s$ respectively, on the closed surface. From the uniqueness theorem, knowledge of the tangential field components on the closed surface gives the equivalent sources.
Figure 4.1: A perspective and top view of the MM waveguide with its completely
tangential electric field profile and equivalent magnetic current sources $M_s$, repre-
sented by double-headed arrows for (a,b) TM$_{00}$ and (c,d) TM$_{01}$ lateral modes.

\[ M_s = -\hat{n} \times E \]  
\[ J_s = \hat{n} \times H \]

where $\hat{n}$ is the surface normal. One can find the exact radiated far-field of the
structure by using the far-field integral expressions (A.1 through A.7) located in
the Appendix A.1.

In analogy to the application of the cavity model to the patch antenna, we
make some approximations of the near-field components of the QC-laser. Specif-
ically, we assume our structure to have a large width-to-height ratio and that the
height is much less than the free space wavelength [75]. For this ideal situation,
fringing fields are negligible, the surface electric fields are tangential to the side-
walls and magnetic fields are normal to the surface so $J_s \approx 0$. We assume an infinite
ground plane, so that one can invoke image theory which doubles the equivalent magnetic current source. Also, any electric surface current that is present on the top surface of the metallic plate will not radiate efficiently since it will cancel with its image. With these approximations, the far-field beam pattern is given by only the equivalent magnetic currents.

The structure of interest is then modelled as an array of radiating equivalent magnetic current elements (see Fig. 4.1), where the array factor is a function of the structure’s dispersion characteristics. For example, in a MM waveguide FP QC-laser, the modelled standing wave is a sinusoidal function with a guided wavelength \( \lambda_g = 2\pi/\beta(\omega) = \lambda_0/n_{\text{eff}} \) where \( \beta(\omega) \) is the dispersive propagation constant. The array factor is then modulated by this sinusoid. For the case of a leaky-wave antenna, the sinusoidal varying field profile also experiences a decaying field factor given by its power attenuation coefficient \( \alpha \), which then dictates the envelope of the array factor along the direction of mode propagation. For example, considering only the two sidewalls of a MM waveguide operating in its TM\(_{01}\) mode as a leaky-wave antenna (Fig. 4.1(c,d)), first an array factor for one sidewall is calculated (along the y direction) using

\[
AF(\theta, \phi) = \sum_{i}^{N} A_0 e^{i(k_0i\Delta y'\sin\theta\sin\phi + \xi_i) - \frac{2}{\alpha}i\Delta y'}
\]

(4.3)

where

\[
\xi_i = -i\Delta y'\beta(\omega)
\]

(4.4)

\[
\theta_{MB} = \sin^{-1}(\beta(\omega)/k_0)
\]

(4.5)

where \( A_0 \) is the normalized element amplitude on the sidewall, \( \theta \) and \( \phi \) are the far-field observation angles, \( \Delta y' \) is the element to element distance in the y direction, \( \alpha \) is the power attenuation coefficient, \( \beta(\omega) \) is the propagation constant along the
leaky-wave antenna, \( i \) is the element index, \( \theta_{MB} \) is the main beam scan angle, and \( k_0 \) is the free-space wave vector. This sidewall is then treated as one radiating source element modified by the appropriate array factor applied in the transverse direction (z direction) to account for the other sidewall.

Using the cavity model’s calculated total radiated power and the structure’s stored energy, the quality factor (radiative loss) can be quantified as shown in the Appendix (A.8). The structure’s time average stored energy is calculated by integrating the electric field within the boundaries of the structure. Of course, this is an approximation since the stored near-field energy is neglected with this method. However, this method does provide a good qualitative understanding of design parameter effects on radiative losses and its accuracy does improve when the structure’s w/h ratio is large and height is much less than its free space wavelength.

Our assumption of an infinite ground plane means that our antenna model is
most accurate for lasers with dry etched facets. However, despite this limitation, we can still obtain insight for THz QC-lasers with cleaved facets provided we consider the following. First, the absence of a ground plane will reduce the effective magnetic image current, which will decrease the radiated power from the facet. Second, the beam pattern will change somewhat as radiation into the lower half-space (previously screened by the ground plane) is now possible (Fig. 4.2).

However, as can be seen from data reported in the literature [5, 76] the beam pattern in the upper half space still exhibits the characteristic fringe patterns that we will show is well described by the cavity model. The cavity model is particularly useful for the emerging designs for THz QC-lasers in MM waveguides with directive beam patterns (such as leaky-wave antennas [77], second and third-order distributed feedback lasers [8], [78], and 2-D photonic crystals [79]), which do not possess cleaved facets.

4.2 MM Waveguide Resonators: Fundamental TM$_{00}$ Lateral Mode

We begin by applying the cavity model to a MM waveguide FP cavity oscillating in an axial mode with index $m = 2l/\lambda_g$. We first consider the radiative quality factor $Q$ for the TM$_{00}$ mode as a function of cavity length using approximated analytic expressions, the cavity model and a full-wave 3-D finite-element solution. The 3-D finite-element simulations for this paper were conducted with HFSS for MM waveguide QC-laser cavities with a 10 $\mu$m or 5 $\mu$m thick active region, 0.2 $\mu$m thick upper metal, 15 $\mu$m ridge width and an infinite ground plane. A 15 $\mu$m ridge width is selected in this study since its TM$_{01}$ mode’s cut-off frequency ($\sim 2.7$ THz with $n_{eff} = 0$) corresponds to a frequency within the THz spectral range and its significance is discussed in greater depth in CH. 6 and CH. 7.1.

In order to obtain the appropriate magnitude of the sidewall magnetic cur-
Figure 4.3: A $w = 15 \mu m$, $h = 5 \mu m$ TM$_{00}$ metal-metal waveguide with a 0.92 facet reflectivity ($0.96e^{-j1.54}$ complex facet reflection coefficient) at 2.7 THz, which agrees with data from [13]. Inset shows the mode’s electric field.

rents, an infinitely long structure is simulated using the finite-element method to obtain the transverse waveguide mode profile for the TM$_{00}$ and TM$_{01}$ modes in the geometries of interest. In this way, the value of the transverse E-field at the sidewalls can be related to the stored energy of the cavity. A polynomial fit of the lateral field profile was used in the calculations for the equivalent magnetic current sources. The same fitted lateral field profile was also used to calculate the stored energy of the MM waveguide resonator.

Additionally, for the MM waveguide cavities pictured in Fig. 4.1, the termination is ideally open and the E-field exhibits an anti-node (maximum) at the facet. In realistic structures, the termination deviates slightly from this condition resulting in a slightly smaller facet field amplitude [80]. This is accounted for by extracting the complex facet reflectivity from a 3-D finite-element simulation (Fig. 4.3) and incorporated into the far-field beam pattern calculations using the cavity model.
Figure 4.4: The cavity model predictions improve with a larger $w/h$ ratio as expected.

Figure 4.5: Quality factor of a MM waveguide FP cavity with $w = 15 \mu m$ and $h = 10 \mu m$ operating at 2.7 THz in its TM$_{00}$ mode as calculated using the cavity model. Analytic calculations (A.9) and (A.11) provided in the Appendix show close agreement with the cavity model and HFSS simulations.
Figure 4.6: A comparison of predicted far-field intensities by the cavity model and HFSS simulation for a MM waveguide with $w = 15 \, \mu m$ and $h = 10 \, \mu m$ operating at 2.7 THz in its TM$_{00}$ mode. (a) Cavity model: radiation due only to the two sidewalls. Far-field intensity due to the sidewalls is three orders of magnitude less than that of the two facets. (b) Cavity model: radiation due only to the two facets. (c) Cavity model: radiation due to two facets and sidewalls. (d) HFSS simulation: radiation due to two facets and sidewalls. Field is primarily polarized in $\phi$ direction.
HFSS eigenmode simulations for MM waveguide QC-lasers resonating (cold cavity) in its TM$_{00}$ mode at 2.7 THz were conducted for structures up to only an axial mode index of $m = 21$, $l = 0.399$ mm, due to simulation size constraints—a limitation that does not exist for the implemented cavity model. Simulations were conducted with a lossless active region, and the metallization was considered to be a perfect electric conductor, therefore, the simulated quality factor reflects only loss associated with radiation. Using the extracted field profile from the simulation, the facet reflectivity was calculated to be 0.84 and the confinement factor 0.79.

A nice feature of the cavity model is that it allows one to study the contributions of each radiating component (sidewalls, facets) separately. Fig. 4.5 illustrates this with the facet and sidewall radiative losses shown separately for a structure with a $w/h$ of 15 µm/10 µm. The radiative losses from the sidewalls are at least three orders of magnitude less than that of the facets—a clear indication that even for MM waveguide lasers with subwavelength dimensions and substantial evanescent field in the air, for the TM$_{00}$ mode, the facets remain the primary source of laser emission. Hence for the TM$_{00}$ mode, the far-field rings in the beam pattern can be considered to originate from the interference of two dipole sources separated by distance $l$. The strong suppression of sidewall radiation is due to two effects: the partial near-field cancellation of the oppositely directed equivalent magnetic current sources along the sidewalls and the far-field cancellation of the rapidly oscillating $M_s$ that occurs for $n_{\text{eff}}>1$, when $l \gg \lambda_0$. Adjacent data points correspond to a difference in MM waveguide length of $\lambda_0/2$. Oscillations in the quality factor with a period of three axial mode indices (corresponding to a total distance of $\lambda_0/2$ since the $n_{\text{eff}} = 3.01$) are therefore due to the constructive and destructive interference of the facets. Lastly, as shown in Appendix A.1 we can also apply the cavity model to derive analytic expressions for radiative Q in the limits where $l \gg \lambda_0$ and $w,h \ll \lambda_0$ for the TM$_{00}$ mode (facets are approximated
to be ideal opens and an uniform lateral field profile is assumed). This allows us to identify scaling trends with dimensions. The small discrepancy between the cavity model and the analytic expressions is due to the nominally more realistic incorporation of the simulated lateral field profile and facet reflectivities. The cavity model predicted $Q$ is in good general agreement with the full-wave 3-D simulations although the cavity model consistently predicts a higher value for the quality factor. This discrepancy results from the assumption that fringing fields can be neglected. Indeed, our calculations show a convergence between HFSS and cavity model simulations for larger $w/h$ ratios. For example for $w/h = 15 \, \mu m/3 \, \mu m$ (Fig. 4.4) the $Q$ values calculated by HFSS are $\sim 80\%$ of those calculated by the cavity model, compared with $\sim 50\%$ for the $w/h = 15 \, \mu m/10 \, \mu m$ case shown in Fig. 4.5. Thus, while the cavity model predictions for $Q$ are at best semi-quantitative for $w/h \sim 1$, they still provide qualitative insight. Furthermore, THz QC-lasers with an active region thickness of $1.75 \, \mu m$ have recently been demonstrated [38], for which the cavity model will be increasingly accurate for calculating radiative losses.

As a representative case, a comparison between the cavity model predicted and simulated (using a HFSS driven modal simulation) far-field beam patterns for a MM waveguide QC-laser with a $w/h=15 \, \mu m/10 \, \mu m$ and an axial mode index of $m = 21$ is shown in Fig. 4.6. We see that the radiation from the facets is the dominant contribution—an observation which is consistent with the cavity model’s prediction of $Q_{\text{sides}}/Q_{\text{facets}} \sim 1000$ shown in Fig. 4.5, and is supported by the decomposed beam patterns. Namely, the radiation pattern from the sidewalls (Fig. 4.6(a)) is expected to give a null along the longitudinal cut of the structure since the equivalent magnetic currents along the two sidewalls are in opposite directions, which leads to destructive interference of their far-field beam patterns directly above the laser ridge (at $\theta = 90^\circ$). However, this is not seen in the overall beam pattern, which is dominated by interference of radiation from the
two facets, and exhibits strong $E_\phi$ polarization. The number of rings (fringe pattern) is directly related to the length of the structure [81]. The radiation pattern predicted by the cavity model matches very well with the full-wave finite-element simulation even though the $w/h$ ratio is close to one, illustrating that the far-field calculations are quite robust.

![Figure 4.7: Quality factor versus effective index for a hypothetical MM waveguide in its TM$_{00}$ mode with $\sim$1000 $\mu$m length. Various effective indices are hypothetically assumed for a MM waveguide with width 15 $\mu$m and height $h = 3$ $\mu$m. Operating frequency is 2.5 THz. Field profile along facet and sidewalls assumed to be ideal with a normalized electric field amplitude of 1 V/m.](image)

The example above illustrated that the facets were the main radiating components for a TM$_{00}$ FP cavity QC-laser, however, the dominant radiating mechanism can change with the mode’s effective index. Consider a hypothetical MM waveguide finite length resonator with an effective modal phase index less than unity; this could be a metamaterial inspired design, or simply a model close to the cutoff frequency. As a representative case, the radiation from the facets and sidewalls of a resonator with a length of $\sim$1000 $\mu$m is analyzed. For effective indices $|n_{eff}| < 1$, the cavity model predicts that the constructive radiation of
Figure 4.8: Dispersion curve for a MM waveguide operating in its TM$_{01}$ mode. Eigen-frequencies are obtained from unit cell eigenmode simulations with periodic boundary conditions corresponding to an infinitely long structure in HFSS. The circuit model for ($L_R = 2.7 \, p\mu H$, $L_L = 2.5 \, p\mu H$, $C_R = 1.3 \, fF$) is in close agreement with the simulation.

the sidewall can be an order of magnitude greater than that of the facets due to the in-phase contributions from the two sidewalls (when $w < \lambda_0/2$) as shown in Fig. 4.7. For larger effective indices, the facet contribution becomes greater than that of the sidewalls, which supports the observations made for the TM$_{00}$ FP cavity QC-laser with effective index $n_{eff} \sim 3.6$ (GaAs/GaAlAs material system). For infinitely long structures with $n_{eff}>1$, sidewall radiation goes to zero as expected for a bound mode.

### 4.3 MM Waveguide Resonators: Higher-order TM$_{01}$ Lateral Mode

Unlike the fundamental TM$_{00}$ mode, which is quasi-TEM and has no low frequency cutoff, the TM$_{01}$ mode exhibits a cut-off frequency $\omega_{sh}$ at which $\beta = 0$ (Fig. 4.8).
Figure 4.9: Quality factor versus effective index for MM waveguide in its TM_{01} mode with \sim 250 \mu m length. Various effective indices are obtained by varying ridge widths from 15 \mu m to 45 \mu m while keeping \( h = 5 \mu m \). Operating frequency is 2.7 THz. Field profile along facet and sidewalls assumed to be ideal sinusoids with a normalized electric field amplitude of 1 V/m. Analytic calculations provided in (A.10) and (A.12) in the Appendix are derived with the same approximations. Insets show the electric field profile in the lateral direction for various ridge widths.
For certain frequencies close to its cut-off, this mode propagates with an effective index $n_{\text{eff}} < 1$, and can be made to couple radiation into a directive beam according to the leaky-wave mechanism. To examine the radiative mechanisms of this in detail, we first consider a MM waveguide finite length resonator operating in its TM$_{01}$ mode. As a representative case, the radiation from the facets and sidewalls of a resonator with a length of $\simeq 250 \ \mu m$ is analyzed (Fig. 4.9). Independent of cavity length, for operation within the light cone ($|n_{\text{eff}}| < 1$), the cavity model predicts that the constructive radiation of the sidewall is orders of magnitude greater than that of the facets due to the in-phase contributions facet contribution become greater than that of the sidewalls. This is a somewhat unexpected result. Since the magnetic currents from the two sidewalls are in phase for a TM$_{01}$ mode, the far-field beam pattern will have even symmetry without a broadside null. However, for structures with $n_{\text{eff}} > 2.3$, the far-field beam pattern is expected to have a null since the facets are the dominant radiating components and have equivalent magnetic currents in opposite directions, as observed in [76] for 130 $\mu m$ wide MM waveguides. This result indicates that examination of the symmetry of the far-field beam pattern alone is not sufficient to identify which lateral mode is lasing. We will see in CH. 6, the polarization of the far-field beam pattern can be used instead if $n_{\text{eff}}$ is unknown.

4.4 Summary

In conclusion, we have proposed the application of the microwave patch antenna cavity model as a general tool for analyzing the radiative properties and beam patterns of THz MM waveguide structures. The method is computational resource non-intensive, allowing for a quick assessment of designs with physical intuition. Its implementation is also not constrained to very narrow wire lasers as in [81], and as such can account for the effects of transverse mode structure and describes
the far-field polarization. As a benchmark, comparisons between full-wave 3-D finite-element method simulations and the cavity model were performed for TM\textsubscript{00} FP cavity QC-laser. Generally speaking, excellent agreement between the cavity model and full-wave simulations was seen for observed beam patterns and a good qualitative agreement was observed for the radiative quality factors. Disagreements in calculated Q-factors generally originated from the approximations invoked to make the cavity model tractable and were greatly reduced for larger width-to-height ratios that reduced fringing fields. Given the flexibility of the cavity model, it is possible for it to be used for other sorts of THz radiating structures. In the next chapter the cavity model is applied to a TM\textsubscript{01} MM waveguide operating as a leaky-wave antenna and a balanced CRLH leaky-wave antenna.
Active THz Metamaterials: Fundamental Mode

The MM waveguide QC-laser can be interpreted as a THz microstrip transmission line with distributed photonic gain. Therefore, we proposed adapting the CRLH transmission line formalism to realize THz CRLH active transmission line metamaterials. In our effort to realize metamaterial inspired THz QC-laser devices, many different designs were investigated. Initial designs were centered around the fundamental TM$_{00}$ waveguide mode [14]. Design efforts focused on two device types: a zeroth-order resonator (ZOR) and a leaky-wave antenna. Unfortunately, high ohmic losses made the ZOR design difficult to realize [12] and although their use as an antenna was promising, fabrication difficulties associated with the stub inductance proved to be impractical. In this chapter we discuss this design and the lessons learned.

5.1 1-D Metamaterials

Our initial efforts in realizing a metamaterial active device focused on a 1-D unbalanced QC-CRLH structure based on the TM$_{00}$ waveguide mode (Fig. 5.1) [14]. The design was based on the MM waveguide platform with distributed left-handed capacitance and inductance realized by periodically loading the MM waveguide with gaps and sidewall stubs, respectively. To maintain electrical isolation between the top contact and ground plane for biasing, the sidewall stub to ground was realized via a large capacitor. Below is a short overview of this initial design and the reader is directed to [12] for greater details.
Although the proposed structure exhibited an unbalanced dispersion, it could still operate as a ZOR. Namely, by imposing open boundary conditions at the end of a 1-D array of an unbalanced QC-CRLH structure, a ZOR operating in its shunt mode would have a field profile with zero variation along the length of the structure. The polarization of the shunt mode is in the growth direction and hence satisfies the selection rules of the MQW, therefore with enough modal gain a zeroth order laser could be realized. Such a device would exhibit the following unique properties: no spatial hole burning, improved electrical pump to THz photon conversion efficiency, gain compression reduction, lasing with cavity lengths independent of the integer multiples of a half guided wavelength and single moded lasing. Fig. 5.2(a) shows the simulation setup of a weakly coupled excitation of a 5 unit cell QC-CRLH structure with open boundary conditions (high reflectivity facets). Material gain is increased until the noted transmission peaks, designating the onset of oscillation and the lasing threshold for the particular mode. An anisotropic dielectric loss tangent was used to model the photonic material gain in the MQW material and with reference to Fig. 5.2(b), the x directed component
Figure 5.2: (a) A THz QC-laser consisting of five unit cells of the proposed balanced CRLH transmission line terminated with open boundary conditions was weakly coupled to waveport excitations in HFSS. Bulk material gain was then increased until threshold gain values for the ZOR oscillation were reached. The blue and red curve represent the transmission through the cold cavity (no gain) and the active cavity, respectively. A bulk material gain of 41 cm⁻¹ is needed to compensate for ohmic and radiative losses; free carrier loss in the MQW region was not accounted for here. (b) Radiative losses were obtained via simulations with and without ohmic losses for the zeroth and higher-order modes. The ZOR exhibits a nearly unity 3-D confinement factor and mode uniformity (inset). (c) E-field plots for the $m = 0$ mode (zero-index CRLH resonator) indicate an uniform electric field across the balanced CRLH resonator at $\omega = 1.8$ THz with a strong out of plane component, which satisfies the selection rules for optical gain; there is a very small longitudinal component across the gap capacitors. (d) E-field plots for $m = 1$ mode for the series resonance at $\omega=2.5$ THz with a strong longitudinal component across the gap capacitors. Figure taken from [14].
(MQW growth direction) is given by

\[ \tan \delta_\perp = \frac{\epsilon'' - (\eta_{\text{bulk}} g_{\text{mat}} C/\omega)}{\epsilon'} \] (5.1)

where \( \eta_{\text{bulk}} \) is the estimated bulk refractive index for the MQW superlattice and \( g_{\text{mat}} \) is the bulk material gain. The other two in plane directions are given by

\[ \tan \delta_\parallel = \frac{\epsilon''}{\epsilon'} \] (5.2)

where the complex permittivity is obtained from Drude's model. Derivation details and HFSS implementation of the material gain are discussed in Appendix A.4

The ZOR has two unique field profile characteristics: increased modal uniformity and mode confinement. Increased modal uniformity, which reduces gain compression due to more efficient pumping of active regions with the desired mode, is expected from a ZOR operating in its shunt resonance (Fig. 5.2(b)), where it is given as

\[ \eta_u = \frac{\left[ \int_{\text{act}} |E_\perp|^2 dv \right]^2}{V_{\text{act}} \int_{\text{act}} |E_\perp|^4 dv} \] (5.3)

and the active region volume is designated as \( V_{\text{act}} \). Increased modal uniformity results in a higher slope efficiency \( (\eta_{\text{slope}} = \frac{dL}{d\Phi}) \) [82], which increases the output power [15] since \( P_{\text{rad}} \propto \frac{dL}{d\Phi} \).

