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Investigation of Phonon Polaritons in an hBN GaN Heterostructure

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Investigation of Phonon Polaritons in an hBN GaN Heterostructure

Catherine G. O'Hearn

Thesis submitted to the
Benjamin M. Statler College of Engineering and Mineral Resources
at West Virginia University
in partial fulfillment of the requirements for the degree of

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in
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Abstract

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Catherine G. O'Hearn

There have been many great advances in the generation and manipulation of optics in the visible and near infrared (IR) range over the past decade. This is largely due to plasmonic enhancement, which has led to new technology in biosensing and molecule detection, solid-state lighting, and solar energy harvesting. The field of plasmonics uses quanta of plasma oscillations, plasmons, formed from the interaction between electromagnetic radiation and free electrons to enhance optical near field magnitudes. However, there is still a large region of the electromagnetic spectrum, covering the mid-infrared (MIR) and terahertz (THz) regions, ranging from 3 μm to 1 mm, that has not benefitted from this research. Polaritonics have recently gained attention from the scientific community to access this region and enhance current technologies. Polaritons are an IR alternative to plasmons; these quasiparticles are formed from light coupling to an elementary material excitation, such as phonons, plasmons, magnons, or excitons.

In this project, we look at the past, present, and future of terahertz technology and the role phonon polaritons play in their advancement. A hexagonal boron-nitride/gallium nitride superlattice is examined through simulated reflection experiments to identify phonon polariton modes.

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Chapter 1: Introduction

There have been many great advances in the generation and manipulation of optics in the visible and near infrared (IR) range over the past decade. This is largely due to plasmonic enhancement, which has led to new technology in biosensing and molecule detection, solid-state lighting, and solar energy harvesting. The field of plasmonics uses quanta of plasma oscillations, plasmons, formed from the interaction between electromagnetic radiation and free electrons to enhance optical near field magnitudes. However, there is still a large region of the electromagnetic spectrum, ranging from 3 μm to 1 mm (covering the mid-infrared (MIR) and terahertz (THz) regions), that has not benefitted from this research. Polaritonics have recently gained attention from the scientific community to access this region and enhance current technologies. Polaritons are an IR alternative to plasmons; these quasiparticles are formed from light coupling to an elementary material excitation, such as phonons, plasmons, magnons, or excitons. These quasiparticles are lighter than electrons and of bosonic nature, making them ideal candidates for realizing Bose-Einstein condensation at higher temperatures [1], [2], extending THz laser source options[3], and emitting optical phonons [4].

For this thesis, a simple multi-quantum well (MQW) design consisting of hBN and GaN was employed to analyze intersubband phonon-polaritons. While there is a new wave of research on phonon-polaritonics and the applications of the unique properties of hBN, this fascinating material has yet to be employed in such a structure. This work aims to contribute to the field of phonon-polaritonics to allow for the generation of optical phonons coupled with an electromagnetic wave.

Self-consistent Schrödinger-Poisson calculation of the wave functions were performed in COMSOL. To determine the nature of the phonon-polariton dispersion in the structure, the reflection is plotted in ω -k space using rigorous coupled wave analysis software. The electric field within the structure were analyzed with the transfer matrix method.

1.1 Scope of Thesis

In the remaining chapter, a review of the limits of current technologies and the future of IR and THz technologies are presented. We reflect on our motivations for this project.

Chapter 2 is a Theoretical Review of the foundational pieces of the project. This includes the various polariton forms, phonon lasers, polariton lasers, and phonon-polariton lasers. Microcavity, interband, and intersubband IR and THz laser designs, challenges, and bottlenecks are discussed. Properties of the materials used in the heterostructure, hBN and GaN, are studied. Chapter 2 also reviews the equations used in the software to determine the wavefunctions and reflection data.

Chapter 3 describes the Simulation Environments used for this study. As this study is purely simulation based, all the experiment properties such as boundary conditions must be explicitly stated.

The simulation results are presented and discussed in Chapter 4. This will include the conduction band diagram, the probability density function, and the reflection in ω - k space.

The conclusion and future work for this project are discussed in the final chapter, Chapter 5. We give a review of the necessary calculations to determine a more accurate electronic structure. A plan for how to fabricate such a device and the obstacles that might be encountered along with the characterization experiments necessary to determine the phonon and polariton properties are presented.

1.2 Applications

As mentioned previously, we would like to see our work lead to the design of a phonon-polariton laser consisting of an hBN heterostructure. Here we give an overview of its applications in industry and research. The past two decades has led to a boom in terahertz generation and detection research, however these tools are still under development [5]–[7]. The broad categories of terahertz sources are thermal sources, vacuum electronics, bound state sources, continuous laser driven sources, and pulsed laser sources [8].

Emitted polaritons could have a large fraction of their energy in the form of optical phonons and could also be considered a phonon laser. Due to the near zero group velocity of optical phonons, there are limited applications for a pure optical phonon laser [9], however a source coherent optical phonons would be useful in condensed-matter studies [10].

Figure 1.1 Electromagnetic spectrum highlighting the visible and terahertz range.

1.2.1 IR and Terahertz Spectroscopy

One unique form of infrared spectroscopy is based on light-matter interaction. This is known as surface-enhanced infrared absorption (SEIRA) spectroscopy and typically uses plasmonic structures such as gratings and nanoparticles. for light-matter coupling. However, one group replaced these plasmonic structures with hBN ribbons to enable phonon-polariton SEIRA spectroscopy [11]. Phonon-polariton spectroscopy could assist in closing the gap in plasmonic enhanced spectroscopy.

The most popular form of tabletop THz spectroscopy is Time Domain Spectroscopy (TDS). In TDS, the emitter and detector are synchronized as they use the same laser pulse train. TDS detects the phase information of the electric field, which is lost when only the amplitude is measured. The pattern produced by the interferometer (the instrument used to bring the split beam back together) is the Fourier transform of the spectrum [8]. Other popular forms are time-resolved THz spectroscopy (TRTS) and THz emission spectroscopy (TES). Through the simultaneous pump-probe set-up of TDS, it measures the static properties. In contrast, TRTS measures the dynamic properties by measuring the time-dependent spectra with a delay from the ultrafast laser pump pulse. TES uses a pulsed source to irradiate the sample and the detector gathers the amplitude and shape of the transient electric field emitted from the sample [5]. Terahertz spectroscopy is an important tool in molecular biology, explosives detection, drug characterization, quality control of paper, leather, food products [6].

1.2.2 Terahertz Tomography

Tomography is an essential aspect of nondestructive testing; however new methods are needed to keep up with the ever-evolving materials of industry. X-rays are the most used electromagnetic region used in tomography. Drawbacks to using X-rays include its ionizing

capabilities, making it harmful to living creatures, and that many materials are transparent to its rays. Microwave imaging systems exist; however, these offer poor resolution due to the long wavelength [12].

Aside from a small range of THz source options, extracting data from THz tomography has also presented challenges. Transmission data of the sample are gathered by placing the object between an X-ray source and detector; from this, mean absorption coefficients are reconstructed from calculating the ray attenuation. Conventional computed tomography programs utilize the linear relationship between the density values, or absorption map, of a slice the device under test and the beam attenuation values to identify defects. However, THz waves do not follow the mostly straight path of X-rays as THz waves diverge faster, leading to more instances of refraction and reflection. Many manufactured materials begin from a CAD model; engineers used this knowledge to create a CT method based on the deviation of experimental THz tomography results from simulated THz tomography results based off a CAD file. New experimental and computational methods will allow for the expansion and wider use of THz tomography across industries [13].

1.2.3 Infrared Thermography

To be kinder to their wallet and environment, many organizations aim to update their buildings for increased energy efficiency. An initial step in this process is performing an energy audit. Infrared thermography can assist in the process to identify regions of inefficiency or malfunction in older buildings and in new buildings to verify design construction [14].