Mode confinement measures the optical mode overlap with the MQW gain medium and a value of unity is desired because the overlap leads to stimulated emission via intersubband radiative transitions. The expression is given by

\[ \Gamma = \frac{n_g \int_{\text{act}} \epsilon |E_\perp|^2 dv}{n_{\text{act}} \int_{-\infty}^{\infty} \epsilon |E|^2 dv} \] (5.4)

where \( n_g \) and \( n_{\text{act}} \) are the group index of the mode and the bulk refractive index of the gain medium, respectively. In its shunt resonant mode, the ZOR has an optical mode field profile that is parallel to the growth direction and confined primarily
in the MQW active region (Fig. 5.2(b inset,c)); the series resonant mode is not desired since the optical field is primarily localized in between the gap of the top plate and hence would not couple well with the intersubband transition of the MQW active region (Fig. 5.2(d)).

In addition to a zeroth order QC-laser, a 1-D balanced QC-CRLH structure based on the TM\textsubscript{00} waveguide mode with an enhanced gap capacitance to close the band gap was investigated for leaky-wave applications. The 1-D balanced QC-CRLH unit cell dispersion characteristics extracted from finite element simulations is shown in Fig. 5.3 and there is a seamless transition between the backward and forward wave propagation regions. The unit cell size of this design remains the same as the unbalanced QC-CRLH unit cell discussed above. However, in order to utilize conventional photolithographic procedures and to close the band gap, the left-handed capacitance and inductance features were changed. In order to compensate for the decrease in left-handed capacitance due to the increase of the gap, which was need for photolithography, a conductive top plate insulated by a 0.12 \textmu m thick layer of silicon dioxide is added above and in between the gap, effectively increasing the achievable series capacitance. Relative to the unbalanced design, the width of the shunt inductor increased to 4 \textmu m, moving the shunt resonant frequency upwards. With those two design changes, a balanced QC-CRLH unit cell with a transition frequency of 1.95 THz is achieved.

Fig. 5.3(a) shows the dispersion curve traversing through the light cone where radiative loss is expected to be the highest since there is efficient coupling to free space. Therefore, a 1-D transmission line radiating structure can be realized with a leaky-wave region that extends from \(~\text{1.65–1.95} \text{ THz}\) and \(~\text{1.95–2.45} \text{ THz}\).
Figure 5.3: (a) Simulation results of the balanced QC-CRLH transmission line metamaterial. Dispersion characteristic of a 1-D structure obtained by finite element method. Inset shows the simulated geometry along with relevant dimensions of the subwavelength inclusions. 2 μm gap covered by a 0.12 μm coating of oxide which is covered by a conductive plate, 4 μm wide stub, 10 μm unit cell length and width result in a balanced CRLH transmission line. Calculated threshold gain values for the $m = -2, -1, 0, 1$, modes for a 5 unit cell long CRLH resonator. (b) Simulated power attenuation for a 10 unit cell long, QC-CRLH transmission line. Shaded region corresponds to frequency range where the dispersion curve lies within the fast wave region. Inset shows the simulated geometry of the 10 unit cell, QC-CRLH transmission line. Figure from [14].

Due to limitations on computational resources, only a 10 unit cell ($\sim 0.67 \lambda_o$ at $f=2.0$ THz) long structure was simulated for analysis. Fig. 5.3(b) shows the power loss coefficient for the balanced QC-CRLH transmission line where the excited $TM_{00}$ mode is swept in frequency. For the purely radiative case, where conductive loss is not considered, radiative loss is observed to significantly increase within the leaky-wave region. With conductive loss included, there is a greater loss over all frequencies. In the lower frequency range, due to a lower group velocity, a substantial increase in loss is observed. The power attenuation coefficient (Fig. 5.3(b)) exhibits oscillations because of the simulation’s finite length resonances and the port to QC-CRLH transmission line impedance mismatch; the terminations are purely right-handed transmission lines (conventional MM waveguides). The purely right-handed portions are removed through de-embedding, however, the impedance mismatch between the purely right-handed
portions with the QC-CRLH unit cells is not negligible and results in reflections and resonances, which then lead to scattering parameters with resonance characteristics as well. From this simulation, however, important information can be extracted, such as an upper bound on the loss associated with the QC-CRLH transmission line structure.

Although the structure was not electrically large, it still achieved a backward to forward scanning beam in the E plane (longitudinal cut) as shown in Fig. 5.4 and Fig. 5.5. The illustrated frequencies, \( \sim 1.7 \) THz and \( \sim 2.3 \) THz, correspond to frequencies that are close to the light line but do not exhibit a large scan angle away from broadside as one would expect given the dispersion relation. Considering array factor analysis, the simulated short antenna structure translates to a broad array factor pattern, which would then explain the less-than-expected scan angle. It is interesting to note that the H plane cut (lateral cut) exhibits a radiation pattern that is not symmetric about the axial direction because of the

Figure 5.4: 10 unit cell TM\(_{00}\) QC-CRLH leaky-wave antenna with backward to broadside to forward frequency scanning capability.
Figure 5.5: Normalized directivity for longitudinal and lateral far-field cuts of the LWA.

Figure 5.6: Magnitude far-field polarization components at (a) 1.7 THz, (b) 2.0 THz, and (c) 2.3 THz.
structure’s asymmetry; there is an inductive stub only on one side. A simulation for a backward scan and forward scan of an unbalanced double sided inductive stub design resulted in a symmetric pattern confirming our assumption (not shown). The polarization of the far field for different frequencies is shown in Fig. 5.6. For the backward scanned beam, the field is dominantly polarized along the ridge \((E_\theta)\), however there are significant cross polarization components at the transition frequency \((2 \text{ THz})\) and in the forward scanned beam at \(2.3 \text{ THz}\). Looking at the axial ratio (AR), the polarization at 1.7 and 2 THz is essentially linear with ARs greater than 10 dB. At 2.3 THz, the AR\(\sim3\) dB corresponding to an elliptically polarized wave with a left-handed polarization \([83]\).

### 5.2 2-D Metamaterials

In addition to 1-D active metamaterials, we were also interested in the feasibility of realizing a 2-D active ZOR structure for scalability and control of the far-field beam directivity. To realize the 2-D active ZOR structure, we needed a 1-D metamaterial design that would scale easily to a 2-D architecture. The 1-D designs mentioned so far did not satisfy the scaling requirement, therefore a new design, which drew inspiration from the Sievenpiper mushroom \([84]\), was selected. The unit cell of the structure consists of a 10 \(\mu\text{m}\) square and 5 \(\mu\text{m}\) tall active region with a via from the top metallization to the ground plane (inset of Fig. 5.7(a)). The top metallization is continuous to maintain DC connectivity, therefore capacitive gaps like those found in Sievenpiper’s mushroom are not present. Since there is no equivalent distributed left-handed capacitance, only a right-handed branch exist with a \(\sim3.45\) THz band edge frequency given by the the left-handed inductance \(L_L\) realized by the via and the right-handed capacitance \(C_R\) \((\omega_{sh} = 1/\sqrt{L_L C_R})\).
Figure 5.7: (a) Dispersion for a 2D THz Sievenpiper-like (no series capacitance) mushroom array. Inset shows the dimensions and field profile for a unit cell along with its circuit model. (b) Equivalent magnetic current sources and (c) electric field profile for a 3x3 array in its shunt resonance along with a top down view of its electric monopole-like far-field radiation pattern. Due to the use of a symmetry plane in the simulation, only half the structure is shown.
Table 5.1: Radiative and ohmic threshold gain values for different 2-D array sizes, where free carrier loss in the GaAs is neglected and the gold metallization is considered with $n = 5.9 \times 22$ cm$^{-1}$, $\tau = 60$ fs.

<table>
<thead>
<tr>
<th>Array size</th>
<th>$f_{sh}$ (THz)</th>
<th>$g_{th,rad}$ (cm$^{-1}$)</th>
<th>$g_{th,met}$ (cm$^{-1}$)</th>
<th>$g_{th,rad+met}$ (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3x3</td>
<td>3.25</td>
<td>178</td>
<td>60</td>
<td>238</td>
</tr>
<tr>
<td>4x4</td>
<td>3.32</td>
<td>178</td>
<td>58</td>
<td>236</td>
</tr>
<tr>
<td>5x5</td>
<td>3.34</td>
<td>146</td>
<td>68</td>
<td>214</td>
</tr>
</tbody>
</table>

When operating at the band edge frequency (zeroth order shunt resonance), the 2-D structure’s radiating mechanism consist of a circular magnetic current configuration, which gives the same radiation pattern as an electric monopole, namely, an omnidirectional pattern with a null at broadside. Fig. 5.7(b-d) shows the equivalent magnetic current sources, electric field profile and far-field pattern for an illustrative 3x3 array example.

Table 5.1 shows the threshold gain values for 2-D arrays with different sizes. The dominant loss mechanism is radiative, and the large ohmic losses (relative to the 1-D designs) is primarily due to the conduction current through the via from the top metallization to ground. Considered in another analysis is the addition of an isolation layer between the via and the MQW active region. To avoid shorting the MQWs, a thin plasma-enhanced chemical vapor deposition (PECVD) SiO$_2$ insulating layer ranging from 25 nm – 100 nm was considered. For oxide layers thicker than 25 nm, the small capacitance, formed by the via, insulator and ground was too small to realize a virtual short, therefore altering the shunt inductance and zeroth order shunt resonance. The thickness of the oxide also posed another challenge, since an applied voltage of 10 V across the active region would most likely reach the typical $\sim$8–11 MV/cm breakdown limit for PECVD SiO$_2$. Although the structure is radiatively efficient, its radiative loss proved too high and its implementation impractical.
5.3 Summary

The 1-D, TM$_{00}$ waveguide mode based designs initially showed promise. However, it was later found that the ohmic and insulator losses associated with the virtual short needed to realize the shunt inductance added an additional $\sim 50 - 70$ cm$^{-1}$ of loss [12]. The sidewall stub also proved to be a fabrication challenge. Although there were fabrication challenges and excessive losses for the initially proposed design, the fundamental concepts and unique features of CRLH metamaterial QC-devices were still conceptually possible. We, therefore, redirected our attention to the planar designs discussed in the next chapter.

Although the 2-D mushroom-like THz ZOR structure addressed scalability concerns, it presented implementation challenges that rendered the design non-feasible. Additionally, unless, a monopole like radiation pattern was desired, there was little control over the beam pattern of the design. We revisit the concern for scalability and beam control in CH. 8 with new designs.
CHAPTER 6

Active THz Metamaterials: Higher-Order Modes

From the lessons learned in CH. 5, attention was redirected towards a planar design using the MM waveguide in its higher-order TM$_{01}$ lateral mode. As mentioned in CH. 4, the MM waveguide in its higher-order TM$_{01}$ lateral mode can be used as a LWA since it exhibits a finite operating bandwidth in the light cone. The mode is associated with characteristics not achievable with the TM$_{00}$ mode such as strong radiative loss, which can be made to exceed unwanted ohmic and material losses for more efficient radiative coupling. For the TM$_{01}$ MM waveguide with a right-handed-only dispersion, only a forward scanning beam can be achieved. By including periodic gap capacitors, a CRLH transmission line metamaterial is realized and a full backward to forward scanning LWA is demonstrated.

6.1 TM$_{01}$ Waveguide Mode, Right Hand Only

The waveguide radiation loss is quite large for the MM waveguide operating in its TM$_{01}$ mode; while this leads to more efficient radiative coupling, one would often like to reduce $\alpha$ for use as a laser or LWA. An obvious strategy is to decrease the height $h$ to reduce the area of the emitting aperture, hence a $h = 5 \mu m$ was chosen for this analysis. A second strategy suggested by the cavity model is to introduce holes with a sub-wavelength periodicity, $p$, into the upper metallization. Then the MM waveguide structure in its TM$_{01}$ mode can be analyzed as repeated unit cells.
Figure 6.1: Dispersion curve for a MM waveguide operating in its TM\textsubscript{01} mode. Two cases are considered; namely, a unit cell with and without holes. In the latter case, a transverse ($h_W$) and longitudinal ($h_L$) hole dimension of $h_W = 3 \ \mu m$ and $h_L = 6 \ \mu m$ is introduced into the unit cell ($p = 8 \ \mu m$) to bring the shunt resonant frequency from 2.75 THz to 2.63 THz. Eigen-frequencies are obtained from unit cell eigenmode simulations with periodic boundary conditions corresponding to an infinitely long structure in HFSS. The circuit model for the case without the hole ($L_R = 2.7 \ pH$, $L_L = 2.5 \ pH$, $C_R = 1.3 \ fF$) and with the hole ($L_R = 2.7 \ pH$, $L_L = 2.8 \ pH$, $C_R = 1.3 \ fF$) are in close agreement with the simulations.
of size $p = 8 \mu m$ (see Fig. 6.1). The addition of the holes has two effects. First, the dispersion relation is altered as illustrated in Fig. 6.1. Without the addition of the holes, the MM waveguide’s $TM_{01}$ mode has a cut-off frequency of $\sim 2.7$ THz, or equivalently, a shunt resonant frequency given by the transmission-line circuit model [10]

$$\omega_{sh} = 1/\sqrt{L_L C_R}. \tag{6.1}$$

In the language of transmission-line metamaterials, increasing the hole size narrows the inductive path leading to a larger shunt inductance $L_L$, and reduces the shunt resonant frequency $\omega_{sh}$ [77]. This is in contrast to a dielectric-only waveguide, where the addition of air holes would decrease the effective index of the mode. The change in the shunt capacitance is not substantial since the electric field has a null in the center of the ridge (Fig. 6.2(a)). In addition to controlling the shunt frequency, the hole size also gives the designer a parameter to control the radiative losses. This can be explained qualitatively using the cavity model by considering additional equivalent magnetic currents at the sidewalls of the holes (see Fig. 6.2(b)). Components labelled $M1$...
are the dominant in-phase components along the sidewalls of the structure and contribute most to the radiated power. The $M2$ components have a negligible contribution due to their quadrupole arrangement. As the hole size in the longitudinal direction is made larger, larger $M3$ components are generated, which leads to a destructive near and far-field contribution relative to that from the $M1$ components; as a result the quality factor should increase. Lastly, the $M4$ components are only present at the ends of the structure since they correspond with the facets and have negligible contribution when operating within the fast-wave region (see Fig. 4.9. A comparison of the radiative losses for an 80 $\mu$m long TM$_{01}$ MM waveguide cavity with varying hole sizes is presented in Table 6.1. The calculated quality factors confirm the trend in radiative losses qualitatively explained by the cavity model. It is important to note that for the finite length structure reported in Table 6.1 there will be a slight shift in shunt frequency compared to that of an infinitely long structure due to the loading effect of radiation from the facets. While the analysis presented shows an increase in the radiative quality factor for an increase in longitudinal hole size, there is also a metal quality factor trade-off. Namely, as the hole size increases, the effective width is decreased leading to an increase in metallic losses, which result in a lower metal quality factor.

Table 6.1: Radiative losses for the TM$_{01}$ mode in its $m = 0$ (zero-index) resonance with different longitudinal hole sizes

<table>
<thead>
<tr>
<th>Longitudinal hole size $h_L$ ($\mu$m)</th>
<th>$\omega_{sh}/2\pi$ (THz)</th>
<th>Q (HFSS)</th>
<th>Q (CM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>no hole</td>
<td>2.814</td>
<td>15.0</td>
<td>14.4</td>
</tr>
<tr>
<td>1</td>
<td>2.813</td>
<td>15.0</td>
<td>15.4</td>
</tr>
<tr>
<td>2</td>
<td>2.806</td>
<td>15.2</td>
<td>16.8</td>
</tr>
<tr>
<td>3</td>
<td>2.792</td>
<td>15.5</td>
<td>18.0</td>
</tr>
<tr>
<td>4</td>
<td>2.770</td>
<td>16.2</td>
<td>19.9</td>
</tr>
<tr>
<td>5</td>
<td>2.736</td>
<td>17.0</td>
<td>21.7</td>
</tr>
<tr>
<td>6</td>
<td>2.689</td>
<td>19.0</td>
<td>23.4</td>
</tr>
</tbody>
</table>
Figure 6.3: Comparison of the longitudinal cut of the far-field beam pattern at 2.74 THz. Inset shows main beam angle predictions from HFSS simulations, the cavity model and measurements for 2.61, 2.74, 2.81 THz, where the LWA is passive and is excited by a master oscillator.
6.1.1 Experimental Results

Operation within the leaky-wave bandwidth of the TM$_{01}$ mode is accompanied by a directive beam launched by the antenna due to the small phase variation between radiating elements as suggested by (4.3); similar microwave microstrip line versions have previously been demonstrated [85].

As an example, we compare cavity model predictions against an experimentally measured beam pattern from a QC LWA presented in [77], namely, with $w = 15 \, \mu m$, $h = 5 \, \mu m$, $p = 8 \, \mu m$, and $3 \, \mu m \times 3 \, \mu m$ holes. Similar to the field profile extraction used for the TM$_{00}$ waveguide mode discussed in CH. 4.2, from the unit cell simulation, the TM$_{01}$ field profile is extracted for calculation of the equivalent magnetic currents. Instead of a standing wave pattern, the fields in the LWA are modelled according to (4.3). The leakage/power attenuation coefficient is obtained from HFSS scattering parameter simulations of the leaky-wave structure, in this case, 51 unit cells long. Having these parameters, the radiation pattern for an arbitrarily long device can be constructed with fairly good accuracy (Fig. 6.3) and as expected a directive, single beam far-field pattern is observed. As the angle of emission is dictated by the dispersion characteristic, the beam can in principle be steered either by varying the frequency or transmission-line characteristics—for instance, by changing the hole size. The inset shows the predicted scan angle as a function of frequency along with the corresponding measured and cavity model prediction. The cavity model also gives qualitative insight for polarization of the far-field beam pattern. For the TM$_{01}$ mode, the far-field pattern along the top of the ridge is expected to have primarily $E_{\theta}$ components (transverse to the length of the ridge) due to the in-phase equivalent magnetic current sources. Cavity model predictions and HFSS simulations (Fig. 6.4 insets) confirm this analysis and is matched by the experimentally measured far-field polarization. Fig. 6.5 shows a longitudinal cut of the beam pattern for the LWA when fed by a master oscillator THz QC-laser operating in the TM$_{00}$ (at 2.50 THz) mode and the TM$_{01}$
Figure 6.4: Total far-field intensity of LWA at 2.81 THz predicted by (a) the cavity model and (b) HFSS. Insets show theta and phi components.

Figure 6.5: Measured far-field beam patterns and spectra under two different bias conditions corresponding to antenna operation in its TM$_{00}$ mode (at 2.50 THz) outside the light cone and TM$_{01}$ mode (at 2.81 THz) within the leaky-wave bandwidth. Data was collected at 77 K with the master oscillator QC-laser biased in pulsed mode (5 $\mu$s pulses repeated at 10 KHz) and the antenna passive.
Figure 6.6: (a) Metamaterial unit cell with symmetric series gap capacitors. (b) Meander metamaterial unit cell with alternating series gap capacitors and its (c) circuit model along with its dispersion relation obtained via unit cell analysis in HFSS. Least squares fit obtained circuit parameters are $L_R = 2.9 \, \text{pH}$, $L_L = 1.3 \, \text{pH}$, $C_R = 2.8 \, \text{fF}$, and $C_L = 1.2 \, \text{fF}$.

(at 2.81 THz) mode. For the TM$_{01}$ mode, the detected radiation is dominantly polarized in the direction perpendicular to the antenna axis, which corresponds to $E_\theta$ components as mentioned above. The TM$_{00}$ mode, on the other hand, exhibited a non-directional beam pattern with many fringes in the far-field and is polarized primarily along the axis of the waveguide, corresponding to the predicted $E_\phi$ components, and is an order of magnitude lower in intensity.
6.2 TM\textsubscript{01} Waveguide Mode, Meander CRLH

The presented TM\textsubscript{01} RH only structure from CH. 6.1 served as a platform for development of a THz CRLH transmission-line metamaterial, namely, a nearly balanced, CRLH metamaterial LWA. This can be achieved with the periodic ($p = 8\mu m$) addition of series gap capacitors in the upper metallization as shown in Fig. 6.6(a). A metamaterial structure comprised of such unit cells exhibits CRLH properties such as left-handed (backward waves) propagation. Compared to the design proposed in [14], where series capacitance and shunt inductance elements are loaded into a MM waveguide operating in its TM\textsubscript{00} mode, this design exhibits greater radiation loss. In this section, we present simulations and cavity model predictions for the radiation pattern and radiative losses of a structure composed of balanced CRLH unit cells.

The unit cell in Fig. 6.6(a), however, does not meet two practical design necessities for active QC-laser structures, namely, the ability to apply an electrical DC bias to the upper metal contact and the ability to achieve a balanced metamaterial design (a large series capacitance is needed corresponding to an unreasonably small gap size). However, with a slight change in design, both concerns can be addressed (Fig. 6.6(b)) with alternating gap capacitors of 238 nm incorporated into the upper metallization, leading to a meander-type structure. Due to its continuous DC connectivity, the device can operate as an active QC-laser as well a purely passive metamaterial LWA. This, however, increases the overall unit cell length to 16 \( \mu m \), which translates to a larger series inductance helping a chieve a nearly balanced condition with \( f_{se} = 2.606 \) THz, \( f_{sh} = 2.616 \) THz (\~10 GHz bandgap reported by HFSS eigenmode simulation). Under the perfectly balanced case, the transition, shunt and series frequencies would be the same \( \omega_0 = \omega_{sh} = \omega_{se} \), where
A circuit model dispersion eigensolver, as described in Appendix A.3, was developed to solve for the meander design’s dispersion. The simple circuit model is qualitatively a good match with the HFSS calculation near the transition point, although there is some discrepancy in the left-handed branch near the light line (Fig. 6.6(c)). The light cone spans from 2.4 THz to 3.1 THz, within which the CRLH waveguide can be used as a LWA.

We have calculated the radiative Q and the associated radiative loss coefficient $\alpha$ (given by (A.17)) for the CRLH structure using both HFSS and the cavity model, as shown in Fig. 6.7. The simulated Q is obtained using HFSS’s eigensolver:

$$\omega_{se} = \frac{1}{\sqrt{L_{R}C_{L}}}.$$  \hspace{1cm} (6.2)
solver with periodic boundary conditions, which estimates radiation from an infinitely long structure. The cavity model is applied to find the $Q$ along with a perfectly balanced analytic dispersion relation obtained from the circuit model (as shown in Fig. 6.6). This calculation is very similar to that shown in Fig. 4.9 and Table 6.1 for a TM$_{01}$ leaky-wave mode, except modified to allow for the inclusion of the series capacitor $C_L$ in the stored cavity energy for $Q$ calculations. In this CRLH structure, electric field energy can be stored in the shunt capacitor $C_R$, which is associated with strong radiation from the sidewalls, and/or $C_L$, which contributes negligible radiation due to the antisymmetric $M_s$ contributions within the metallization gaps.

Fig. 6.7 shows generally good agreement between the cavity model and HFSS calculations of the radiative loss coefficient. However, near 2.6 THz the HFSS calculation shows a discontinuity in $Q$ and $\alpha$ due to the fact that in the numerical simulation the CRLH structure is not perfectly balanced, and a residual 10 GHz bandgap remains. In the cavity model simulation, a perfectly balanced circuit model was used which exhibits no bandgap, and thus the radiative loss characteristic is smooth. For comparison, the loss coefficient is also plotted for the right handed (RH) only leaky-wave structure whose dispersion lies between the two cases given in Fig. 6.1 (15 $\mu$m wide waveguide with 3 x 3 $\mu$m holes). This structure exhibits a power loss coefficient that diverges as the cutoff frequency $f_{sh}$ is approached, due to a group velocity that approaches zero. The CRLH structure on the other hand maintains a non-zero group velocity even at $\beta=0$, and hence there is no divergence in loss. This makes this structure highly attractive for use as a LWA.

Using the HFSS derived dispersion relation, the radiation pattern for an arbitrarily long device is constructed with fairly good accuracy using the cavity model. The backward to forward scanning of the main beam for the balanced metamaterial structure of 10 unit cells (160 $\mu$m) is observed (Fig. 6.8 (a-c)). There is good
Figure 6.8: HFSS and cavity model longitudinal far-field beam pattern cuts for different regions of operation: (a) left-handed (2.5 THz), (b) transition frequency (~2.61 THz), and (c) right handed (2.80 THz). Insets: HFSS and cavity model rectangular contour plots of the far-field intensity.
agreement between the simulated and cavity model predicted beam patterns along the longitudinal direction of the structure for all scan angles. The largest deviation occurs around the transition frequency where the dispersion characteristic of a simulated finite length structure will differ slightly from that of an infinitely long one, which is how the dispersion relation was obtained; this could also be associated with larger uncertainty in the vicinity of $\omega_0$. For observation angles far from the longitudinal cut of the device, slight deviations are seen compared to the simulated radiation patterns from HFSS (Fig. 6.8 insets). The deviation is due to the fact that the TM$_{01}$ mode is not highly confined and hence the effective transverse dimension is effectively larger than the physical size. In our cavity model, the distance separating the equivalent magnetic current elements along the side-walls is modelled to be the same distance as the physical ridge width (in this case 15 $\mu$m). Indeed, in [85], Menzel also considers an effective width due to fringing fields, which we have neglected in order to simplify the model. By separating the equivalent magnetic current sources with a greater element spacing (i.e. a wider equivalent ridge width), the cavity model resulted in a beam pattern that was less divergent in the transverse dimension, closely matching that predicted by HFSS (not shown here).

### 6.2.1 Experimental Results

After a successful demonstration of the RH only LWA, my colleague Amir Tavalaei fabricated and experimentally characterized the proposed balanced CRLH design (Fig. 6.9). Backward directed beams were successfully demonstrated and as predicted by the cavity model analysis, the far-field pattern at 2.594 THz is primarily polarized transverse to the ridge. However, the far field at 2.484 THz, unexpectedly, is dominantly polarized in the longitudinal direction along the ridge. For ideal dimensions, i.e. equal-sized gaps in the top metallization and perfectly centered etched holes in the waveguide ridge, the LWA exhibits a far-field beam
Figure 6.9: (a) SEM image of fabricated CRLH antenna-coupled device. (b) Intensity measurements showing backward directed beams corresponding to left handed operation. Figure adapted from [15].
Figure 6.10: (a) A 30 unit cell (480 μm) long CRLH LWA excited by a tapered QCL master oscillator.

Figure 6.11: (a) The out of plane and (b) in plane E-field distribution inside the waveguide and within the gaps, respectively, at 2.4 THz, which is in the leaky wave regime along the left hand branch of the dispersion.
pattern with an expected dominant transverse polarization due to the tangential fields along the sidewalls; this was confirmed with a full-wave finite element method simulation (Ansys’s HFSS) of a 30 unit cell long (480 μm) structure. To account for fabrication imperfections, we introduced an asymmetry in the gap length, for example, by having an etched hole size that is slightly larger on one side (1.5 μm) (Figure 6.10). Even for the nonideal case simulated here, the electric field for adjacent gaps on opposite sides of the ridge are out of phase (Figure 6.11), but the equivalent magnetic current source associated with the shorter gap is effectively reduced and results in an imperfect cancellation of the near and far field. Because of the intense fields in the gap capacitors, its radiated far field is then comparable, if not greater, than that of the sidewalls; the far-field beam pattern is then dominantly polarized along the waveguide ridge (Figure 6.12(a)) versus in the transverse direction for the ideal case (Figure 6.12(b)). Additionally, the larger holes’ sidewalls’ equivalent magnetic current sources no longer perfectly cancel [86], which contribute also to a longitudinal component of the far field.

Figure 6.12: Polar representation of the simulated far-field beam patterns of the CRLH LWA in the backwards direction (a) non-ideal case and (b) ideal case. Components of the electric field along the longitudinal (|E₀|²) and transverse (|E₉|²) directions are shown for each case.
6.3 TM\textsubscript{01} Waveguide Mode, Symmetric CRLH

The previous TM\textsubscript{01} waveguide mode based designs (both the RH only and CRLH case) are fantastic radiators with radiative losses that are greater than the ohmic losses, making them more efficient radiators than a conventional MM waveguide where the reverse is true. The radiative losses, however, were too high ($\sim 100 \text{ cm}^{-1}$) to realize a ZOR. An approach involving near and far-field cancellation via etched holes showed a slight reduction in the radiative losses (increased $Q\text{rad}$) as mentioned in section 6.1. A similar approach that yields a reduction in radiative loss of $\sim 20 \text{ cm}^{-1}$ or $\sim 20\%$ relative to the previously mentioned TM\textsubscript{01} CRLH meander design in CH. 6.2 requires two openings in the top metallization, one on each side of the virtual short (Fig. 6.13(a,b)). Additionally, this design maintains DC electrical connectivity across the top metallization. The reduction in radiative loss is attributed to the large destructive equivalent magnetic current sources $M3$ as shown in Fig. 6.13(c). The electric field profile associated with the $M3$ equivalent source is larger than in the previous TM\textsubscript{01} design since that aperture in this case is relatively closer to the field’s maximum in terms of a guided wavelength and larger along the longitudinal direction with respects to the unit cell size (Fig. 6.13(c)).

Similar to the TM\textsubscript{01} CRLH waveguides described so far, the primary source of radiation is due to the sidewall and hence the far-field radiation is expected to be dominantly polarized transverse to the ridge. A HFSS simulation of a 10 unit cell long LWA shows backward to broadside to forward scanning with a main beam that is transversely polarized, as predicted (Fig. 6.14).
Figure 6.13: TM$_{01}$ symmetric CRLH (a) unit cell, its dispersion and (b) field profiles at the series and shunt resonance. (c) Equivalent magnetic current sources of the unit cell; equivalent sources $M_5$ in the gap would be negligible exactly at the gamma point.
Figure 6.14: (a) TM$_{01}$ symmetric CRLH, 10 unit cell (150 $\mu$m) long LWA scanning from the backward to broadside to forward direction. Only half the structure is shown since a symmetry E plane was used to reduce the simulations space and time. (b) Rectangular and (c) polar plots of the far-field intensity components exhibit a negligible longitudinal ($\theta$ direction) component.

6.4 TM$_{02}$ Waveguide Mode, CRLH

To further reduce the radiative losses, a CRLH design focused around the higher-order TM$_{02}$ mode is analyzed. In the previous TM$_{01}$ mode based designs, the main radiating mechanisms were the sidewalls, where holes were introduced to
tailor the radiative efficiency. The approach with the TM$_{02}$ mode similarly uses destructive and constructive interference to control the radiative losses. However, the sidewalls now do not provide constructive interference and instead, openings in the top metallization are utilized to control the radiation. The dispersion and unit cell of the proposed TM$_{02}$ CRLH design and its field profiles are shown in Fig. 6.15(a,b). The radiative losses were reduced by $\sim$75% compared to the original TM$_{01}$ meander CRLH design presented (Fig. 6.18). The cavity model shows that the primary source of radiation is from the gap capacitors, which would hint at a longitudinally polarized far-field beam pattern, which is corroborated by an eight unit cell LWA simulation (Fig. 6.16). The CRLH LWA can be driven with a feed operating in either the fundamental TM$_{00}$ or higher order TM$_{02}$ mode (Fig. 6.17).
Figure 6.15: (a) Unit cell of the TM\textsubscript{02} CRLH structure and its dispersion. (b) Equivalent magnetic current sources of the unit cell.
Figure 6.16: (a) TM$_{02}$ CRLH, 8 unit cell (80 µm) long LWA scanning from the backward to broadside to forward direction. Far-field intensity (b) rectangular and (c) polar plots show negligible and barely noticeable transverse $E_\phi$ components; longitudinal $E_\theta$ components dominate.
Figure 6.17: Either the (a) higher order TM$_{02}$ or (b) fundamental TM$_{00}$ mode can excite a TM$_{02}$ propagating mode in the CRLH LWA (8 unit cell, 80 $\mu$m long). A far-field intensity plot shows scanning from the backward to broadside to forward direction. An electric field magnitude plot for a 2-D in-plane cut reveals the gradual transition from a fundamental mode excitation to a propagating TM$_{02}$ mode.

### 6.5 Summary

Over the course of the project a few different THz, 1-D CRLH transmission line designs were investigated for resonator and LWA applications. The initial TM$_{00}$ design proved to be too lossy and impractical for either application, while the planar, higher-order TM$_{01}$ waveguide mode designs successfully demonstrated frequency scanning when operating as a LWA excited by a master oscillator MM waveguide QC-laser. It also exhibited gain via increased measured intensity with increased device bias \cite{12, 15}. Analysis of other 1-D designs to control and understand the radiative losses continued for two primary reasons: to increase the effective aperture size of the 1-D THz CRLH LWA by increasing its power extinction length and to meet the requirements for lasing, namely, for ZOR operation. A
summary of the threshold gain values for the ZOR mode for the five different 1-D CRLH THz transmission line designs are shown in Fig. 6.18, where the radiative losses dominate for all designs other than design 5, the TM$^{0}_{2}$ mode based design.

Figure 6.18: Threshold gain values for the 1-D, ZOR mode for the mentioned designs: (1) TM$^{0}_{01}$ RH only-no holes (2) TM$^{0}_{01}$ RH only-3x3 $\mu$m hole (3) TM$^{0}_{01}$ meander CRLH (4) TM$^{0}_{01}$ symmetric CRLH (5) TM$^{0}_{02}$ CRLH. The TM$^{0}_{00}$ based design was not included here given its fabrication difficulties and large ohmic losses.

A comparison of the radiative power attenuation within the leaky-wave bandwidth is shown in Fig. 6.19 for four different designs: TM$^{0}_{00}$ CRLH, TM$^{0}_{01}$ meander CRLH, TM$^{0}_{01}$ symmetric CRLH, and TM$^{0}_{02}$ CRLH. The TM$^{0}_{02}$ mode based design, over most of its leaky-wave regime, exhibits a lower radiative loss than all the designs. Although the TM$^{0}_{00}$ CRLH design proved to be impractical, its analysis is included here because its leaky-wave fractional bandwidth is comparatively larger than the other designs, so if it is possible to overcome the fabrication hurdles, perhaps this design could be used as a LWA since meeting lasing threshold gain requirements is not necessary.
Figure 6.19: The radiative power attenuation coefficients and their corresponding normalized eigenfrequencies relative to the design’s band gap center frequency is plotted for the leaky-wave regime. The last data point on the left and right side of the figure corresponds to the intersection of the dispersion curve with the light line. The largest band gap of $\sim$20 GHz out of 4 different CRLH designs is represented in the figure.

In conclusion, we used the antenna cavity model and CRLH transmission line theory to guide our understanding of the presented metamaterial QC-devices, which led to a successful demonstration of an active CRLH LWA with backward to forward beam scanning. Although a zeroth order QC-laser was not demonstrated due to excessive losses, engineering the losses with a similar design strategy i.e. manipulating destructive and constructive interference of near and far-field components, may lead to a feasible design.
Passive THz Metamaterial Metasurfaces

Experimental verification of the first passive THz CRLH transmission line was conducted in parallel with verification of the active QC LWA of CH. 6.1 and prior to the CRLH active LWA of CH. 6.2. The intension was to experimentally characterize both bound and leaky-wave modes in passive THz CRLH waveguides to prove the feasibility of THz CRLH metamaterial MM waveguides. Since it is non-trivial to measure the S-parameters of a single waveguide in the THz range, we instead fabricated an uniaxial metasurface composed of dense arrays of passive THz CRLH waveguides and experimentally mapped their dispersion relation using angle-resolved reflection spectroscopy. The waveguides were implemented using metal-insulator-metal topology and exhibited dispersion relations that are well fit by a circuit model; bound surface wave modes are obtained with Otto (prism) coupling [87]. Depending upon the incident polarization, either a RH-only, or a CRLH waveguide mode is excited; a behavior which is explained by invoking the microwave cavity antenna model. It is shown that the cavity antenna model can provide an understanding of the polarization dependence of the radiative coupling to $\text{TM}_{00}$ and $\text{TM}_{01}$ waveguide modes. Along with transmission line theory, an effective surface impedance model to describe CRLH waveguide array metasurfaces is derived. This model is in good qualitative agreement with experiment and correctly predicted the coupling and mode splitting (i.e. anticrossing) between $p$-incident radiation and RH only waveguide modes. These modes are similar to the spoof surface plasmon polariton modes that are supported on structured
metal surfaces that exhibit large inductive surface impedance [88–90]. The CRLH waveguide mode is shown to form s-polarized surface waves which do not exhibit such a splitting. Furthermore, these s-polarized CRLH modes can be considered as a type of magnetic spoof surface plasmon which are supported when the surface impedance of the metasurface becomes large and capacitive [91, 92].

7.1 CRLH Metamaterial Metal-Metal Waveguide

Figure 7.1: (a) A perspective and (b) top view of the metal-metal waveguide operating near $\beta = 0$ with a unit cell size, $p$, with its x component, E-field profile and equivalent magnetic current sources $M_s$, given by double-headed arrows for the higher-order lateral TM$_{01}$ waveguide mode. (c) Circuit model and (d) typical dispersion. (e) Side view of the E-field profile from a full-wave finite element simulation (Ansys’s HFSS) of an infinitely long structure operating at the series band edge mode $\omega_{se}$ and (f) shunt band edge mode $\omega_{sh}$.

To reiterate the points mentioned in CH. 6.2, a THz CRLH waveguide can be realized in the MM waveguide configuration by introducing gaps with subwave-
Figure 7.2: A perspective and top view of the metal-metal waveguide operating near $\beta = 0$ with a unit cell size, $p$, with its x component, E-field profile and equivalent magnetic current sources $M_s$, given by double-headed arrows for the fundamental TM$_{00}$ waveguide mode with its equivalent circuit model.

length period into the top metallization, which can be represented as distributed series capacitance $C_L$. When the waveguide is operating in its fundamental lateral TM$_{00}$ mode, only a right-handed branch of operation is observed. However, operation in its higher-order lateral mode can be qualitatively represented using a circuit model with two coupled parallel transmission lines, as shown in Fig. 7.1(c). The conduction currents in the transverse direction can be represented by an effective shunt inductance $L_L$. The odd symmetry of the mode introduces a virtual ground plane along the center of the waveguide. Proper choice of dimensions and introduction of other structures (such as holes, overlay capacitors, etc.) allows control of the four circuit parameters for realization of a CRLH metamaterial, which exhibits both forward and backward wave propagation. [74] In general, such a transmission line is “unbalanced” and exhibits a bandgap between the LH and RH ranges bounded by the shunt ($\omega_{sh} = (L_LC_R)^{-1/2}$) and series ($\omega_{se} = (L_RC_L)^{-1/2}$) resonant frequencies (see Fig. 7.1(d)). For operation at or near $\beta \approx 0$ the shunt or series resonant frequency is associated with stored energy in either the series $L_RC_L$ or shunt $L_LC_R$ tank (field profiles as shown in Fig. 7.1(e,f) respectively). The dispersion can be “balanced” by choosing parameter values such that $\omega_{se} = \omega_{sh}$; a balanced line has no bandgap and is characterized by propagating modes at $\beta = 0$. The shunt resonance frequency $\omega_{sh}$ corresponds to the standing-wave resonance condition where the waveguide width $w$ is approximately equal to one half of the wavelength in the dielectric ($w \approx \lambda_o/2\pi$).
When the waveguide is operating in its fundamental lateral TM$_{00}$ mode (see Fig. 7.2), the effective shunt inductance $L_L$ does not exist, and only a RH branch of operation in its dispersion relation is observed. If series gap capacitors are present, propagating modes are cut-off below the series resonant frequency $\omega_{sc}$.

For our geometry, due to the presence of the ground plane, and the orientation of the magnetic field, the effect of electric currents can be neglected for low-profile structures with minimal fringing fields. Considering operation near $\beta = 0$ for the fundamental lateral TM$_{00}$ waveguide mode (Fig. 7.2), the equivalent magnetic current sources along opposite sidewalls of the proposed CRLH metal-metal waveguide are out of phase, leading to destructive interference. On the other hand, the equivalent sources in the gaps are in phase, which gives rise to far-field radiation that is polarized in the $\theta$-direction or along the waveguide axis. The E-field is concentrated within the gap capacitor and has a field profile similar to the HFSS field plot shown in (Fig. 7.1(e)). Hence, for the fundamental mode, coupling to radiation takes place almost entirely through the series gap capacitors—we represent this phenemologically by placing a radiation conductance $G_{rad}$ across the series capacitance $C_L$ in its circuit model (see Fig. 7.2).