1.2.4 Electronics Fabrication

Terahertz lasers allow for the fabrication of laser induced periodic surface structures (LIPSS) an interesting feature that is useful in a variety of applications. These periodic structures are from self-induced polariton-laser interference [15], [16].

Figure 1.2 Laser induced periodic surface structures. [15]

LIPSS or ripple fabrication is often non-uniform over large regions due to multiple independent seed locations. Large area LIPSS can be employed as diffractive gratings enabling laser marking, anti-counterfeiting measures, and enhanced color displays. Surface plasmon polaritons have been frequently investigated in LIPSS formation, however surface phonon-polaritons exhibit a larger lifetime allowing for larger area fabrication [15].

Biomedical engineers have also found use for LIPSS in neuroelectrode design. Previous studies had indicated that topographical functionalization of electrodes can improve performance by limiting tissue encapsulation of the electrode caused host immune response to the foreign object. In a recent study by Kelly et al., the addition of LIPSS to electrodes showed reduced electrochemical impedance, increased the active surface, and increased the charge injection capacity in comparison to planar electrodes [17].

1.2.5 Superconductivity Research

Much of the fundamentals of superconductivity have yet to be understood. The first superconducting material operated at 4.2° Kelvin, or roughly -450°F, while recent high temperature superconductors operate up to 100°K, or -280°F [18]. These fascinating materials were first characterized by their ability to conduct an electric current perfectly, hence the name

“superconductor.” However, an equally important characteristic is perfect diamagnetism- when a magnetic field does not enter a superconductor. This is known as the Meissner effect [19].

Terahertz radiation has been used to alter the electronic and magnetic properties of a material in condensed-matter physics research. LO phonons coupling to electrons has been shown to be the cause of superconductivity in SrTiO_3 [20], specifically through phonons operating in the adiabatic regime [21]. The adiabatic regime refers to a system that does not lose energy in the form of heat, and all energy transfer is through work [22]. It has been predicted that optical phonon pumping of certain materials can have weak effects on their electronic properties and strong effects on the magnetic modes, which can have effects on superconductivity [10], [23]. To identify new materials for superconductivity it is important to understand the electronic and magnetic modes causing such effects. A source of coherent optical phonons would allow for such probing experiments.

1.3 Motivation

There are a limited range of terahertz sources and detectors, with few capable of operating in higher, near room-temperature conditions. Research in the strong-coupling and ultra-strong coupling regime has exploded in the past five years, with 249 articles from 2015-2020 found on Web of Science compared with the 147 articles from 2010-2014 when searching for “phonon polariton.” And while hBN has attracted some research due to its similarities to other popular research materials; graphene, black phosphorous, transition metal dichalcogenides; it has yet to be applied in a superlattice for light source and detection. While there are industrial applications for such a THz active region, future projects could lead to emission of electromagnetic radiation and phonons, a fascinating new category, of which there is only one [4].

Chapter 2: Theoretical Review

2.1 Important Quasiparticles

2.1.1 Phonons

Like all forms of energy, vibrational oscillations can be analyzed as a quantum particle, known as the phonon. Simple solids are represented by a single atom primitive cell and we analyze phonon propagation through these by determining the displacement from an equilibrium position and the restoring force by Hooke's law. The vibration of the atoms is represented by the dispersion equation and is related to the wave vector k by the following equation; where C is the force constant, m is the mass of the atom, and d is the equilibrium distance between atoms of adjoining primitive cells.

$$\omega(k) = 2 \sqrt{\frac{C}{m}} \left| \sin \left(\frac{kd}{2} \right) \right| \quad 2.1$$

For a more complex solid, we look at a two-atom primitive cell. As shown in the dispersion equation below, there are two possible solutions which produce the upper optical branch and the lower acoustic branch.