The case is reversed for the higher-order lateral TM$_{01}$ waveguide mode (Fig. 7.1(a,b)). Here, the equivalent magnetic current sources along opposite side walls are in phase and give rise to far-field radiation polarized in the $\phi$-direction or transverse to the waveguide axis. Because the E-field within the series capacitive gaps follows the symmetry of the mode, the equivalent magnetic current sources in the gaps are out of phase, which leads to destructive interference and cancellation of its far field at broadside. Therefore, the coupling to radiation takes place mostly through the fields associated with the shunt capacitors, which we can represent with a shunt radiation conductance $G_{rad}$ across $C_R$ (Fig. 7.1(c)). This is essentially the same radiation mechanism as a patch antenna. [75] For non-zero values of $\beta$, there will be a phase shift ($\sim \beta p$) between $M_s$ from adjacent unit cells, which
leads to both steering of the beam away from surface normal ($\theta = 90^\circ$ relative to coordinate system in Fig. 7.2(a)) and a change in the radiated power.

The cavity antenna model can be used to derive analytic expressions for the radiation conductance in limiting cases. We use the formalism and approximations that are described in the Appendix A.1 to calculate the total radiated power $P_{rad}$ from a waveguide. The difference here is that we consider radiation from arrays of waveguides spaced with a lateral period $\Lambda$ rather than a single waveguide; we choose this geometry to be consistent with the surface impedance model described next in 7.2. We assume the ideal limiting conditions for the ridge width $w \ll \lambda_0$, height $h \ll \lambda_0$ and length $\ell \gg \lambda_0$, and consider only the leaky-wave regime, where the effective modal index obeys $|n_{eff}|<1$ (where $n_{eff} = \beta c/\omega$). A value for the radiation conductance can be derived by invoking the circuit theory relation for time averaged dissipated power $G_{rad} = 2P_{rad}/|V_0|^2$. $V_0$ is the equivalent voltage across $C_L$, which is approximately related to the E-field $E_0$ within the gap of length $a$ by the expression $V_0 = E_0 a$. For a single waveguide operating in its TM$_{00}$ mode within $|n_{eff}| < 1$, the radiation conductance is then given by

$$G_{rad,00} = \frac{1}{\eta_0 \cos \alpha \Lambda} \frac{w^2}{2p}$$

(7.1)

where $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$, $p$ is the unit cell size, $w$ is the ridge width, and $\alpha$ is the incident angle relative to the surface normal. Similarly, for the TM$_{01}$ mode, we obtain

$$G_{rad,01} = \frac{\cos \alpha}{\eta_0} \frac{1}{F} \frac{2p}{\Lambda}$$

(7.2)

However, in this case the voltage appears across the shunt capacitor $C_R$, so that $V_0$ is related to the E-field at the waveguide sidewall. The presence of $\cos \alpha$ in these expressions reflects the dependence of the free-space characteristic impedance of a plane wave incident upon a surface with angle of incidence $\alpha$ relative to the surface normal. The factor $F$ appears as a correction factor that accounts for the
sinusoidal lateral E and H-field variation along the width of the waveguide ridge \( (w \approx \lambda_0/2n) \) for the TM\(_{01} \) mode. It is necessary to ensure that conservation of energy is satisfied for calculations of the radiative power and is consistent between the field model and the circuit model. For the ideal analytic case where the top waveguide metallization is continuous in the lateral direction (Fig. 7.1(a,b)) then \( F = \pi/4 \). As the structure becomes more complicated, such as by the introduction \( F \) will increase — eventually reaching unity in the lumped element limit.

### 7.2 Surface Impedance Model

![Image](image.png)

**Figure 7.3:** (a) Transmission line model for a CRLH metasurface with its fundamental TM\(_{00} \) waveguide mode excited by p-polarized incident light. (b) HFSS simulations and surface impedance model predictions for surface reactance for p-polarized incident light at an incident angle \( \alpha = 40^\circ \) relative to the surface normal. The surface impedance model qualitatively captures the reactive transitions in the dispersion. The inset maps the regions of capacitive and inductive reactance.

It is convenient to characterize the dispersion characteristics of both bound and leaky-wave modes of CRLH waveguides using angle dependent reflection spectroscopy. If arrays of waveguides are fabricated, spaced with a periodicity \( \Lambda < \lambda_0/2 \) in the lateral direction, only the zeroth order diffractive component will contribute to the far-field reflected power (i.e. specular reflection). Provided the
Figure 7.4: (a) Transmission line model for a CRLH metasurface with its higher order lateral TM$_{01}$ waveguide mode excited by s-polarized incident light. (b) HFSS simulations and surface impedance model predictions for surface reactance for s-polarized incident light at an incident angle $\alpha = 40^\circ$ relative to the surface normal. The surface impedance model qualitatively captures the reactive transitions in the dispersion, either from capacitive to inductive or inductive to capacitive. The inset maps the regions of capacitive and inductive reactance.

The metamaterial unit cell length is $p < \lambda_0/4n$ (where $n$ is the refractive index of the dielectric), we operate sufficiently far from the 1st Brillioun zone edge that Bragg scattering will not significantly contribute to the dispersion, and we can use the previously described TL metamaterial model to describe the propagating waveguide modes. The subwavelength structure of the waveguide will determine the detailed dispersion relation $\beta(\omega)$, both through the fundamental and higher-order Floquet-Bloch terms, whose contribution can be captured via the effective lumped element values for the TL ($C_R, L_R, C_L, L_L$). However the higher-order Floquet-Bloch terms contribute only to the evanescent near field and do not radiate into the far field. We can then treat this as a metasurface described by a surface impedance $Z_s$ and in turn calculate the reflection coefficient for incident plane waves. When plane waves are incident upon the metasurface with the plane of incidence along the waveguide axis (z-axis in Fig. 7.3(a), Fig. 7.4(a)) and with incident angle $\alpha$, incident light will couple with propagating waveguide modes when $\beta(\omega)=k_0 \sin(\alpha)=k_z$, where it is either absorbed (due to dielectric or ohmic
losses), or reradiated (specular reflection). Depending upon the polarization of an incident propagating plane wave, either the TM$_{00}$ or TM$_{01}$ waveguide mode will be excited. While at higher frequencies higher order lateral modes can be excited, we will confine our treatment here to the lowest order odd and even modes.

7.2.1 P-Polarization

As shown in Fig. 7.2, along with the cavity model discussion in CH. 4.1 and CH. 7.1, the symmetry of the TM$_{00}$ waveguide mode dictates that radiation from the waveguide is mediated via E-fields in the series capacitor. For a p-incident polarized plane wave, the E-field is polarized along the axis of each waveguide, and by reciprocity couples to the TM$_{00}$ waveguide mode via the series gap capacitors. Hence we define a transmission line model where we place an input port across the series capacitance $C_L$ in each unit cell, as shown in Fig. 7.3(a). The incident wave induces a voltage $V'(z) = V_0' e^{-jk_z z}$ and current $I'(z) = I_0' e^{-jk_z z}$, which defines an input impedance for the unit cell as $Z_{in,p} = V'(z)/I'(z)$. We obtain

$$Z_{in,p}(k_z, \omega) = \frac{Z_1 Z_2 + k_z^2 p^2}{Y_1 Z_1 + Y_1 Z_2 + k_z^2 p^2},$$  \hspace{1cm} (7.3)

where $Z_1 = 1/(j\omega C_L + G_L)$, $Z_2 = j\omega L_R + R_R$, $Y_1 = j\omega C_R + G_R$. If there are no metal ohmic losses ($R_R = 0$) and no dielectric losses ($G_L = G_R = 0$), we obtain the lossless case where $Z_1=1/j\omega C_L$, $Z_2 = j\omega L_R$, $Y_1 = j\omega C_R$. The input impedance is then

$$Z_{in,p}(k_z, \omega) = \frac{-j}{\omega C_L} \frac{\omega^2 - k_z^2 p^2 / L_R C_R}{\omega^2 - \omega_c^2 - k_z^2 p^2 / L_R C_R}.$$ \hspace{1cm} (7.4)

It should be noted that $Z_{in,p}$ is different from the characteristic impedance often defined for a CRLH line. [10] We now convert $Z_{in,p}$ to a surface impedance $Z_{s,p}$.
The input impedance was rescaled by multiplying $Z_{in,p}$ by the factor $Z_0 G_{rad}$ where $G_{rad}$ is the radiation conductance in the series branch (Eq. 7.1), and $Z_0$ is the characteristic wave impedance in a vacuum for p-polarized plane waves ($Z_0 = \eta_0 \cos \alpha$, $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$). The rescaling of $Z_{in}$ to $Z_s$ accounts for both the aspect ratio of the metamaterial unit cell area ($p \times \Lambda$) and cases where ridges of width $w$ may have a fill factor below unity ($w<\Lambda$). The dispersion relation for the waveguide modes, $\beta(\omega)$, can be extracted from the poles of $Z_{in}$ by replacing $k_z$ with $\beta$. For normal incidence and unity fill factor ($w = \Lambda$), $Z_{s,p}$ is equivalent to that of a Sievenpiper mushroom surface. [84]

Results from the analytic surface impedance model were compared with the surface impedance extracted from a HFSS full-wave 3D simulation of a plane-wave reflection coefficient of a lossless CRLH waveguide metasurface. Lumped element circuit parameters for Eq. 7.3 were extracted from a circuit model fit to the dispersion relation obtained from a full-wave 3D simulation. The details of the simulated CRLH waveguide are not important for this comparison and are left for discussion in CH. 7.3. All dielectrics were lossless and all metals were simulated as a perfect electric conductor (PEC), so that the surface impedance is purely reactive. For p-polarized incident light at an incident angle $\alpha = 40^\circ$ relative to the surface normal, for example, the metasurface is inductive at low frequencies and is capacitive above $\sim 3.6$ THz (Fig. 7.3(b)). The crossover frequency where $Z_s^{-1} = 0$ reflects the frequency of the propagating mode; the fact that there is only one crossover reflects the fact that p-polarized light excites the TM$_{00}$ waveguide mode, which has only a RH branch of the dispersion.
7.2.2 S-Polarization

The cavity model predicts that the TM$_{01}$ waveguide mode couples with s-polarized incident light (E-field polarized transverse to the ridge) through the sidewalls’ surface equivalent magnetic current sources. Hence, the incident E-field induces a voltage $V'(z)$ across the shunt capacitor $C_R$, and we can place the coupling input port to free space across the shunt branch of each unit cell, as shown in Fig. 7.4(a). Because of the odd symmetry of the TM$_{01}$ mode, the TL shown represents only one branch of the odd-mode line, so that a unit cell occupies area $p/2 \times \Lambda$. We obtain for the input impedance for one unit cell:

$$Z_{in,s}(k_z, \omega) = \frac{1}{Y_{sh} + k_z^2 p^2 / Z_{se}},$$  \hspace{1cm} (7.6)

where $Z_{se} = j\omega L_R + R_R + 1/(j\omega C_L + G_L)$, and $Y_{sh} = j\omega C_R + G_R + 1/(j\omega L_L + R_L)$. Once again, we obtain the lossless relation by setting the resistances and conductances to zero:

$$Z_{in,s}(k_z, \omega) = j\omega L_L \frac{\omega^2_{sh} \omega^2_{se} (1 - \omega^2 / \omega^2_{se})}{\omega^2_{sh} \omega^2_{se} + \omega^2_{sh} \omega^2_{se} + \frac{k_z^2 p^2}{L_R C_R}}.$$

The surface impedance is given by

$$Z_{s,s} = Z_{in,s} Z_0 G_{rad,01} = Z_{in,s} \frac{1}{F} \frac{2p}{\Lambda}.$$  \hspace{1cm} (7.7)

For s-polarized radiation, $Z_0 = \eta_0 / \cos \alpha$ and once again, the rescaling accounts for the non-square aspect ratio of the unit cell as well as the voltage correction factor $F$ necessary to satisfy conservation of energy.

We compare the surface impedance calculated analytically from Eq. (7.7) with that extracted from full-wave 3D reflectivity simulations. The surface reactance for an incident angle of $\alpha = 40^\circ$ is shown in Fig. 7.4(b). Unlike the p-polarized
Table 7.1: Circuit parameters

Even mode (TM\textsubscript{00})

<table>
<thead>
<tr>
<th>Sample</th>
<th>Patch A</th>
<th>L\textsubscript{R} (pH)</th>
<th>C\textsubscript{R} (fF)</th>
<th>C\textsubscript{L} (fF)</th>
<th>f\textsubscript{se} (THz)</th>
<th>G\textsubscript{R} (mS)</th>
<th>R\textsubscript{R} (Ω)</th>
<th>G\textsubscript{L} (mS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>6.8</td>
<td>0.98</td>
<td>5.1</td>
<td>2.2</td>
<td>3.38</td>
<td>1.2</td>
<td>0.49</td>
<td>1.3</td>
</tr>
<tr>
<td>S2</td>
<td>7.6</td>
<td>0.98</td>
<td>5.1</td>
<td>3.1</td>
<td>2.86</td>
<td>1.2</td>
<td>0.49</td>
<td>1.3</td>
</tr>
<tr>
<td>S3</td>
<td>8.6</td>
<td>0.98</td>
<td>5.1</td>
<td>3.8</td>
<td>2.60</td>
<td>1.2</td>
<td>0.49</td>
<td>1.3</td>
</tr>
</tbody>
</table>

Odd mode (TM\textsubscript{01})

<table>
<thead>
<tr>
<th>Sample</th>
<th>Patch A</th>
<th>L\textsubscript{L} (pH)</th>
<th>C\textsubscript{L} (fF)</th>
<th>C\textsubscript{L} (fF)</th>
<th>f\textsubscript{se} (THz)</th>
<th>f\textsubscript{sh} (THz)</th>
<th>G\textsubscript{R} (mS)</th>
<th>R\textsubscript{R} (Ω)</th>
<th>G\textsubscript{L} (mS)</th>
<th>R\textsubscript{L} (Ω)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>6.8</td>
<td>3.2</td>
<td>2.4</td>
<td>0.65</td>
<td>0.51</td>
<td>3.98</td>
<td>4.03</td>
<td>0.45</td>
<td>1.5</td>
<td>0.32</td>
</tr>
<tr>
<td>S2</td>
<td>7.6</td>
<td>3.2</td>
<td>2.4</td>
<td>0.65</td>
<td>0.59</td>
<td>3.66</td>
<td>4.03</td>
<td>0.45</td>
<td>1.5</td>
<td>0.32</td>
</tr>
<tr>
<td>S3</td>
<td>8.6</td>
<td>3.2</td>
<td>2.4</td>
<td>0.65</td>
<td>0.81</td>
<td>3.13</td>
<td>4.03</td>
<td>0.45</td>
<td>1.5</td>
<td>0.32</td>
</tr>
</tbody>
</table>

case, for s-polarized radiation the metasurface exhibits two crossover frequencies where $Z_{s}^{-1} = 0$, corresponding to the LH and RH branches of the dispersion respectively. $Z_{s} = 0$ at $\omega = \omega_{se}$, where the series resonance shorts out the surface (see inset of Fig. 7.4(b)). With an accurate circuit model fit of the metasurface’s dispersion, the surface impedance model qualitatively captures the metasurface’s different reactive regions with good agreement.

7.3 Large Area Passive CRLH Metamaterial

We now apply the surface impedance model to analyze the experimentally realized CRLH waveguide metasurface reported in Ref. [93]. Passive, large area (1 cm $\times$ 1 cm) CRLH TL metamaterial arrays were fabricated in metal-insulator-metal waveguide technology using Benzocyclobutene (BCB) as the insulating layer (Fig. 7.5). The series capacitance $C_{L}$ was realized by gaps in the top conductor of the metal-metal waveguide; $C_{L}$ was further enhanced by metal top patches that were isolated with a thin layer of SiO$_{2}$ in order to achieve a close-to-balanced dispersion. Three sample variations were fabricated, where the series capacitance
Figure 7.5: (a) A perspective and (b) cross section side view of the metal-metal waveguide’s unit cell of length $p$, with its equivalent circuit model. (c) Perspective and (d) cross section view of large area array along with an illustration of the two different measured polarizations. (e) Scanning electron microscope images of the fabricated CRLH waveguide array (perspective view) and a top down view of a unit cell (inset).
was increased by increasing the longitudinal dimension of the 6.5 μm wide overlay top metallization from $A = 6.8$, 7.6, and 8.6 μm for samples referred to as S1, S2, and S3, respectively (Fig. 7.5(a)). This allows the series resonance frequency \( \omega_{se} = 1/\sqrt{L_R C_L} \) to be varied with respect to the shunt resonance frequency \( \omega_{sh} = 1/\sqrt{L_L C_R} \).

Circuit parameters in Fig. 7.3(a) and Fig. 7.4(a) were extracted using circuit model fits to the dispersion relations obtained from HFSS simulations of the unit cell (Fig. 7.5(a-b)). Lossy component values $G_R, G_L, R_R, R_L$ were chosen using lumped element approximations for a parallel plate waveguide with appropriate material parameters (i.e. loss tangents, skin depths).

Lossy component values were obtained with approximations:

\[
G_R = C_R \omega \tan(\delta_{BCB}) \tag{7.8}
\]

\[
R_R = \frac{1}{\sigma} \frac{A_l}{l_t} \pi \tag{7.9}
\]

\[
G_L = C_L \omega \tan(\delta_{SiO_2}) \tag{7.10}
\]

\[
R_L = \frac{1}{\sigma} \frac{A_l}{l_t} \frac{4}{\pi} \tag{7.11}
\]

For (7.8), $C_R$ is the parallel plate capacitance between the top plate and the ground plane calculated by assuming a voltage given by the electric field along the sidewall and a sinusoidal transverse E-field profile; the BCB has a loss tangent of 0.01 [94]. For (7.9), the Drude conductivity for gold was calculated for room temperature [95], $A_l$ is the cross sectional area (skin depth x $w/2$) for charge flowing along the axial direction of the waveguide, $l_t$ is the unit cell length $p$, and the factor $\pi$ is needed to account for the half sinusoidal variation and loss for two conductors. Similar methods for (7.10) and (7.11) were used where the series capacitance $C_L$ was extracted from the circuit parameter fit and the loss in SiO$_2$ was obtained from Ref. [96]. For the fundamental TM$_{00}$ lateral waveguide mode,
(7.9) and (7.11) would not have the factors associated with a sinusoidal variation.

### 7.3.1 Leaky Waves

Both the TM$_{00}$ and TM$_{01}$ waveguide modes exhibit a propagating mode with a finite bandwidth that falls within the light cone ($|\beta| < \omega/c$). The dispersion is experimentally characterized with angle-resolved Fourier transform infrared (FTIR) reflection spectroscopy. In this technique, incident light is coupled into the waveguide array when the in-plane wave-vector of the incident light matches the waveguides’ propagation constant $\beta$. This coupling condition is marked by an absorption dip in the reflectivity spectrum.

For the FTIR reflection spectroscopy setup, a continuous incident scan angle from $\theta = 10^\circ$ to $90^\circ$ was measured with the 1 cm $\times$ 1 cm sample and detector mounted on a $\theta - 2\theta$ rotary stage (schematic shown in Appendix. A.5). An eight inch focal length off-axis paraboloid (OAP) mirror was used to focus the FTIR’s broadband

![Figure 7.6](image-url)
light to a spot size $\approx 0.7$ cm, which resulted in an incident angle variation of less than $\pm 3^\circ$. A small spectral linewidth broadening of less than $\sim 10^\circ$ is estimated from the waveguide dispersion. A wire grid polarizer placed between the FTIR and eight inch OAP was used to select either s- or p-polarization. The device sample was mounted vertically relative to the optical bench such that the incident light’s plane of incidence was perpendicular to the sample surface and parallel to the waveguide axis (Fig. 7.5(d)). To reduce the effects of water vapor absorption, the measurement was conducted under a N$_2$ purge. For a reference spectrum, a $\sim 1$ cm x $\sim 1$ cm gold mirror was used and all measurements were conducted at room temperature.

Absorption spectra were measured at multiple angles of incidence for each of the three samples, and then plotted as a contour plot as a function of $\beta$ in Fig. 7.6(a-c). As predicted by the cavity model, s-polarized (E-field transverse to the waveguide axis) incident light couples to the TM$_{01}$ waveguide mode which exhibits the CRLH characteristic dispersion relation. Notably, both left-handed (backward-wave) and right-handed (forward-wave) branches of the dispersion relation are seen. We compare this experimental data surface impedance model, as shown in Fig. 7.6(d-f). Good agreement is observed in the dispersion relation, except for slightly broader spectral features observed in the experimental data. This suggests an underestimate of the lossy lumped element values ($G_R, G_L, R_R, R_L$) used in the surface impedance model.

As larger overlay patches are used to increase the series capacitance $C_L$, we observe the dispersion transition from nearly balanced (sample S1) to increasingly unbalanced with a significant bandgap opening (sample S2 and S3). We also observe the absorption in the LH branch become relatively weaker for the unbalanced samples, particularly near the $\beta = 0$ point. This can be understood by considering the distribution of energy in an unbalanced CRLH line as a function of $\beta$. At $\beta = 0$, the band-edge resonant modes at $\omega_{sh}$ and $\omega_{se}$ (see Fig. 7.1(d)), correspond
to resonance purely in the shunt $L_L C_R$ tank or series $L_R C_L$ tank circuits, respectively. As $|\beta|$ increases above zero, although the energy is no longer solely stored in the shunt or series tank, nevertheless each dispersion branch retains its “shunt-like” or “series-like” character to some degree. The more unbalanced the line, the larger the bandgap, and the larger the value of $|\beta|$ for which this modal character persists. As we described in CH. 7.1, due to the odd-symmetry of the $\text{TM}_{01}$ mode in our CRLH waveguide, the series resonance does not radiate significantly — it is a “dark” mode. Therefore, s-polarized incident light does not efficiently couple to the “series-like” branch of the dispersion relation, a phenomenon which is observed experimentally and is accurately reproduced by the surface impedance model. The fact that the LH branch of the dispersion relation is “series-like” near $|\beta| \approx 0$ for samples S2 and S3 simply reflects the fact that $\omega_{se} < \omega_{sh}$. Were $C_L$ made to be smaller, the case would easily be reversed and the RH branch would be “series-like”. Hence, reflection spectroscopy is a useful technique to identify the band edge frequencies as either $\omega_{se}$ or $\omega_{sh}$, something which cannot be determined solely from looking at a dispersion relation.

Although we have not plotted the corresponding absorption data for p-incident polarization, it too is well fit by the surface impedance model. [93]

### 7.3.2 Surface Waves

In addition to leaky-wave modes within the light cone, we expect the waveguide array to support bound surface waves for operation outside the light cone. As an example, for the $\text{TM}_{01}$, the magnitude of the averaged H-field components across the unit cell for such a bound mode, calculated at 2.97 THz (on the LH branch), is shown in Fig. 7.7. The field is observed to decay exponentially away from the metasurface as shown in Fig. 7.7, therefore confirming the existence of the bound surface wave. We also plot for comparison the expected field decay obtained from the perpendicular component of the wavevector $H \sim \exp(-k_z x)$. Significant E-
Figure 7.7: Simulated H-field taken over the unit cell of the CRLH metal-metal waveguide (sample S1). Insets show the magnitude of the E-field for a cross section along the direction of propagation for a unit cell and the placement of the polyethylene prism relative to the sample (Otto-coupling configuration) used to map the waveguides’ dispersion outside the light cone.

Figure 7.8: Measured spectra for sample S3 for (a) p-incident and (b) s-incident angles with coupling distance between the sample and prism of 10 μm. Measured absorption for (inset of (a)) p-incident light and (inset in (b)) s-incident light at a prism-to-air gap incident angle of $\theta_{inc} = 41.5^\circ$ for different prism-to-sample coupling distances.
Figure 7.9: Measured dispersion and HFSS simulations for all three samples for (a) p-polarized and (b) s-polarized light inside and outside of the light cone. Dispersion captured by the surface impedance model for (inset of (a)) p-polarized incident light with a 40 $\mu$m prism-to-sample coupling spacing and (inset of (b))) s-polarized incident light with 10 $\mu$m prism-to-sample coupling spacing.

Field enhancement is observed in the 1 $\mu$m BCB layer compared to the evanescent field — the field within the SiO$_2$ series capacitors is stronger still (Fig. 7.7 inset).

In order to access the bound-mode region using variable angle FTIR reflection spectroscopy, we used the Otto-coupling configuration [87], where a prism is mounted close to the sample with an air gap of $\Delta$, as shown in the inset of Fig. 7.7. The setup is shown in Appendix A.5. Incident waves couple evanescently across the gap to the metasurface at wavenumbers in the range $\omega/c < k_z < n\omega/c$. A polyethylene prism is used, with a 90° apex, 1 cm sides, and a refractive index of $n = 1.52$, which has a critical angle $\theta_{mc} = 41.1^\circ$. The prism position was fixed and the sample was located on a single axis translation stage. Alignment was performed by bringing the prism into contact with the metasurface manually and then varying the coupling distance from $\sim 5 – 300$ $\mu$m with a piezoelectric translation stage. FTIR reflection spectra were measured using a globar blackbody source with a resolution of 1 cm$^{-1}$ and a silicon composite bolometer detector under a N$_2$ purge. To obtain a reflectivity spectrum, the reference background spectrum was taken with the prism in place and the metasurface sample several
millimeters away so that total internal reflection occurs at the prism face without any evanescent field interaction.

A set of the reflection spectra outside the light cone for p and s-incident polarization is shown in Fig. 7.8 for a fixed prism-to-sample coupling distance of $\Delta = 10 \, \mu m$. Compared to the reflection spectra within the light line [93], the signal to noise ratio (SNR) is degraded due to insertion loss of the prism. For p-polarization, only a single absorption feature is observed corresponding to the RH branch, while for s-polarization, two features are seen, corresponding to the LH and RH branches. The absorption features shift with varying angle according to the dispersion relation.

Dispersion relations outside the light line were obtained by fitting Lorentzian curves to the reflection spectra to obtain the absorption peak at each angle. The data from the Otto-coupled measurements are plotted in Fig. 7.9 alongside the data measured within the light cone that was published in Ref. [93]. The solid lines represent data from HFSS simulations. The prism line designates the calculated dispersion mapping limit for the polyethylene prism. Similar to operation inside the light cone, a tuning of the bound mode dispersion outside the light cone is observed for an increase in series capacitance. For p-incident polarization, an anticrossing gap is observed as the waveguide dispersion crosses the light line, leading to formation of a bound mode and radiative mode. This gap indicates the formation of a polariton as the TM$_{00}$ waveguide mode become strongly coupled with p-polarized plane waves of grazing incidence. This is to be expected since the fundamental TM$_{00}$ mode is characterized by electric fields in the gap capacitors that couple well to p-polarized incident light at grazing incidence. No anticrossing gap is observed for s-polarized incident light interacting with the CRLH TM$_{01}$ mode. This too is expected, since the incident E-field component is polarized transverse to the ground plane such that it “shorts” with its image. This is also reflected in the fact that radiative quality factors for the CRLH modes within the
light cone are higher than those for the TM\textsubscript{00} mode.

The surface impedance model accurately predicts the dispersion, as shown in the insets of Fig. 7.9 (sample S1 shown). Each inset contour plot is comprised of two calculations: one within the light cone and one outside the light cone. Inside the light cone, the reflection coefficient is calculated simply for a plane wave incident upon the metasurface from free space. Outside the light cone, the presence of the prism and air gap were accounted for by transforming the surface impedance using transmission line formalism. For the TM\textsubscript{00} waveguide mode, the surface impedance model predicts a relatively broad resonance compared to the TM\textsubscript{01} waveguide mode because of a lower radiative quality factor.

We also examined the effect of the prism-to-air gap \( \Delta \) spacing on the spectra for a fixed incident angle of \( \theta_{\text{inc}} = 41.5^\circ \), which is very close to the light line. For the p-polarized spectra, there is little effect on the spectrum for gaps up to \( \Delta = 50 \, \mu\text{m} \); for \( \Delta = 100 \, \mu\text{m} \) the peak redshifts slightly, and for \( \Delta = 300 \, \mu\text{m} \) the absorption is highly redshifted, broadened, and nearly too weak to distinguish (see Fig. 7.8(a)). This redshift with increased coupling distance is also captured by the surface impedance model (not shown). This measurement suggests that at this particular angle of incidence, for prism distances of \( \Delta \leq 50 \, \mu\text{m} \) the prism is slightly overcoupled to the metasurface and perturbs the bound surface wave mode. As \( \Delta \) increases beyond this, the apparent broadening and redshift of the absorption feature results from the bound mode returning to its unperturbed state and “hugging” the light line at \( \beta = \omega/c \) as it becomes more light-like; this is seen in the contour plot (inset of Fig. 7.9(a)). In contrast, for s-polarized incident light, no clear shift in frequency is observed as a function of coupling distance — at least to the degree distinguishable from noise (inset in Fig. 7.8(b)). This finding is consistent with fact that no anticrossing gap is observed at the light line.
7.3.3 Comparison to Spoof-Surface-Plasmon Structures

It is instructive to compare our CRLH waveguide metasurface with other reported metasurfaces that support spoof surface plasmons. While THz frequencies are too far below the plasma frequencies of noble metals to support true surface plasmon polaritons, so called “spoof surface plasmons” (i.e. p-polarized surface waves) are supported even for perfectly conducting metal surfaces, provided they are structured to present an inductive surface impedance. [88–90] One example is a metal surface corrugated with a subwavelength lattice of metal grooves or holes slightly less than a quarter wavelength deep so that the impedance of the surface is tuned from zero to be large and inductive [97–99]. However, at THz frequencies the necessary groove depth may be as large as several tens to hundreds of microns, which can be prohibitive for planar fabrication processes. Compared to such a corrugated surface, our CRLH metasurface has several differences. First, the height of our metasurface is approximately 1.7 \( \mu \text{m} \) — approximately 50-60 times smaller than the free-space wavelength. Such thin structures are often advantageous for microfabrication in a planar process compared to a high-aspect ratio quarter-wavelength deep trench. It is made possible by using a multi-layer metal-insulator-metal geometry, where a quarter-wave transmission-line transformer has been replaced by low-profile folded circuit elements to achieve the high inductive impedance required to support a p-polarized surface wave. Second, while our CRLH structure exhibits a p-polarized polariton anticrossing signature, it is not proper to describe the p-polarized surface wave as a spoof surface plasmon because the p-polarized surface wave is a coupling of a plane wave to a propagating waveguide mode. At high wavenumbers, the dispersion asymptotically tends to the waveguide dispersion and not a single resonant “plasmon” frequency.

Our CRLH waveguide metasurface is closer in form to the Sievenpiper mushroom surface [84], with the exception of several differences. First, since there is a defined axis for the waveguides, our structure is not isotropic. Second, our struc-
ture has no via to the ground plane, which eases fabrication. Otherwise, there are similarities: Sievenpiper surfaces support both p-polarized spoof-surface-plasmon polariton bound modes (below the surface LC resonance frequency where the surface impedance is inductive) and s-polarized surface wave modes (above the LC resonance frequency where the surface is capacitive). [91] The existence of s-polarized surface waves is expected when a surface exhibits a capacitive surface impedance, and these can be considered to be magnetic spoof surface plasmons. [92] Although it was not observed in Ref. [91], the p-polarized surface wave on a Sievenpiper surface can even exhibit LH behavior if the series capacitance is made sufficiently large. [100] Our metasurface has a third important difference: its CRLH behavior exists only for s-polarized light, and hence is not characterized by an anticrossing gap. As discussed below, this difference is important for the development of THz CRLH leaky-wave antennas.

7.4 Summary

We were first to experimentally demonstrate the existence of leaky-wave and bound modes within passive CRLH THz metamaterial waveguides. The waveguide’s dispersion in and outside the light cone was mapped using angle-resolved FTIR reflection spectroscopy; mapping of the dispersion outside the light cone also required prism-coupling. Two sets of leaky-wave and bound modes were observed: p-polarized RH only modes associated with the waveguide TM$_{00}$ mode and s-polarized CRLH modes associated with the waveguide TM$_{01}$ mode.

The polarization dependence of the response of the RH-only fundamental TM$_{00}$ mode and CRLH higher order lateral TM$_{01}$ mode is qualitatively explained using the cavity antenna model. In particular the TM$_{00}$ waveguide mode is shown to strongly anticross with p-polarized plane waves at the light line, leading to the formation of surface waves. Although the CRLH TM$_{01}$ waveguide mode couples
with s-polarized radiation to produce a surface wave, the coupling is much weaker, and no anticrossing gap at the light line is observed. Indeed, finite element simulation confirms that these s-polarized surface waves exhibit magnetic spoof surface plasmon characteristics with strong field enhancement at the surface and magnetic field loops in the waveguide’s axial direction. The E-field enhancement present within the capacitive structures suggests that such metasurfaces may be useful to enhance nonlinear optical effects.

Second to the importance of demonstrating the feasibility of a CRLH transmission line is the tunability of the CRLH transmission lines’ dispersion with small changes in the series capacitance. The wide tuning in and outside the light cone could offer THz QC-lasers the advantage of single mode frequency tuning. If the capacitive tuning is made dynamic, the in situ tuning scheme could be faster and less bulky than mechanically tuned [101] or externally tuned [102] approaches.

As another modeling tool to guide our understanding, we presented a surface impedance model to support analysis of CRLH waveguide metasurfaces and their radiative properties. The surface impedance model quantitatively reproduces the experimentally measured reflection spectra, using as inputs lumped element transmission line circuit parameters extracted from the dispersion relation. Furthermore, this model correctly predicts the surface reactance of the metasurface, which can be used to predict the presence of p- or s-polarized surface waves. It is computationally non-intensive, allowing for a quick assessment and physical understanding of a design’s features: polarization response, dispersion relation, and loss.

These results guided our understanding of these CRLH waveguides for one particular application: as leaky-wave antennas fed by monolithically integrated THz QC-lasers [15,77] (CH. 6). Endfire operation is particularly interesting, since it allows directive beams to be achieved from THz QC-laser waveguides with subwavelength transverse dimensions [78]. The TM$_{00}$ waveguide mode is clearly not
suitable for LWA operation. It can only achieve RH propagation, so only a forward directed beam is possible. Also, the strong radiative coupling will result in a small radiative quality factor and a large radiation loss coefficient — as discussed in CH. 6.1 for a typical $h = 5 \, \mu m$, the power attenuation coefficient (radiation loss) is greater than $500 \, cm^{-1}$ near $\beta = 0$ [74]. The fast attenuation leads to a small effective emitting aperture and a non-directive beam. Most importantly, feeding the waveguide structure at a single frequency at $n_{eff} = 1$ for endfire operation is not possible due to the anticrossing gap between the radiative and bound mode. The TM$_{01}$ waveguide mode is more favorable for LWA operation. First, it can achieve CRLH operation, which allows backward-to-forward beam scanning, and if properly balanced has no stopband at $\beta = 0$ [71]. Second, the radiative loss coefficient is more modest with values of $\sim 120 \, cm^{-1}$ for a typical $h = 5 \, \mu m$ design near $\beta = 0$; it can be further reduced if desired by decreasing the height of the waveguide or introducing holes, as discussed in the next chapter [74]. Third, no anticrossing will occur at the light line, and the waveguide can be excited exactly at the end-fire condition, $n_{eff} = 1$. However, it must be noted that due to the orientation of the radiating magnetic current dipoles on the waveguide sidewalls, such an end-fire mode from a single waveguide will radiate an azimuthally polarized donut-shaped beam in the far field, rather than a focused spot.
CHAPTER 8

Active THz Reflectors and Metasurfaces

Currently, THz QC-laser output power performance ranges from 1–130 mW in continuous wave (CW) and 248 mW pulsed power [4]. Greater output power could benefit applications such as imaging by improving the signal to noise ratio [103]. From the survey (Table 1.1) of current beam tailored QC-devices discussed in CH. 1, the most promising, in terms of beam quality approaches are the large area surface emitting (broadside) Bragg lasers [41, 79] and the endfire 3rd order DFBs [9]. To improve the total output power or directivity, a larger aperture size is needed. However, neither design scales in size well. Scaling of the surface emitting designs would lead to a large current and heat dissipation; the heating reduces the population inversion and hence degrades high-duty cycle performance. The nearly perfectly phase matched 3rd order DFB in [43] results in a directive beam with a divergence angle that scales with the square root of the device length ($\propto \sqrt{L}$ [104]). For example, a 1.9 mm and 5.65 mm long device result in 10°×17° and 6°×11° directive far-field beams, respectively. Scaling to longer lengths becomes increasingly more challenging because of difficulties in phase matching.

The research so far has primarily focused on implementing metamaterial inspired concepts to tailor the radiation from 1-D/2-D MM waveguide QC-based devices. Another possibility is to tailor the beam of any THz device with a beam collimator, i.e. reflectarray, which would allow for scalability. A reflectarray is a powerful tool that could help reduce the beam divergence (increase far-field directivity), control the main beam direction (scanning), and improve the beam
intensity (with an active design) of a THz source. In this section, analysis for the feasibility of a passive and active reflectarray in the THz regime will be discussed. Additionally, we present an active metasurface that leverages our understanding of TM\textsubscript{01} RH transmission lines of CH. 6. With this active reflector, one could perhaps realize a scalable THz vertical external cavity surface emitting laser.

8.1 Reflectarray

Antennas with high gain and directivity are needed for long range applications such as JPL and NASA’s Deep Space Network (DSN) [105]. Usually, such antennas consist of parabolic reflector antennas. In general reflector antennas can include many different antennas such as corner reflectors, planar reflectors, and parabolic reflectors, to name a few [106]. The objective of a reflector antenna is to provide increased gain and directivity through its larger effective aperture where there are two main components: a feed and a reflector. The feed radiates a spherical wavefront and at the reflector surface, the wave is locally treated as a plane wave, with a phase proportional to the distance from the phase center of the
Figure 8.2: Reflection phase needed for each element is a function of location on the reflectarray. Figure taken from [17].
feed to the reflector. A parabolic reflector compensates for the phase difference due to the path length difference (Fig. 8.1) and reradiates a planar wavefront in order to have a highly directive far-field pattern. However, parabolic reflectors are difficult to manufacture due to their curved surfaces and consequently have the disadvantage of a large footprint. Another option is to use a planar surface with radiating elements that provide the necessary phase compensation, namely, a reflectarray. A reflectarray imitates a parabolic reflector by using a planar array of resonant elements designed to have a reflected beam with the necessary phase shifts to create a planar phase front \[16\]. A very similar concept is the generation of phase discontinuities at the interface of a surface using resonant structures that are organized in a subwavelength configuration \[107\]. The underlying concept shared by both is phase engineering.

Usually implemented in the microwave regime, but also recently shown to be feasible in the infrared \[108\], the resonant elements of a reflectarray can be square patches, circular patches or their derivatives. The phase front of the reflected beam can be arbitrary designed (depending on the obtainable phase swing of the resonant element) to collimate the beam and also to steer the main beam to some desired angle \((\theta, \phi)\). With reference to Fig. 8.2, the reflection phase provided by the \(ij\)th element to steer a main beam to some desired angle \((\theta, \phi)\) for a given feed distance \(R_{ij}\) is given by \[16\]

\[
\psi_R(x_{ij}, y_{ij}) = k_o R_{ij} - k_o \mathbf{r}_{ij} \cdot \hat{\mathbf{r}} - 2\pi N \\
= k_o R_{ij} - k_o \sin(\theta) \cos(\phi)x_{ij} - k_o \sin(\theta) \sin(\phi)y_{ij} - 2\pi N \tag{8.1}
\]

where the first term represents the total accumulated phase by the incident beam from the feed’s focal point to the \(ij\)th element. The second term

\[
k_o \mathbf{r}_{ij} \cdot \hat{\mathbf{r}} = k_o \{\hat{x}x_{ij} + \hat{y}y_{ij} + \hat{z}z_{ij}\} \cdot \{\hat{x}\sin(\theta)\cos(\phi) + \hat{y}\sin(\theta)\sin(\phi) + \hat{z}\cos(\theta)\} \quad (8.2)
\]

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is the progressive phase shift needed at each element for beam steering and is
a function of the element’s position and desired main beam angle (observation
point). The last term is to account for phase wrapping. Some important design
parameters in a reflector antenna, which are revisited later in the chapter, include
the desired gain \( G = \eta_{ap}D, D = 4\pi A/\lambda^2 \), desired aperture efficiency (for the
most simple case: \( \eta_{ap} = \eta_{spillover}\eta_{taper/illumination} \)) a.k.a. feed efficiency, and the
F/D ratio.

8.1.1 Feasibility in the THz

In both the passive and active reflectarray study, rectangular resonant patch ele-
ments with MQWs in between the two metallization layers is assumed (GaAs/AlGaAs
material system). One approach in reflector design involves choosing a desired gain
and from there calculate the other required parameters of interest. However, a
slightly different approach was taken given the current dissipation/consumption
concerns of an active reflectarray. To be conservative, a maximum current density
\( J_{\text{max}}=1000 \, \text{A/cm}^2 \) [64] was used for my calculations (for the FL86Q-M11 active
region designs, the max current \( J_{\text{max}} \) is closer to \(~575\,\text{A/cm}^2\) [77]). Since the
current supply available at the time has a 2 A maximum output, a reflectarray
diameter of \( D = 2.25 \, \text{mm} \) was chosen for the study (Fig. 8.3), translating to a
maximum reflector directivity of 36 dB and gain of 30 dB for an assumed aperture
efficiency \( \eta_{ap} = 81\% \); the gain translates to an increase in power density of 1000
times.