$$\omega^2 = \frac{2C(m_1+m_2) \pm \sqrt{4C^2(m_1+m_2)^2 - 8m_1m_2C^2(1 - \cos(kd))}}{2m_1m_2} \quad 2.2$$

$$\omega^2(k=0) = \begin{bmatrix} 2C \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \left(1 - \frac{k^2 d^2}{4} \right) & \text{optic} \\ \frac{C}{2(m_1+m_2)} k^2 d^2 & \text{acoustic} \end{bmatrix} \quad 2.3$$

There are two modes of operation for the two atoms in the primitive cell. When the atoms move in opposite directions, they follow the upper solution and are considered optical phonons; when the atoms move together in the same direction, they follow the lower solution and are considered acoustic phonons [24]. The acoustic phonons correspond to shear and compressive waves in a lattice. Optical phonons are furtherer split into transverse optical (TO) and longitudinal optical (LO) phonons due to their polarization. TO phonons oscillate perpendicular to the propagation direction and LO phonons oscillate parallel to the propagation direction [25].

2.1.2 Polaritons

A polariton is a quasiparticle caused by the coupling of a photon with a material excitation, such as excitons, plasmons, magnons, or phonons. When a system has large light-matter coupling it is operating in the strong-coupling regime, which occurs when the normalized coupling η is larger than the inverse quality factor of the light and matter resonances [3]. In the strong-coupling regime the light-matter interaction is shorter than the relaxation time of the system; meaning there is more time before relaxation is complete for the light-matter coupling [26].

The amount of light-matter coupling is determined by the Rabi frequency and Rabi splitting. Taking a photon and material excitation as two oscillators in a system, we consider the case when the quality factors are near to each other and examine their frequency dependency. If the eigenmodes of the system are superimposed, the oscillators beat at the Rabi frequency [27]. Rabi splitting is the separation between the normal modes at the anti-crossing point. Strong coupling occurs when the Rabi splitting is experimentally observable, or when the coupling is large enough so that the linewidths are clearly distinguished [28], [29]. A case of strong coupling or large Rabi splitting is shown in Figure 1.3 (a), while weak coupling is shown in Figure 1.3 (b).

Figure 2.1 (a) Strong coupling allowing for distinct separation between energy lines. (b) Weak coupling preventing clear separation of energy lines. Rabi splitting is the distance between the closest points of the energy lines. [28]

The polariton's light mass in comparison to other Bose-Einstein condensates enables quantum effects to appear at higher temperatures [1].

2.2 Phonon and Polariton Lasers

2.2.1 Phonon Lasers

The first phonon analog for the laser, or rather saser (sound amplification through stimulated emission of radiation), came far after the laser due to the nature of phonons. In

conventional lasers there are two requirements to reach emission into the lasing mode: the occupation of the mode reaches unity and population inversion [30]. This is generally done by a photon amplifier and a positive feedback circuit [31]. While their bosonic nature allows lasing, the large density of states causes difficulty in achieving gain. Furthermore, in the best-case scenario for phonon lasing (assuming the phonons have linear dispersion and states 1 and 2 are dispersionless), the threshold is orders of magnitude larger than for photon lasing. This is due to the lower velocity of sound, which also leads to a shorter mean free path [9].

In the case where an emitted LO phonon decays into an optic and acoustic phonon, or states A) and B), it was suggested that to maximize gain the densities of phonons N_A and N_B should be as far apart as possible [9]. This decay process is shown below in Figure 1.4 and was initially used in the design for acoustic phonon lasing in 1996 [32]. Most phonon lasers generate acoustic rather than optical phonons, this is due to the significantly larger energy of optical phonons coupled with the inability to meet the inversion requirements under quasistationary conditions makes achieving amplification difficult [33].

Figure 2.2 LO phonon emission process. [9]

A more recent proposal for optical phonon lasing utilized the same mechanism described above in Figure 1.4, placing the LO phonon at the Γ point and the decay at the L point. Here they proposed optical phonon lasing from an optically pumped double quantum dot (DQD) system. The DQD couples to two LO modes, and since these modes do not diffuse due to their small group velocity, it does not need a cavity or resonator [34], [35]. It was suggested that materials with

longer optical phonon lifetimes than GaAs be used in future designs, leading us to believe this DQD system would serve as suitable application for graphene or hBN.