We can also estimate the beam divergence, a.k.a. the half power beam width
(HPBW), since the directivity varies inversely with the beam solid angle \( (D = 4\pi/\Omega) \), where \( \Omega \) is the solid angle that captures all the power radiated if the
radiation intensity through that solid angle were the same as the maximum of
the beam. For a Gaussian beam, there are no minor lobes, so the radiation is
contained only in the main lobe, therefore, we can approximate the beam solid
Figure 8.3: In the very rough and conservative estimate, two reflectarray shapes were considered: square and circular. The element periodicity is assumed to be $\lambda_0/2 = 50 \, \mu m$ and elements are assumed to completely cover the reflectarray. A comparison, when using square resonant patches, shows that the circularly shaped reflectarray would draw the least amount of current. When using slightly smaller resonant elements (smaller in the nonresonant direction) a larger aperture size can be obtained for the same total current consumption of 2 A.
angle as a product of the principal planes’ HPBW, $\Omega \approx HP_E HP_H$. Generally, however, there are sidelobes and gain is used in practice. Therefore, the HPBW is approximated with $G = \frac{4\pi}{HP_E HP_H}$ [109]. Assuming equal HPBWs for the two principal planes, a 5° HPBW is estimated.

Next, the diameter $D$ is used to calculate the F/D (focal length to aperture diameter) ratio for a 60° apex angle requirement resulting in F/D=0.866. A 60° apex angle formed by the feed and the reflectarray is assumed because optimal performance is achieved for broadside illumination of the reflectarray elements. This restriction is due to practical purposes; the various-sized elements’ reflection phase and loss were characterized only at broadside. One could increase the accuracy of the study by characterizing the elements for different incident angles, but that was beyond the scope of this feasibility study. Some figures of merit for a reflectarray element include: maximum range of the reflection phase, sensitivity (to changes in dimension), and element bandwidth [110]. In this study, focus was placed on the first two figures of merit. To decrease current consumption a smaller nonresonant dimension was elected resulting in a rectangular shaped element. The reflection phase plots of 10 $\mu$m tall resonant patches with attached bias lines, for various resonant length dimensions (Fig. 8.4(a)) gives a reflection phase curve (‘S’ curve) with a range of $\sim$320°(Fig. 8.4(b)). Fig. 8.5 outlines the steps that were taken to obtain a full EM simulation of the THz reflectarray’s far-field beam pattern.

8.1.2 Far-Field Modeling with the Cavity Model

HFSS simulations of the reflectarray were resource and time intensive, so a reflectarray far-field model using the cavity antenna model was generated to quickly give a rough idea of the reflectarray’s performance. Since each resonant element is essentially a patch antenna, the cavity model implemented in the previous sections was reused along with a few adjustments to calculate the far-field beam pattern.
Figure 8.4: (a) Reflection phase from resonant elements for various resonant lengths (y direction) and the resulting (b) ‘S’ curve. Inset shows the phase sensitivity to changes in dimension. For an active implementation, elements have bias lines connected along the non resonant direction.

The resonant element’s far-field beam pattern from HFSS simulations was closely predicted by the cavity model. For example, for a structure with length 19.75 $\mu$m in the resonant direction, the cavity model initially predicted close but not extremely accurate (Fig. 8.6) principal plane cuts. However, by accounting for fringing fields, the cavity model predicted the element’s pattern very well (Fig. 8.7).

Similar to the process in Fig. 8.5, to calculate the reflectarray’s far-field beam pattern, the required phase shift at a particular location is calculated using Eq. 8.1 and an array factor and far-field component is calculated to account for the element’s contribution to the reflectarray’s total far-field pattern. Fig. 8.8 details the process flow.

As an example, we considered a reflectarray with a diameter of 600 $\mu$m to keep the benchmark HFSS simulation reasonable in size. The reflectarray was assumed to be center fed, and was designed for a broadside far-field beam. Given the calculated reflection phase and position of the elements (Fig. 8.9(a)), the corresponding
Figure 8.5: Reflection phase from resonant elements for various resonant lengths (y direction) is obtained from HFSS simulations. A matlab script then calculates the placement and necessary phase shifts to be provided by the element, looks up the corresponding element dimensions, and outputs a visual basic script that sets up the HFSS model, where an assumed Gaussian feed illuminates the reflectarray giving a directive far-field beam pattern. Note that a symmetry E plane is used in the above HFSS reflectarray model to minimize the simulation size and time.
Figure 8.6: A comparison between the cavity model predicted far field and HFSS simulation. Inset shows one resonant element and its dimensions used for this comparison; the double headed arrows designate the radiating equivalent magnetic current from the radiating slots.
Figure 8.7: By adjusting the resonant length in the cavity model to account for fringing fields, which make the structure look effectively larger, the cavity model predicted far field matches the HFSS simulation almost perfectly.
Step 1: Acquire far field beam pattern for a single resonating element using the cavity model. Only the two radiating slots are modeled and was compared with closed form expressions.

Step 2: Calculate phase shift needed for different locations on the reflectarray. Look up corresponding element dimensions acquired from Step 1.

Step 3: For each element:
- calculate phase
- calculate the array factor
- add element contribution to the far field

\[ \psi_{ij}(x_j, y_j) = \frac{k}{c_106} R_{i,j} - \frac{k}{c_106} \sin(\theta_{xj}) x_j - \frac{k}{c_106} \sin(\theta_{yj}) y_j - 2\pi N \]

\[ \text{AF}_{ij} = \frac{\hat{z}}{2R_{ij}} \exp(i2\pi k R_{ij}(x_j - x_i)) \]

\[ E_{\text{total}} = E_{\text{element}} \cdot \text{AF}_{ij} \]

Figure 8.8: Cavity model predicted reflectarray far-field beam pattern process flow. As a side note, a small nonsymmetry in the H plane cut predicted by HFSS shown above for an example reflectarray with D=600 μm is due to the nonuniform/nonsymmetric meshing generated by HFSS’s adaptive meshing algorithm. The nonsymmetry is not noted in the E plane cut because a symmetry plane is used for the bottom half of the reflectarray. Additional considerations such as resonator loss and Gaussian beam feed profiles were accounted for in the elements’ far-field intensity contribution.
amplitude loss due to the inherent loss of the off/on resonance elements is shown in Fig. 8.9(b). The overall intensity of the reflected beam is also dependent on the intensity of the incident beam. Since the incident beam is assumed to be Gaussian, its field decay in the transverse direction (xy plane) must also be accounted for at the plane of the reflectarray (Fig. 8.9(d)). Lastly, only certain reflection phases can be obtained for two reasons: a minimum 0.5 μm change in the physical dimension was assumed and the resonant element’s inability to provide a full 2π phase shift. Therefore, relative phase differences between the required phase reflectarray and what is obtainable will exist and is detailed in Fig. 8.9(c). However, even with such phase errors, the cavity model predicted far-field beam pattern proved to be quite robust compared to the HFSS results (Fig. 8.10, Fig. 8.11).

Two possible reasons for the differences seen away from the main lobe include element pattern effects and specular reflection of the elements/ground plane that attributes to side lobe levels. The former is related to the discussion above pertaining to the chosen 60° subtended angle between the feed and the reflectarray, namely, the radiation pattern of the element is not isotropic. Ideally, elements in the center should have narrow beamwidth with higher gain, and elements close to the edge should have a wider beamwidth. Specular reflection is a source of loss and inefficiency in reflectarrays for the edge elements. The reflected power is not a reradiated contribution to the main lobe and instead contributes to the side lobe levels [16].
Figure 8.9: The (a) required reflection phase shift, (b) electric field amplitude decay due to resonant element losses, (c) phase error/difference between what is required and what is obtainable, and (d) incident Gaussian beam profile for a reflectarray with a diameter of 600 μm.
Figure 8.10: Cavity model and HFSS predicted intensity for a reflectarray with diameter $D=600 \mu m$. 

![Cavity model and HFSS predicted intensity for a reflectarray with diameter $D=600 \mu m$.](image)
Additional benchmarking was done for a reflectarray scanned main beam of 30° from broadside along the H plane cut (x axis in Fig. 8.8)) of the reflectarray. Fig. 8.12 details the element design considerations. The H-plane cut between the HFSS sim and cavity model prediction match nicely around the main lobe (Fig. 8.13). Although away from the main lobe there are some small discrepancies (differences < -12 dB), the main lobe prediction is of primary concern.

We therefore have two tools to predict the performance of a reflectarray: HFSS simulations and a much quicker antenna cavity model calculation. The next phase of the study involved characterizing the feed, a third order distributed feedback
Figure 8.12: The (a) required reflection phase shift, (b) electric field amplitude decay due to resonant element losses, (c) phase error/difference between what is desired and what is obtainable, and (d) incident Gaussian beam profile for a reflectarray with a diameter of 600 μm and a scanned main beam at 30° off from broadside along the H plane.
8.1.3 Feed

In the microwave regime, the feed usually takes for the form of an open-ended waveguide or horn antenna. For this analysis the feed was assumed to be a 3rd order DFB THz QC-laser. Our post doctoral scholar Zhijun Liu had fabricated 3rd order DFB designs based on the design reported in [9] and was in the process of characterizing them. Unfortunately, beam data was not yet available. Therefore, I assumed a Gaussian beam with its waist placed at the focal point in the HFSS reflectarray simulations and cavity model predicted far fields discussed above. Simulations (Fig. 8.14) of the 3rd order DFB revealed a close-to-endfire beam.
Figure 8.14: (a) Simulation of a 12 unit cell DFB with a close-to-endfire beam pattern at 2.992 THz. A little more than 5 unit cells and only half the structure is shown, where a symmetry H plane has been used along the length of the structure. Only one end of the two end-fire patterns is shown for (b) a finite sized ground plane and an (b) infinite sized ground plane.
In the previous sections, the required reflection phase for the $ij$th element is based on the assumption that the phase center of the feed is situated at the focal point of the reflectarray. To acquire the phase center of the 3rd order DFB, the origin of the “infinite sphere”, which is used by HFSS to calculate the far-field pattern, is parametrically swept along the ridge of the DFB until the most stable phase over the widest solid angle is located. The corresponding location along the ridge of the DFB is considered the phase center and is placed at the focal point of the reflectarray. The phase center was found to be $\sim 200\mu$m inset from the facet of the 3rd order DFB with a maximum phase variation of $\sim 10^\circ$ from the observation angles $\theta = 70^\circ \rightarrow 90^\circ$ with respect to the coordinate system drawn in the inset of Fig. 8.14. Since the DFB does not have a perfect endfire pattern, using it as a feed for the reflectarray would require one of two adjustment. One could redesign the reflectarray’s chosen element and placement to adjust for a beam maximum that is not at the center of the reflectarray. Consequently, the required reflection phases would need to be recalculated for the desired main beam direction. The other option is to tilt the reflectarray similar to an offset fed parabolic design [106].

8.1.4 Summary

A set of tools were generated to design and analyze the performance of a THz passive/active reflectarray and results were benchmarked with HFSS simulations. For our sample analysis, a maximum reflectarray diameter, limited only by the maximum current output of the lab’s pulse generator, of 2.25 mm resulted in a directivity of 36 dB and a gain of 30 dB (a 3 order increase in power density). An estimated divergence of $5^\circ \times 5^\circ$ can be obtained! A passive/active THz reflectarray is certainly realizable, but it is not without it’s challenges. Some of the more challenging aspects of a THz reflectarray is obtaining a feed with a well defined phase center and beam pattern. For example, the close-to-endfire 3rd order DFBs
realized by Amanti [78] [9], with an experimentally acquired $\sim 10^\circ \times \sim 10^\circ$ divergence does not exhibit a perfectly symmetric beam pattern. The alignment between the feed and the reflectarray is another challenge as well that needs to be addressed in a practical implementation.

8.2 Active Metasurface

After studying the feasibility of a passive/active reflectarray, our attention focused onto another possible solution for tailoring the beam pattern and out coupling power of THz QC-devices. Namely, an active metasurface reflector, similar to the ones in CH. 7, but comprised of TM$_{01}$ MM waveguides sandwiching MQWs, where the active metasurface reflector would provide optical gain to overcome losses. From our previous work, we recognized that the MM waveguide operating in its TM$_{01}$ mode radiates efficiently in the broadside direction when operating at its shunt resonant frequency [74]. The shunt resonance field profile also satisfied the selection rules of the MQW active region and therefore, optical gain could be obtained. An amplification of an incident beam reflecting off a surface comprised of a sparse array of such antenna-coupled THz QC-laser active sub-cavities could be possible assuming that there is enough optical gain to overcome the losses: ohmic loss from the ground plane and top metallization and free-carrier loss in the MQWs. Such an active metasurface reflector could provide the gain necessary to sustain a lasing high-Q cavity mode formed between the active metasurface reflector and another passive reflector, i.e. an output coupling mirror.

8.2.1 Modeling and Engineering Losses

Using HFSS, an infinite array of MM waveguides spaced less than a wavelength away (to avoid lossy higher order diffraction) is illuminated with an incident plane wave and loss is systematically removed to quantify the bulk material gain ($g_{\text{mat}} = \ldots \ldots$).
Figure 8.15: Example of a 2 mm × 2 mm active large area array of TM$_{01}$ waveguide reflectors with a tranverse period of 100 μm.
Figure 8.16: The (a) reflectivity, (b) effective mirror loss power attenuation coefficient, (c) waveguide loss power attenuation coefficient and (d) total power attenuation coefficient at the interface between the $TM_{00}$ waveguide and taper.
Figure 8.17: The (a) reflectivity, (b) effective mirror loss power attenuation coefficient, (c) waveguide loss power attenuation coefficient and (d) total power attenuation coefficient at the interface between the TM$_{01}$ waveguide and taper. The cutoff frequency (shunt resonant frequency) is $\sim 2.7$ THz.
\( \frac{\text{ohmic}}{1} \) needed to overcome the losses. While increasing the material gain, we note the reflectivity at the surface of the metasurface and find that a total material gain of \( \alpha_{\text{ohmic,fc}} = 32.5 \text{ cm}^{-1} \) is needed to reach transparency (a lossless reflector) for TM\(_{01}\) waveguides operating its shunt resonant frequency of 2.7 THz and an active region height of 5 \( \mu \text{m} \). The gain needed to overcome ohmic and free carrier loss in the MQW are \( \alpha_{\text{ohmic}} = 12.5 \text{ cm}^{-1} \) and \( \alpha_{\text{fc}} = 20 \text{ cm}^{-1} \), respectively.

In a practical realization, only a finite sized array can be fabricated, which requires proper termination of the array of waveguides. Lasing in either the fundamental TM\(_{00}\) or higher order TM\(_{01}\) waveguide mode is not desired. Therefore each waveguide is terminated with an impedance transforming taper that connects to a bond pad region, which then tapers to free space. Fig. 8.15 is an example of a 2 mm\( \times \)2 mm active region array with terminations that have a total length of 500 \( \mu \text{m} \). The termination is designed not to present any gain (there is an insulating oxide layer between the top contact layer and the active region) and minimal reflection for both waveguide modes. The HFSS waveport driven results of the termination shown in Fig. 8.16 and Fig. 8.17 detail the total power attenuation coefficient across the frequency range of the gain medium for the TM\(_{00}\) and TM\(_{01}\) modes. At the designed shunt frequency of the TM\(_{01}\) mode, the total power attenuation for the TM\(_{00}\) and TM\(_{01}\) mode is \( \sim 58 \text{ cm}^{-1} \) and \( \sim 65 \text{ cm}^{-1} \), respectively. Since, a bulk material gain of \( \alpha_{\text{ohmic,fc}} = 32.5 \text{ cm}^{-1} \) is needed for transparency, there is a difference of \( \sim 32.5 \text{ cm}^{-1} \) before any possibility of lasing in the TM\(_{01}\) mode. Bulk material gain ranging from \( \sim 50-100 \text{ cm}^{-1} \) is possible, but lasing in either mode is greatly reduced with this termination.

### 8.2.2 Experimental Results

Testing on preliminary devices did not yield conclusive results illustrating gain compensated reflection off the metasurface. However, experimental findings are included in this section for thoroughness.
Figure 8.18: Pulsed (10 KHz repetition frequency with a 500 ns pulse width) light-current-voltage (L-I-V) characteristic of a 2.2mm long, 15μm wide MM waveguide with one etched and one cleaved facet operating at 77 K.
Figure 8.19: IV comparison between three devices: (1) a 1 mm x 1 mm array, herein known as device 1.9, comprised of 11 elements, (2) a MM waveguide from the same processed wafer piece as shown in Fig. 8.18 (NGB17952.A fabricated: 07/23/13) and (3) a MM waveguide from the same wafer but different processed piece (NGB17952.1 fabricated: 11/18/09). No noticeable negative differential resistance (NDR) was observed for any of the devices and higher current draw is likely due to poor ohmic contacts.
The objective of the experiment is to obtain transparency and eventually gain in the metasurface reflected beam as a function of increased device bias. To effectively couple to the waveguide’s shunt resonant mode, normal incident reflection upon the device with a polarization transverse to the ridge is achieved with the setup shown in Appendix A.6’s Fig. A.9. Devices were fabricated by Zhijun Liu and Chris Curwen, our lab’s post doctoral scholar and Ph.D. student, respectively. Active region growth was provided by Dr. Qi-Sheng Chen of Northrop Grumman Aerospace Systems (NGAS) at Redondo Beach, CA. Devices from two separately processed pieces were tested. One piece was over etched, where surface roughness was visible on the copper ground plane (herein known as NGB17952.A) and the other piece was under etched leaving ~100 nm of quantum wells left (herein known as NGB17952.B).

Three types of devices were tested: a MM waveguide, a smaller 1 mm x 1 mm array and a larger 2 mm x 2 mm array. Many devices were tested, but only representative data for each type will be presented. The MM waveguide was tested to obtain an understanding of the electrical and optical characteristics of the devices on the same processed piece. Light-current-voltage (L-I-V) measurements of a MM waveguide at 4 K from NGB17952.B exhibited a lasing threshold current density value that was three times larger than the expected \( \sim 450 \text{ mA/cm}^2 \) \cite{77} of previously tested devices from the same growth, but different fabrication. A MM waveguide from NGB17952.A at 77 K exhibited a lasing threshold current density of \( \sim 545 \text{ mA/cm}^2 \) (Fig. 8.18). Therefore, testing focused primarily on devices from NGB17952.A.

Initial array device testing focused on 1 mm x 1 mm devices, where L-I-V measurements were taken to verify that there was no lasing (Fig. 8.19). To address the possibility of a single bad ridge shorting the entire array, the 11 ridge device was electrically separated into 5 and 6 ridges through a 20 µm gap between the bias pads. The scheme also allowed biasing flexibility, namely, 5, 6 or 11 ridges.
Figure 8.20: Mapping of device 1.9’s location with reflectivity measurements. A reflective gold piece was used as a background reference and blue nonreflective tape was used as an aid to align the device.
Figure 8.21: IV comparison between three devices: (1) a 2 mm x 2 mm array, herein known as device 1, comprised of a total of 21 elements (only 11 contiguous elements were biased), (2) a MM waveguide from the same processed wafer piece as shown in Fig. 8.18 (NGB17952.A fabricated: 07/23/13) and (3) a MM waveguide from the same wafer but different processed piece (NGB17952.1 fabricated: 11/18/09).
could be biased at a particular instance. Device and optical path alignment were verified with reflectivity mapping; the signal level of the interferogram was noted for varied x, y and z device locations until a figure like Fig. 8.20 was obtained. Continuous scans successfully revealed absorption dips corresponding to the shunt resonance at expected wavenumbers (~ 97 cm\(^{-1}\)). Unfortunately, at the time of testing the smaller 1 mm x 1 mm arrays, the duty cycle was limited to 2% by the Avtech AV0-6HF-B pulse generator’s 4% duty cycle limit and the pulse trains 50% duty cycle. Therefore a continuous scan did not yield any difference in the absorption spectra as a function of device bias. The other testing alternative, step-scanning, did not result in an interferogram with a noticeable center-burst due to high device thermal emission. If there was any gain compensated reflection from the device, the signal was overwhelmed by thermal emission. Two checks were conducted to verify that the signal was thermally dominated: a variation in repetition rate from 500 Hz to 20 KHz and a blocking of the signal within the experiment’s optical path. In the former check, as the repetition rate is increased, the lock-in signal dropped, presumably due to a reduction in thermal emission. The second check involved blocking of the radiation from the FTIR, which resulted in a lock-in signal level comparable to the case where the FTIR’s radiation was not blocked.

To address the need for higher duty cycles and still provide the necessary bias voltage and current, the AE Techron 7224 amplifier was acquired and implemented into the test setup with the Agilent 8114A pulse generator. Focus shifted to the larger 2 mm x 2 mm devices in hopes of more easily detecting amplified reflection. The Janis cryostat was replaced with the Infrared Laboratories device dewar to present a larger thermal body to the device in hopes of reducing thermal emission. The objective was to perform a continuous scan with increased duty cycle; step-scans were taken but were still dominated by thermal emission. Similar to the smaller arrays, the 2 mm x 2 mm arrays were electrically separated into 5, 11
Figure 8.22: Mapping of device 1’s location with reflectivity measurements. A reflective gold piece was used as a background reference and blue nonreflective tape was used as an aid to align the device.