Figure 2.3 Inversion condition for optical phonons. [33]

Rather than change the material, a novel optical phonon lasing design coupled a GaAs heterostructure to a surface array of metallic dog-bone resonators. As shown above in Figure 1.5, it is difficult to achieve gain while the electron distribution is centered around the Γ point, and rather performs absorption. Using a THz optical pump pulse the initial LO phonons are generated, and the electron distribution f_e is shifted allowing for $f_e(k) > f_e(k-q)$, thus fulfilling the inversion condition for gain [33].

2.2.2 Intersubband Polariton Lasers

In the previous sections we stated how polaritons are quasiparticles of light coupled with a material excitation. ISB transitions fundamental to QC structures can be one such material excitation, and when coupled with light is an ISB polariton [36]. Technically, “ISB transition” is clearly a verb, therefore not a material excitation quasiparticle; what the photons are coupling with is the ISB plasmon quasiparticle.

Figure 2.4 Conduction band diagram of a QCL structure with squared wave functions in the active area. [37]

Integral to conventional intersubband laser operation, such as quantum cascade lasers, are electron-phonon scattering. Electron-phonon scattering allows for efficient relaxation of the electron from level 2 into level 1, as shown in Figure 1.3. Only optical phonons polarized along electron the path are allowed, thus only allowing LO phonons [25]. A similar scattering pathway was employed in the initial proposal for the lasing ISB cavity polaritons. In the ISB polariton laser, a polariton is optically pumped into the upper polariton branch, relaxes via an LO phonon to the lower polariton state, from where coherent polaritons are emitted. This process is depicted in Figure 1.4, where n_2 is the polariton density of the upper polariton state, n_1 is the polariton density of the $k = 0$ polariton state, τ_{21} is the LO phonon assisted scattering time, and τ_{2NR} is the upper polariton lifetime [38].

In a recent demonstration of an optically pumped polaritonic device, experimental evidence of resonant ISB polariton-LO phonon coupling was found. The magnitudes larger ISB polariton-phonon scattering time τ_{21} in comparison to the electron-phonon scattering time in standard QCLs, indicates larger coupling and led researchers to believe this ISB polariton laser could serve as a coherent source of mid-IR light and LO phonons [39].

While the demonstration of an intersubband polariton laser has yet to come, we expect its imminent development as it would offer room temperature operation and higher output powers

than exciton-polariton lasers. This is due to the limiting factor of the Mott transition density in exciton-polariton lasers, above which excitons and polaritons are no longer bosonic in nature. Bosonic operation in ISB polariton lasers is not fixed and can be engineered via doping [38].

Figure 2.5 ISB polariton dispersion and phonon relaxation pathways in a MIM cavity. Solid blue lines are the polariton eigenmodes, while the green and red dashed lines are the bare cavity and ISB eigenstates. [38]

2.2.3 Phonon-Polariton Laser

There have been laser designs seeking to operate in the strong and ultra-strong regimes. Such designs include the previously discussed intersubband polariton lasers and those exploiting coupling between ISB electronic transitions and LO phonons, known as polarons.

Figure 2.6 Tripartite coupling for phonon-polariton laser operation. [40]

In a recent 2019 paper from the Faist group, employing a quantum cascade structure, the first phonon-polariton laser was developed. Their previous work laid the theoretical ground work for such a device by determining the necessary elements and calculating the gain equation in [40]. This laser operation is based on three distinct components: ISB transitions, TO phonons, and the optical cavity mode; this tripartite coupling is shown in Figure 1.8.