Figure 8.23: Continuous scan absorption spectrum from device 1. Two absorption dips are visible: one around $95 \text{ cm}^{-1}$ corresponding to device 1’s shunt resonance and another around $91 \text{ cm}^{-1}$ corresponding to an adjacent device which had a wider ridge width (15 $\mu$m).
and 5 ridges. The data presented next is from a device herein known as device
1. Only 11 (contiguous) of its 21 elements were biased, each element having
a 15 $\mu$m ridge width and 2 mm length. It exhibited an IV similar to the MM
waveguide from the same wafer piece (Fig. 8.21). Continuous scans were taken
after device location mapping was performed (Fig. 8.22) and a strong absorption
(Fig. 8.23) around $\sim 95$ cm$^{-1}$ for different device bias was noted. An additional
absorption dip is observed and is due to an adjacent device with 15.5 $\mu$m width
ridges corresponding to a shunt resonance around $\sim 91$ cm$^{-1}$. With each increase
in duty cycle a continuous scan was conducted until the device was damaged at
a 40% duty cycle. Unfortunately, no noticeable reduction in absorption with an
increase in duty cycle was observed.

8.2.3 Summary

For the first design cycle, the radiative, ohmic and free carrier losses were not
optimized. Instead, the focus was to suppress unwanted lasing and to show gain
compensated reflectivity. Testing of fabricated active metasurface devices sug-
jest that thermal emission may be swamping any gain compensated reflection,
therefore, a method to address the thermal dissipation needs to be implemented.
Additionally, the devices were fabricated on a wafer’s edge piece and may not
have yielded the most reliable devices, therefore leading to their early failure at
low duty cycles. Among the devices tested, device failure ranged from 20-40%
duty cycle. For future designs, perhaps, a reduction in device length could reduce
the likelihood of a single point failure in the array. Also, biasing from the sides of
the ridges with high impedance lines could also address nonuniform gain due to
the voltage drop along the ridge.

In conclusion, simulations for a sparse array of antenna-coupled THz QC-
lasers operating in its shunt resonance (a.k.a. the half wavelength resonance in
a patch antenna) support the feasibility of an active metasurface reflector that
can compensate for losses and even provide gain. Unfortunately, testing of first-round, fabricated devices did not show any gain compensation. To be left for future work, the successful demonstration of this concept could lead to an external cavity laser, where a high Q TEM$_{00}$ cavity mode could mode lock the multiple THz QC-laser sub-cavities, which would provide the optical gain necessary to sustain lasing. Such a scheme could provide scalable power and a near-diffraction-limited Gaussian beam pattern, along with the flexibility that comes with external cavity design, i.e. various tuning schemes, insertion of intracavity elements, etc.
CHAPTER 9

Conclusion: THz Device Engineering

To summarize, I have detailed the techniques used in the design of THz CRLH transmission lines realized with passive BCB/active QC-material in the MM waveguide configuration. The focus of the research was to adapt metamaterial dispersion engineering concepts to MM waveguide QC-lasers for the purpose of improving the directivity of their far-field beam pattern. Many designs based on different lateral waveguide modes were investigated. Eventually, passive and active CRLH transmission lines based on the higher-order lateral TM$_{01}$ waveguide mode were successfully demonstrated.

Two measurement techniques were used to verify the existence of a left handed and right handed branch, a signature of CRLH metamaterials. Namely, polarization-dependent angle-resolved reflection spectroscopy mapped out the dispersion of large area arrays of CRLH transmission lines via momentum matching. Second, an equivalent but reciprocal measurement technique used a conventional FP QC-laser to excite an active CRLH leaky-wave antenna. The resulting frequency scanned backward to forward far-field beam, being a function of the CRLH transmission line’s dispersion, is then a verification of a left and right handed branch in its dispersion.

In my research, the most notable accomplishments include:

- Modeling of QC-devices based on the MM waveguide configuration, such as the conventional FP MM waveguide and CRLH metamaterial waveguides with a set of general analytic, numeric and full-wave FEM simulation tools.
Based on the antenna cavity model, expressions for the quality factor and far-field beam patterns of MM waveguide based devices were derived. Quality factor calculations qualitatively agreed with full-wave FEM simulations, where closer agreement is achieved with larger ridge width to height ratios, which would approach the cavity model approximation. The antenna cavity model predicted far field notably predicted relative roles of the sidewall and facet radiative contributions for different waveguide modes, which was a limitation for the previous wire laser model by Orlova [81]. A general circuit model eigensolver that extracts the dispersion and circuit parameters such as voltage/current across different components was used for the CRLH waveguides. Lastly, threshold intersubband gain for MM waveguide based devices were acquired via full-wave FEM simulations; its implementation is documented in Appendix A.4.

- Modeling of the surface impedance of a waveguide array metasurface using the antenna cavity model along with transmission-line theory, which can give the absorption spectra/dispersion of the metasurface. The model also correctly captures the polarization dependent mode coupling with the light line, which can aid in the design of devices operating near the light line.

- Design and analysis of various CRLH transmission line designs for zeroth order QC-laser and leaky-wave antenna applications. Comparison of loss mechanisms showed that the $TM_{01}$ waveguide mode is too radiatively lossy for ZOR applications. Reduction in its radiative efficiency is introduced via near and far-field engineering, however, the reduction is not enough to meet lasing requirements. On the other hand, because of the large radiative efficiency, designs based on the $TM_{01}$ mode are good candidates for leaky-wave applications. The balanced CRLH leaky-wave antenna exhibits a directive broadside radiation relative to a right-handed only leaky-wave antenna, where broadside radiation is nondirective due to its zero group
velocity. Additional simulations for a new $TM_{02}$ design show a $\sim 50\%$ reduction in total losses (radiative, metallic and free carrier losses) relative to the other designs, making it a possible candidate for a zeroth order QC-laser. It also could make for a more directive leaky-wave antenna given its longer effective aperture size.

- First demonstration of passive THz CRLH transmission lines by verifying left handed and right handed branches in its dispersion via polarization-dependent angle-resolved reflection spectroscopy measurements of a large area array. Dispersion tuning via the series capacitance for small changes in physical dimensions suggest sensitive tuning capability in and out of the light cone. A dynamically tunable series capacitance would be great for in situ tuning of QC-lasers, which currently require mechanical or external cavity approaches [101,102].

- Proposal and feasibility analysis of a THz passive/active reflectarray for increased beam directivity and intensity of a THz feed. Both full-wave FEM simulations and numeric modeling suggest that directive beam patterns and power scalability are possible. For example, a reflectarray with a diameter $D = 600 \mu m$ would give a beam divergence of $\sim 5^\circ \times \sim 5^\circ$ and an increase of 1000 times in intensity relative to its feed.

The most important aspect of this thesis that I’ve presented is the design tools/methodology used to analyze our proposed CRLH transmission lines. Because they are general-purpose tools they can be used for other devices based on the MM waveguide configuration. The original goal of tailoring the beam pattern of MM waveguide QC-lasers has been successfully achieved with a leaky-wave antenna where it also had an added functionality of beam scanning with frequency. A related and important concern is the output power level and the scalability of the LWA-based designs. As mentioned in [12], reaching the full potential of these
designs depends on their optimization, for example, feeding efficiency between the master oscillator and the leaky-wave antenna, radiative loss engineering of the leaky-wave antenna to extend its effective aperture size, to name a few.

The understanding acquired from this research has led to a promising future prospect, namely, a vertical external cavity surface emitting laser, which has a scalable output power and directive beam. A critical component is the active reflective metasurface, which will provide the optical gain needed for lasing of the external cavity mode. A successful demonstration of the metasurface to not only reach reflective transparency but to also provide gain would be an important first step towards a new approach for THz sources.
Technology hardening of microwave devices is a continuing field of research. Protection schemes used at lower frequencies such as resistors and diodes have been used for pulse shaping and electrostatic discharging, respectively. However, these protection schemes are not suitable at microwave frequencies. A possible solution is the use of field-emitter based electrostatic discharge (ESD) protection circuits, which require additional, but standard, transistor technology processing steps [111]. Unfortunately, the above mentioned protection schemes only provide limited protection. Since the first observations of powerful electromagnetic shock waves in the 1940s from atmospheric nuclear detonations, high power microwave (HPM) weapons capable of similar characteristics have been created [112]. The beauty of such a weapon is its benign nature to human life and its effectiveness in shutting down an enemy's communication system since modern day telecommunication systems are comprised of metallized components that are extremely sensitive to high power pulses. Even with protection circuitry, such components represent the weakest link in the communication chain. There are some conventional front-end protection schemes such as ESD protection with and without diodes, which have been made suitable for microwave frequencies [113] and also more exotic ones like plasma limiters [114]. However in the former there exist a voltage limit and a finite rise time. In the later, there exist a finite rise time as well, but also the necessity to use very sharp conductive electrodes, where sharpness of
the metallized electrodes may degrade with continuous HPM pulses, which would degrade the effectiveness of the limiter. There are also cascaded configurations, which consist of a plasma limiter in series with a PIN limiter [115]. Simulated microwave leakage in the cascaded configuration showed dramatic reduction, but such a system still suffers from the finite breakdown time of the gas in the plasma limiter.

To continuously and instantaneously provide protection against electromagnetic radiation from HPM weapons, an all-dielectric non-electronic radio front-end (ADNERF) technology was proposed in [116–118]. A good analogy of the system would be a low frequency opto-coupler. A microwave signal is converted to an optical signal and finally back to a microwave signal, which eventually may be fed into a traditional MMIC low noise amplifier. This methodology electrically isolates the sensitive metallization-based microwave electronics from the electromagnetic pulse attack. The system in [116–118] consists primarily of a cylindrical dielectric resonator antenna (DRA) to enhance the electromagnetic fields across a resonant electro-optic (E-O) field sensor, which together provide a microwave receiver front-end that is made of only dielectrics.

My research focused on an unconventional dielectric rod antenna to be used as a dielectric field enhancer (DFE). It is unconventional in terms of design methodology, its feed and its proposed incorporation into the ADNERF system. The use of the DFE further increases the enhanced field in the cylindrical DRA and hence modulated field intensity in the E-O field sensor, which could increase the system’s sensitivity [117].

The design methodology for the DFE is detailed and a microwave verification of the design is conducted with a preexisting annular ring DRA. The objective is to verify the increase in the annular ring DRA’s gain after the inclusion of the DFE, and hence the DFE’s field enhancing capability. Lastly, simulations of the DFE and a stand-alone (without any metallization) DRA combination are presented.
Figure 10.1: Dielectric field enhancer dimensions.

10.1 Analysis and Design

Early work from Mueller [119] highlighted the dielectric rod antenna’s directive, wide band, and light weight properties and because of those properties, the dielectric rod antenna has been a great candidate for antenna feed applications [120]. Also, due to low material loss, dielectric rod antennas have been suggested for millimeter wave applications where ohmic losses are no longer negligible [121]. Finally, other applications include ground penetrating RADAR and its use as an array element [122, 123].

The dielectric rod antenna is usually fabricated with a circular or rectangular cross section, where its propagating field configuration is primarily dictated by its feed’s field configuration; a metallic rectangular or circular waveguide feed is usually used depending on the desired mode. There are a few other excitation variations which include a helix wound around the dielectric rod antenna, an aperture coupled excitation, and a dipole coupled excitation[6-8], to name a few, but metallic waveguide feeds have been the most prevalent.

The design of the DFE requires consideration of the far-field radiation pattern, as for a traditional dielectric rod antenna, as well as the near-field interaction with the excitor/feed antenna. Far-field gain is optimized by controlling the cross sec-
tion, permittivity and length of the structure while the near-field consideration is
done by controlling the coupling aperture section’s (E-plane sectoral horn section)
flare angle. The excited mode, TE_{11}^z, with reference to Fig. 10.1(a), in the DFE
is well suited for coupling to and from an annular ring DRA that is resonating
in its electric monopole TM_{010+δ} mode. Efficient coupling is achieved due to the
co-polarized near fields of the DFE and annular ring DRA.

10.2 Dielectric Field Enhancer

In a traditional dielectric rod antenna, the length of the guided region dictates
the achievable gain of the antenna, as mentioned in [124], [119], for a given cross
section and permittivity. The objective is to design a DFE, with a certain gain,
that will provide the maximum achievable coupling to an annular ring DRA.

The DFE was designed in two steps. First, using the phase velocity versus cross
sectional dimension design curves in [124], a rectangular cross section dielectric
rod was designed. This portion of the design consisted of a free space to dielectric
impedance transforming terminal taper and a waveguiding section. The above
is done to insure a well coupled and guided mode in the dielectric rod. The
terminal taper dimension of slightly greater than half a wavelength was found
to be sufficient in our simulations for good coupling. As a starting point, an
assumed gain of 16 dBi for a traditional rod antenna was made and the cross
sectional dimensions were acquired from [124]. A cross-linked polystyrene is used
for the dielectric with permittivity of 2.6, and a loss tangent of 0.0007. This results
in a square cross-section having a side of 9.7 mm at 10.45 GHz. The length of the
guided region based on the dielectric permittivity, desired gain and cross section
comes out to be 143.5 mm (5λ_0).

It is mentioned in [124] that a feed taper and body taper are included after the
waveguiding section in a typical dielectric rod antenna for an efficient transition
Figure 10.2: Field distribution at the center of the dielectric rod along the axis for three different configurations.
from the exciting source, typically, a metallic waveguide and to suppresses side lobes, respectively. However, in the present scheme, the other end of the DFE was designed to have an E-plane flare similar to those described in [125]. This allows for control of the near field for near-field coupling to the DRA. A flare length of 1.25$\lambda_0$ and flare angle of 12.5 degrees were chosen based on the desire to maximize achievable near-field strength for the given guide length and cross section acquired from step 1. The E-flared section provides an impedance mismatch between its face and free space where a reflected wave is generated in the rod. Fig. 10.2 shows three simulation results for the field distribution at the center of the dielectric rod along the axis. The various configurations for the end-section highlight the need for the E-flared section. We will compare case 1 with a tapered section, case 2 with a non-tapered section, and case 3 with a flared section. The simulations consist of a plane wave incident upon the terminal taper of the DFE. In case 1, the field amplitude of the guided propagating wave is seen to grow along the length of the guide due to the continuous coupling of the incident plane wave to the guide. The field amplitude then decays in the taper, where the guided wave is slowly impedance matched to free space. In case 2, a flare angle of 0 degrees is introduced and a resulting increase in the electric field at the face of the end-section is noted. The resulting field distribution in the guide shows a periodic variation along the length of the guide with a period of $\sim$12.75 mm ($\lambda_g/2$); $\lambda_g$ is the guided wavelength for the TE_{11} mode in the guide where the propagation constant of $\beta_z=246$ rads/m in the axis direction is obtained using Marcatili’s method [126]. In case 3, a flare angle of 12.5 degrees is introduced. A similar periodic variation in the field distribution of the guided mode exists, while the electric field at the face of the end-section is higher than that of case 2. The increase in the electric field at the face for case 2 and 3 relative to case 1 is due to a mismatch between the face and free space, where a field distribution much like a standing wave is generated. Therefore, with a flare angle of 12.5 degrees,
a strong field at the face can then be near-field coupled to the DRA. The final dimensions of the DFE are shown in Fig. 10.1(b). Traditionally, dielectric rod antennas are considered travelling wave antennas, however in this case, the DFE in such a configuration can certainly be considered unique in the sense that it is a traveling/standing wave hybrid structure.

### 10.3 Measurements and Discussions

To verify the field enhancing capability of the DFE, a measurement in the microwave was conducted. An annular ring DRA operating in the electric monopole $\text{TM}_{010+\delta}$ mode was fabricated [127], [128]. A ground plane for the annular ring DRA much smaller than a wavelength was selected so as to allow for close coupling between the annular ring DRA and DFE, which then leads to a radiation pattern that is not exactly that of an ideal monopole, as will be shown. Following this approach, an annular ring DRA, as shown in Fig. 10.3, with permittivity of 43, height of 3.45 mm ($0.12\lambda_0$), radius of 3.05 mm ($0.11\lambda_0$), center cutout radius of 0.815 mm ($0.03\lambda_0$), and ground plane radius of 6.45 mm ($0.22\lambda_0$) was designed.

![Figure 10.3: $\text{TM}_{010+\delta}$ mode monopole DRA reflection coefficient and its millimeter dimensions shown in the inset.](image)
and fabricated to verify the simulations. The designed resonant frequency was 10.35 GHz. After fabrication and measurements, it was found to have resonated at 10.45 GHz. With this information, the design for the DFE discussed above (CH. 10.2) was then made to center around 10.45 GHz. Fig. 10.3 shows the simulated and measured reflection coefficient for the electric monopole \( \text{TM}_{010,+} \) mode annular ring DRA, which was coaxially excited. The results are in close agreement, with only a 100 MHz, or 1% shift in frequency. The shift could be due to a small chip on the cylindrical DRA created during the machining process, some possible air gap between the DRA and the ground plane as mentioned in [129], [130], or a difference in the reported relative permittivity due to manufacturer tolerances. The \( H \) (xz plane) and \( E \)-plane (yz plane) radiation patterns of the DRA are illustrated in Fig. 10.4 and as expected, resemble those of a monopole, but with a noticeable amount of scalloping due to the finite ground plane. The simulated gain of the monopole DRA is 1.5 dBi and the maximum measured gain is 1.30 dBi. The slight difference in gain and radiation pattern is most likely due to the mentioned imperfections. However, the point of interest is the relative increase of the gain and its resulting radiation pattern after the inclusion of the DFE and hence this annular ring DRAs characteristics are adequate.
After verifying the annular ring DRA’s performance, the DFE was then closely coupled, namely, 4 mm away. Fig. 10.5 illustrates the test setup with the annular ring DRA and the DFE, which is supported by a styrofoam stage. The results qualitatively followed the simulations. For example, at a 4 mm coupling distance, the measured gain is 9.07 dBi, giving a gain increase of 7.77 dB (compared to the measured gain of the monopole excited DRA alone). From simulations, at a 4 mm coupling distance, the gain with and without the DFE were 10.64 dBi and 1.5 dBi respectively. Therefore, a simulated difference of 9.14 dB was predicted. The difference between the simulated difference, 9.14 dB, and measured difference, 7.77 dB, is 1.37 dB.

Figure 10.4: TM<sub>010±δ</sub> mode monopole DRA (a) H-plane and (b) E-plane far-field gain patterns. Simulated cross polarization in both cases is extremely small.
7.77 dB, could be attributed to a possible misalignment between the DRA and the DFE. The gain was found, in simulations, to be sensitive to the relative positioning (parallelism) of the annular ring DRA to the DFE. Additionally, the loss in the polystyrene may be higher than expected leading to a smaller increase in gain from the DFE.

Figure 10.5: Measurement setup of DFE coupling to the TM_{010+\delta} mode monopole DRA.

To ensure a fair comparison, it is important to note that a decrease in power illuminating the antenna under test (the annular ring DRA, DFE combination) was made relative to the power level used for the annular ring DRA only system. Namely, the signal generator output level was decreased with the addition of the DFE to ensure that the plane wave incident on the DRA, DFE combination had the same power density as the case with only the annular ring DRA. Fig. 10.6 details the H (xz plane) and E-plane (yz plane) cuts. For both cuts, it is interesting to note that the radiation pattern is a hybrid of the directional pattern of the DFE and the pattern of the annular ring DRA. The half-power beamwidth (HPBW) in the H-plane is measured to be \(~18\) degrees compared with the simulation of \(~19\) degrees. The HPBW in the E-plane is measured to be \(~18\) degrees compared with the simulation of \(~21\) degrees. In both planes, the measured and simulated HPBWs are in close agreement with simulations.
10.4 DFE and Cylindrical DRA Combination Without Metallization

Fig. 10.7 illustrates the simulation setup used to quantify the extra field enhancement that could be achieved within a stand-alone (no metallization) DRA similar to the one used in the ADNERF system [116]. The excited mode of the DFE has an electric field component that is co-polarized with the near field distribution of the $\text{TM}_{010+\delta}$, cylindrical DRA. The near-field distribution of the co-polarized
Figure 10.7: Electric field distribution of DRA and dielectric rod antenna.

Figure 10.8: Electric field z component in the cylindrical DRA and theoretical change in minimal detectable power level given by equation 1 for a given coupling distance.
electric field component $E_z$ of the DFE is used to predict the increase in electric field within the cylindrical DRA. For example, for a plane wave excitation of 1 V/m incident upon the terminal taper of the DFE, the simulated near-field $E_z$ component is 4.67 V/m at a distance of 4 mm from the aperture of the E-flared section, translating to an increase of 13.39 dB. The difference in enhanced field intensity in the cylindrical DRA before and after the addition of the DFE is clearly seen by looking at the $E_z$ component. The $E_z$ component distribution for the TM$_{010+4}$ mode is a Bessel function distribution [127]. Fig. 10.8 shows the increase in the $E_z$ component at the center of the DRA due to the DFE. The increased field enhancement $\beta$, which is defined as the ratio of DRA-enhanced field strength to the incident free-space field gives an improved minimal detectable power level compared to the stand-alone DRA case. In [117], the minimal detectable power level is given by

$$P_{\text{min}} \propto \frac{1}{\beta^2}. \tag{10.1}$$

For a 2 mm and 7 mm coupling distance, a theoretical relative improvement in minimal detectable power level of 13.64 dB and 11.06 dB, respectively, is expected.