The light-matter coupling constant is provided in Equation 1.4, where ω_p is the phonon plasma frequency, f_a^0 is the filling factor of the cavity by the mechanical oscillators.

$$\Omega = \frac{\omega_p}{2} \sqrt{\frac{\omega_{cq}}{\omega_{LO}} f_a^0} \quad 2.4$$

To measure the phonon-photon coupling of the polariton we look at the Rabi coupling energy Ω_R .

$$\Omega_R = \frac{\omega_p}{2} \sqrt{f_a^0} \quad 2.5$$

We get the polariton dispersion by solving for equation 2.3,

$$\left(\omega^2 - (\omega_o^2 + \omega_p^2)\right)(\omega^2 - \omega_c^2) = f_p \omega_c^2 \omega_p^2 \quad 2.6$$

ω_c is the bare cavity frequency, ω_p is the plasma frequency associated with the phonon excitation having resonance energy $\hbar\omega_o$, f_p is the filling factor of the phonon-containing material in the cavity. The bare cavity frequency ω_c is given by

$$\omega_c - \omega_A = \frac{c}{n_g} \left(k - \frac{\omega_A n_{eff}}{c} \right) \quad 2.7$$

The AlInAs barriers served as the AlAs TO phonon source and confinement region. In both the resonant tunneling diode and QCL simulations, the gain was largely due to typical dipole coupling, however with design optimization, phonon coupling could play an even a larger role [40]. Such optimizations were enacted with their demonstration of an electrically pumped phonon-polariton laser. By coupling phonons to photons, the large density of states issue discussed in the Phonon Lasers section, is alleviated. Coupling of the particles decreases the density of states close to the anti-crossing point, reducing the threshold. [4].

2.3 Materials

2.3.1 Hexagonal Boron Nitride

The isolation of graphitic films in 2004 by Novoselov *et al.*, has sparked research interest in 2D materials, such as hBN, black phosphorous, and the transition metal dichalcogenides [41], [42]. Materials such as graphene derive their honeycomb structure from sp^2 -hybridized covalent bonds and layered bulk structure from van der Waals forces. hBN nanosheets have parameters $a = 0.250$ nm, $c = 0.666$ nm, interlayer spacing of 0.33nm and can form AA' or AB stacked layers [43].

hBN is a unique and fascinating material that has gained interest due to its hyperbolic properties and polar dielectric nature. We will review the meaning and implications of these properties, but first, a review of its electronic structure.

2.3.1.1 Electronic and Dielectric Properties

hBN's bandgap was largely disputed until a 2016 experiment from Cassabois et al. Previous *ab initio* studies predicted an indirect bandgap; however, this was remained experimentally unsupported. By a two-photon excitation scheme, the Cassabois team was able to detect new lines in the photoluminescence intensity vs energy plots, a weak doublet at 5.93 eV and another weak line at 5.955 eV. This large bandgap and hBN's optical transparency make it a suitable choice for a barrier material or as an active layer in tunneling devices [43]. These lines were previously undetected due to stray light in the one-photon spectroscopy scheme. From this two-photon scheme, an exciton binding energy, the minimum energy necessary to remove both the electron and hole components from their locations [44], of 128 ± 15 meV was determined and the ZA, TA, LA, TO, and LO phonon modes were identified. This large exciton binding energy is larger than diamond or AlN, suggesting strong luminescence from exciton recombination [45] and thermal stability. Exciton binding energy and oscillator strength have a direct relationship, where high levels of one indicate high levels of the other [46], this interaction leads to exciton-photon coupling [45].

2D hBN exhibits many tunable properties for the engineering the desired device. It has been shown that the tunneling current, breakdown voltage, and piezoelectric coefficient are all layer dependent. The tunneling current and breakdown voltage exponentially increase with increasing hBN thickness [47]. Bulk 3D hBN is centrosymmetric with a D6h point group, causing it to have no piezoelectric properties; however, since 2D hBN is antisymmetric with a D3h point group, it does have piezoelectric properties when stacked in an odd number of layers. The piezoelectric coefficient decreases with increasing number of layers, given by Equation 1.4, where $e_{1.11}(N_u = 1) = 7.31 \times 10^{-5} \text{ C} \cdot \text{cm}^{-2}$ [48].