### 10.5 Conclusion

Through the use of numerical simulations and measurements, a DFE is shown to be an effective field enhancing passive element that can be used for radiation pattern modification and gain enhancement. An annular ring DRA was used to help characterize and verify the characteristics of the DFE. By characterizing the realized gain of the annular ring DRA before and after the addition of the DFE, it was concluded that the DFE changed the omnidirectional radiation pattern to that of a directional pattern. The directional field pattern was also found to have increased gain in the main lobe, which can be interpreted as a field enhancement.
within the DRA when illuminated by a plane wave in the same direction as the main lobe. The DFE demonstration here centered about the resonant frequency of the DRA, however, the DFE can potentially be used for applications with larger bandwidth requirements.

Although, the only mode discussed is a $\text{TM}_{010+\delta}$ in the DRA, different mode profiles and DRA geometries could possibly be used. The coupling between the DFE and the DRA is primarily determined by the matching of the polarization between the DRA and the DFE. For example, if a $\text{TE}_{010+\delta}$ mode cylindrical DRA is used, the DFE can efficiently couple to the DRA by rotating the DRA such that its electric field component is co-polarized to that of the DFE. With the above in mind, a variety of other non dielectric based antennas could be used as well.
APPENDIX A

Appendix

A.1 Far-Field Expressions

Following the treatment of Balanis [75], the far-field integral expressions are given as

\[ A = \frac{\mu}{4\pi} \int_S J_s \frac{e^{-jkR}}{R} \, ds' \simeq \frac{\mu e^{-jkr}}{4\pi r} N \]  
(A.1)

\[ N = \int_S J_s e^{jk'r'\cos\psi} \, ds' \]  
(A.2)

\[ F = \frac{\epsilon}{4\pi} \int_S M_s \frac{e^{-jkR}}{R} \, ds' \simeq \frac{\epsilon e^{-jkr}}{4\pi r} L \]  
(A.3)

\[ L = \int_S M_s e^{jk'r'\cos\psi} \, ds' \]  
(A.4)

where we have defined our closed surface to extend conformally over the surface of the MM waveguide cavity and ground plane. \( \psi \) is the angle between the vector \( r \) and \( r' \). \( A \) is the magnetic vector potential induced by an electric current \( J_s \) and \( F \) is the electric vector potential induced by a magnetic current \( M_s \). The E field components in the far-field can then be written as:

\[ E_r \simeq 0 \]  
(A.5)
\[ E_\theta \simeq \frac{-jke^{-jkr}}{4\pi r} (L_\phi + \eta N_\phi) \quad (A.6) \]

\[ E_\phi \simeq \frac{jke^{-jkr}}{4\pi r} (L_\theta - \eta N_\phi). \quad (A.7) \]

A.2 Analytic Quality Factor Expressions

The cavity model can be used to derive analytic expressions for the radiative quality factor for FP modes in a MM waveguide cavity under certain limiting conditions. For a cavity of width \( w \), height \( h \) and length \( \ell \), as shown in Fig. 4.1, we consider the radiation from the mode when \( h \ll \lambda_0, \ w \ll \lambda_0, \) and \( \ell \gg \lambda_0 \).

As shown in detail in [80], and when \( h \ll \lambda_0 \), the edges of the MM waveguide ridge act as nearly ideal open terminations. Additionally, a uniform or perfect half sinusoid is assumed for the TM\(_{00}\) and TM\(_{01}\) lateral field profiles, respectively. Under these conditions the necessary integrals simplify.

The tangential electric fields at the surface are used to obtain the equivalent magnetic currents \( M_s = -2\hat{n} \times \mathbf{E} \) which in turn enters into the expressions for \( L \) given in (A.4), and in turn is used to calculate the far-field radiated power \( P_{rad} \).

We calculate the radiative quality factor by considering the ratio of the stored electromagnetic energy within the cavity to the total radiated power integrated over the far-field half-space over the ground plane:

\[ Q = \omega \frac{\iiint_{\text{cavity}} \frac{1}{2} \varepsilon |\mathbf{E}|^2 dV}{\int_0^{\pi} d\phi \int_0^{\pi} d\theta r^2 \sin \theta P_{rad}(\theta, \phi)}. \quad (A.8) \]

We use this to obtain expressions for the quality factor due to radiation separately from the facets or sidewalls, in either the TM\(_{00}\) or TM\(_{01}\) lateral modes:

\[ Q_{\text{facets,00}} = \frac{3}{8} \frac{\varepsilon_r \ell \lambda_0}{hw}, \quad (A.9) \]
\[ Q_{\text{facets},01} = \frac{15\pi^2 \varepsilon_r \ell \lambda_0^3}{256 h w^3}, \]  
(A.10)

\[ Q_{\text{sides},00} = \frac{\varepsilon_r \ell \lambda_0}{h w f_0(n_{\text{eff}})}, \]  
(A.11)

\[ Q_{\text{sides},01} = \frac{\pi^2}{4} \frac{\varepsilon_r w \ell}{h \lambda_0 f_1(n_{\text{eff}})}, \]  
(A.12)

where

\[ f_0 = 5n_{\text{eff}}^2 - \frac{13}{3} - \frac{1}{n_{\text{eff}}} \tanh^{-1} \left( \frac{1}{n_{\text{eff}}} \right) (5n_{\text{eff}}^2 - 1)(n_{\text{eff}}^2 - 1), \]  
(A.13)

and

\[ f_1 = \frac{3n_{\text{eff}}^2 - 1}{n_{\text{eff}}} \tanh^{-1} \left( \frac{1}{n_{\text{eff}}} \right) - 3. \]  
(A.14)

In these expressions, \( \varepsilon_r \) is the relative permittivity of the cavity dielectric, and \( n_{\text{eff}} \) is the effective index of the propagating mode. It should be noted that the expressions for \( Q_{\text{sides}} \) given above are only valid when \( n_{\text{eff}} > 1 \). For \( n_{\text{eff}} < 1 \), i.e. a hypothetical CRLH MM waveguide operating in the TM\(_{00}\) mode,

\[ Q_{\text{sides},00} = \frac{\varepsilon_r \lambda_0^2}{4\pi^2 h w \sin^4(\cos^{-1}(n_{\text{eff}}))}. \]  
(A.15)

For a MM waveguide in the TM\(_{01}\) mode

\[ Q_{\text{sides},01} = \frac{\varepsilon_r w}{4h(1 - n_{\text{eff}}^2)}. \]  
(A.16)

For a Fabry-Pérot cavity characterized by counter-propagating modes with group velocity \( \nu_g \), we can relate the radiative Q to the power attenuation coefficient \( \alpha \) using the relation

\[ \alpha = \frac{\omega}{Q \nu_g}. \]  
(A.17)
A.3 Circuit Model Dispersion Eigensolver

The asymmetric CRLH design of Fig. 6.6(b) has a unit cell circuit model from transmission line theory given by Fig. A.1. The structure can be interpreted as two transmission lines coupled together through the distributed inductance $L_L$. The meander design is effectively comprised of two subcells, where each subcell is 8 $\mu$m long. For the first subcell, the eigenvalue problem describing the voltage and current through the left and right branch are given as

$$
\begin{bmatrix}
V_{LB\ text{cell }1,\text{out}} \\
I_{LB\ text{cell }1,\text{out}} \\
V_{RB\ text{cell }1,\text{out}} \\
I_{RB\ text{cell }1,\text{out}}
\end{bmatrix} = [T1] \begin{bmatrix}
V_{LB\ text{cell }1,\text{in}} \\
I_{LB\ text{cell }1,\text{in}} \\
V_{RB\ text{cell }1,\text{in}} \\
I_{RB\ text{cell }1,\text{in}}
\end{bmatrix}
$$

(A.18)

where $T2$ for the second subcell would also take the same form. For the 16 $\mu$m unit cell (both subcells together), we have

$$
\begin{bmatrix}
V_{LB\ text{cell }2,\text{out}} \\
I_{LB\ text{cell }2,\text{out}} \\
V_{RB\ text{cell }2,\text{out}} \\
I_{RB\ text{cell }2,\text{out}}
\end{bmatrix} = [T2][T1] \begin{bmatrix}
V_{LB\ text{cell }1,\text{in}} \\
I_{LB\ text{cell }1,\text{in}} \\
V_{RB\ text{cell }1,\text{in}} \\
I_{RB\ text{cell }1,\text{in}}
\end{bmatrix}.
$$

(A.19)
Figure A.2: Comparison between circuit model eigensolver and HFSS

where $T_1$ and $T_2$ combine to give

$$
\begin{bmatrix}
1 + \left( \frac{B_1}{T_1} + \frac{C_1}{T_1} \right) & -(A_1 + B_1 + \frac{A_1 B_1}{T_1} + \frac{A_1 C_1}{T_1}) & -(\frac{B_1}{C_1}) & \frac{A_1 B_1}{T_1} \\
-(\frac{1}{T_1}) & (1 + \frac{A_1}{T_1} + \frac{C_1}{T_1}) & (\frac{1}{T_1}) & -(\frac{2}{T_1}) \\
-(\frac{C_1}{T_1}) & -\left( \frac{A_1 C_1}{T_1} \right) & (1 + \frac{C_1}{T_1} + \frac{C_1}{T_1}) & -(C_1 + D_1 + \frac{C_1 D_1}{T_1}) \\
(\frac{1}{T_1}) & -(\frac{A_1}{T_1}) & -(\frac{1}{T_1}) & (1 + \frac{B_1}{T_1} + \frac{D_1}{T_1})
\end{bmatrix}.
$$

The equivalent impedance and admittances are given below.

$$A_1 = j\omega(0.25L_R)$$

$$B_1 = C_2 = D_2$$

$$C_1 = j(\omega(0.25L_R) - \frac{1}{\omega 2C_L})$$

$$D_1 = A_2 = B_2$$

$$Y = j\omega(4L_L)$$

$$Z = \frac{1}{j\omega(0.5C_R)}$$
The eigensolver’s predicted dispersion for the TM$_{00}$ and TM$_{01}$ waveguide mode for the unit cell in Fig. 6.6(b) is shown in Fig. A.2. There is close agreement between the eigensolver and HFSS simulation for the TM$_{01}$ mode. For the TM$_{00}$ mode, the eigensolver predicts a series resonant frequency that coincides with the series resonant frequency for the TM$_{01}$ mode. However, HFSS simulations predicted a higher series resonance (not shown in figure). The discrepancy is due to the difference in field profile between the two modes. The actual effective capacitance for the TM$_{00}$ mode is less than that of the TM$_{01}$ mode given the lateral variation of the field profile. Nonetheless, the dispersion for the mode of interest TM$_{01}$, is well described by the eigensolver and a qualitative trend is obtained.

A.4 Drude Model Implementation

The bulk Drude model was used in our simulations to model the free carrier loss in the active region as previously done in [13, 14]. The following implementation is adopted from [63, 131, 132]. Ansys’ HFSS uses the electrical engineering convention $e^{j\omega t}$ where the complex permittivity is given by

$$\epsilon(\omega) = \epsilon'(\omega) - j\epsilon''(\omega) = \epsilon_0\epsilon'_r(\omega) - j\epsilon_0\epsilon''_r(\omega) = \epsilon'(\omega) - j\frac{\sigma(\omega)}{\omega}. \quad (A.28)$$

Using Drude’s model for conductivity

$$\sigma(\omega) = \frac{ne^2\tau}{m^*(1+j\omega\tau)} \quad (A.29)$$
and plugging it into Eq. A.28 we get the relative permittivity

\[
\frac{\epsilon(\omega)}{\epsilon_0} = \epsilon_{r,\text{core}} - \frac{\omega_p^2 \tau^2}{(1 + \omega^2 \tau^2)} - j \frac{\omega_p^2 \tau}{\omega(1 + \omega^2 \tau^2)}
\]

\[
= \frac{\epsilon'(\omega) - j \epsilon''(\omega)}{\epsilon_0}
\]

(A.30)

where \(\epsilon_{r,\text{core}} = 12.9\) for GaAs and \(\omega_p = \frac{ne^2}{m^*\epsilon_0}\) is the plasma frequency. The loss tangent that accounts for free carrier loss is then given as

\[
\tan\delta = \frac{\epsilon''(\omega)}{\epsilon'(\omega)} = \frac{\epsilon''(\omega)}{\epsilon_r(\omega)} = \frac{\frac{ne^2}{m^*(1+\omega^2\tau^2)}\omega_0}{\epsilon_r(\omega)}
\]

(A.31)

We then add the term for material gain. From [131, Chapter 8] we have the electric displacement vector

\[
D = \epsilon_0(E) + P + P_{\text{trans}} = \epsilon \left[ 1 + \frac{\epsilon_0}{\epsilon} \chi(\omega) \right] E
\]

\[
= \epsilon'(\omega)E
\]

(A.32)

where \(\epsilon = \epsilon_0\epsilon_r\). The polarization has been separated into two parts: \(P_{\text{trans}}\) represents the resonant component due to an atomic transition and \(P\) is due to all other contributions to the polarization. \(\chi = \chi' - j\chi''\) is the complex electric susceptibility found via a density matrix derivation in [131]. Assuming some propagating wave in a medium with complex permittivity given by Eq. A.28, it will have a
wavevector given by

\[ k' = \omega \sqrt{\mu \epsilon} \]

\[ \approx k(1 + \frac{\epsilon_0}{2\epsilon}) \]

\[ \approx k \left[ 1 + \frac{\chi}{2n^2} - j \frac{k \chi''(\nu)}{2n^2} \right] \tag{A.33} \]

where it is assumed that \(|\chi| \ll 1\) and \(k = \omega \sqrt{\mu \epsilon}\). The forward propagating plane wave then takes the form

\[ E(z, t) = \text{Re}[E_0 e^{j\omega t - j(k+\Delta k)z + (\gamma/2)z}] \tag{A.34} \]

where there is a phase shift and amplitude decay due to the atomic polarization.

The amplitude decay is given by the attenuation coefficient \(\gamma(\nu) = \frac{-k \chi''(\nu)}{\nu^2}\). By treating the attenuation coefficient as a positive number, we effectively have a gain coefficient and solving for the imaginary part of the susceptibility gives

\[ \chi'' = \frac{n^2 G}{k} \]

\[ = \frac{n^2 G}{n\omega/c} \]

\[ = \frac{n_r G c}{\omega} \tag{A.35} \]

The loss tangent then becomes

\[ \tan \delta = \frac{n_r^2 \epsilon_r}{m^* \epsilon_r \omega(1+\omega^2/\tau^2)} - \frac{\epsilon_0 \chi''}{\epsilon_0} \]

\[ = \frac{n_r^2 G c \epsilon_0}{\epsilon_0 \omega(1+\omega^2/\tau^2)} + \frac{\omega^2 \tau^2}{1+\omega^2/\tau^2} \tag{A.36} \]
Figure A.3: For GaAs with a dopant level of $5 \times 10^{21}$ (m$^{-3}$), the plasma frequency is $\sim 0.5$ THz. The (a) relative permittivity and (b) loss tangent using Drude’s model shows a non-negligible difference compared to HFSS. HFSS’s library definition for GaAs is by default lossless. Inset is a zoomed in view.

Fig. A.3 shows a comparison between the HFSS library definition for GaAs and the Drude model.

Ohmic losses in the metallization were captured by the conductivity. From Ampere’s equation, we can represent loss through the conductivity.

$$\nabla \times \mathbf{H} = \mathbf{J} + j \omega \mathbf{D}$$

$$= \sigma(\omega)\mathbf{E} + j \omega \varepsilon(\omega)(\mathbf{E})$$

$$= j \omega \varepsilon(\omega)\mathbf{E}$$

$$= (j \omega \varepsilon'(\omega) + \omega \varepsilon'')(\mathbf{E})$$

$$= \omega \varepsilon''(\omega)\mathbf{E} + j \omega \varepsilon'(\omega)\mathbf{E} \tag{A.37}$$

$$\sigma = \omega \varepsilon''(\omega)$$

$$= \omega \left( \frac{\omega_p^2 \tau \varepsilon}{1 + \omega^2 \tau^2} \right)$$

$$= \frac{ne^2}{m^* (1 + \omega^2 \tau^2)} \tag{A.38}$$
The material definitions and parameters used for the HFSS simulations are given in Table. A.1 and Table. A.2. A comparison between the HFSS library defined gold, which assumes DC conductivity of $\sigma=4.1e7$ S/m versus the Drude model is shown in Fig. A.4.

Figure A.4: (a) Relative permittivity and (b) conductivity of gold. HFSS library definition for gold has a frequency independent conductivity $\sigma=4.1e7$ S/m.

Table A.1: Summary of Expressions used in HFSS

<table>
<thead>
<tr>
<th>Material</th>
<th>$\epsilon_r$</th>
<th>$\sigma$</th>
<th>$\tan\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>$\Re$(Eq. A.30)</td>
<td>0</td>
<td>Eq. A.31</td>
</tr>
<tr>
<td>GaAs w/ Gain</td>
<td>$\Re$(Eq. A.30)</td>
<td>0</td>
<td>Eq. A.36</td>
</tr>
<tr>
<td>Gold</td>
<td>$\Re$(Eq. A.30)</td>
<td>Eq. A.38</td>
<td>0</td>
</tr>
</tbody>
</table>
Table A.2: Material Parameters. *Where not explicitly stated, these lifetimes were used in simulations.

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Gold</th>
<th>GaAs/AlGaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carrier density, $D$ (m$^{-3}$)</td>
<td>5.9e28</td>
<td>5e21</td>
</tr>
<tr>
<td>Effective mass, $m^* = m_0 m_e$ (kg)</td>
<td>(9.11e-31)(1)</td>
<td>(9.11e-31)(0.067)</td>
</tr>
<tr>
<td>Drude Relaxation lifetime, $\tau$ (fs)</td>
<td>17 @295 K, 39 @77 K [95]*</td>
<td>500 @77K</td>
</tr>
<tr>
<td>Relative Permittivity, $\epsilon_{r,core}$</td>
<td>1</td>
<td>12.96</td>
</tr>
<tr>
<td>Charge, $q$ (C)</td>
<td>1.6e-19</td>
<td>1.6e-19</td>
</tr>
</tbody>
</table>

A.5 Ottocoupling Experimental Setup

Polyethylene (HDPE) was chosen as the prism material for its low loss in the THz and ease of fabrication (easily machinable, yet rigid). A $\sim$1 cm$^{-1}$ power attenuation coefficient around 2.7 THz was extracted from a transmission spectra measurement of a 0.125 inch slab of polyethylene (Fig. A.5). The measured power transmission was fitted to the magnitude squared of the field transmission coefficient for a single slab which is given by [133, Chapter 13]

$$T_{\text{slab}} = \frac{T_{12} T_{23} e^{-\gamma_2 d} e^{-\gamma_3 d}}{1 + \Gamma_{12} \Gamma_{23} e^{-2\gamma_2 d}}$$  (A.39)

where the subscripts 1 and 3 correspond to air and 2 is the polyethylene. The extracted permittivity (Fig. A.6) and loss (Fig. A.7) agree well with those reported in literature [134, 135]. A tradeoff study involving the transmission loss through the prism, beam walk off and prism size concluded that the optimal prism size to be 1 cm $\times$ 1 cm with a 90° apex angle. Fig. A.8 is a schematic of the measurement setup.
Figure A.5: Measured and fitted power transmission through a 0.125 in slab of polyethylene (HDPE). A moving average was applied to smooth out the Fabry Pérot oscillations due to the thickness and smooth polish of the slab. The oscillations are seen in the analytically fitted data.

Figure A.6: Extracted permittivity from the fitted data.
Figure A.7: Transmission measurement extracted power attenuation coefficient and loss tangent.
Figure A.8: (a) Diagram of the FTIR reflection spectroscopy setup with the Ottocoupling setup. (b) Top view photograph of the components in the purge box; featured without the detector and micrometer translation stage that moves the device sample to achieve different coupling distances with the HDPE prism. (c) Top view photograph of the micrometer translation stage along with the HDPE prism.
Figure A.9: (a) Diagram of the active reflector FTIR reflection spectroscopy setup for both continuous and step scanning. A (b) top down and (c) front view of a portion of the experimental setup.

THz radiation from the FTIR’s blackbody source traverses through a Tydex high resistivity float zone (HRFZ) silicon beam splitter with 52% transmittance. The transmitted THz beam is focused onto the sample with a three inch focal length off axis parabola (OAP). The device reflected THz beam is then focused onto the Ge:Ga photodetector with a four inch focal length OAP. Translation stages in x, y and z directions were used to achieve fine alignment of the device dewar/cryostat.
Two types of measurements were conducted: step and continuous spectrum scans. For step scans, the lock-in amplifier integration time was set to one second and the bias repetition rate was set to 10 KHz. For continuous scans, the FTIR mirror velocity was set to 0.4747 cm/s with a 30 sample average and 2 cm\(^{-1}\) resolution.
References


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