$$e_{1.11}(N_u) = \frac{e_{1.11}(N_u = 1)}{N_u} \quad 2.8$$

2.3.1.2 Hyperbolicity

A material's electro-optical properties are defined by their electric displacement **D** and magnetic induction **B**, given by the formulas

$$\mathbf{D} = \varepsilon_0 \boldsymbol{\varepsilon}_r \mathbf{E} \quad 2.9$$

$$\mathbf{B} = \mu_0 \boldsymbol{\mu}_r \mathbf{H} \quad 2.10$$

where ε_0 and μ_0 are the vacuum permittivity and vacuum permeability, $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields, and $\boldsymbol{\varepsilon}_r$ and $\boldsymbol{\mu}_r$ are the relative permittivity and relative permeability, respectively. Throughout this text, variables representing matrices and tensors will be in bold. Since the permittivity matrix is always symmetric, $\boldsymbol{\varepsilon}_r = (\boldsymbol{\varepsilon}_r)^T$, it can be represented by a diagonal matrix, as shown below [49].

$$\boldsymbol{\varepsilon}_r = \begin{bmatrix} \varepsilon_{xx} & 0 & 0 \\ 0 & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix} \quad 2.11$$

There are two main categories of crystals, isotropic and anisotropic, these represent crystals with equal permittivity components i.e. $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz}$, and varying permittivity components, such as in biaxial crystals where $\varepsilon_{xx} \neq \varepsilon_{yy} \neq \varepsilon_{zz}$ and in uniaxial crystals where $\varepsilon_{xx} = \varepsilon_{yy} \neq \varepsilon_{zz}$.

To understand hyperbolic materials, we must examine the dispersion relation first. We derive the dispersion relation by taking the plane wave equations

$$\mathbf{E} = \mathbf{E}_0 e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})} \quad 2.12$$

$$\mathbf{H} = \mathbf{H}_0 e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \quad 2.13$$

and placing them in Maxwell's equations

$$\Delta \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad 2.14$$

$$\Delta \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} \quad 2.15$$

yielding

$$\mathbf{k} \times \mathbf{E} = \omega \mu_0 \mathbf{H} \quad 2.16$$

$$\mathbf{k} \times \mathbf{H} = -\omega \varepsilon_0 \boldsymbol{\varepsilon} \mathbf{E} \quad 2.17$$

with wavevector $\mathbf{k}$. Combining these equations gives us $\mathbf{k} \times (\mathbf{k} \times \mathbf{E}) + \omega^2 \mu_0 \varepsilon_0 \boldsymbol{\varepsilon} \mathbf{E} = 0$ or as a matrix

$$\begin{bmatrix} k_0^2 \varepsilon_{xx} - k_y^2 - k_z^2 & k_x k_y & k_x k_z \\ k_x k_y & k_0^2 \varepsilon_{yy} - k_x^2 - k_z^2 & k_y k_z \\ k_x k_z & k_y k_z & k_0^2 \varepsilon_{zz} - k_x^2 - k_y^2 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} = 0 \quad 2.18$$

Here we encounter the wavevector of free space $k_0 = \frac{\omega}{c}$ and the speed of light in a vacuum $c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$. If we set the optical axis along the z direction, we get the dispersion relation

$$(k_\perp^2 + k_z^2 - \varepsilon_\perp k_0^2) \left(\frac{k_\perp^2}{\varepsilon_\parallel} + \frac{k_z^2}{\varepsilon_\perp} - k_0^2 \right) = 0 \quad 2.19$$

$$\varepsilon_{xx} = \varepsilon_{yy} \equiv \varepsilon_\perp \quad 2.20$$

$$\varepsilon_{zz} \equiv \varepsilon_\parallel \quad 2.21$$

$$k_\perp = \sqrt{k_x^2 + k_y^2} \quad 2.22$$

The first and second terms in the dispersion relation correspond to TE and TM polarized incident light, respectively. These terms give us the isofrequency plots for isotropic and anisotropic media. If one component of the permittivity tensor is negative, the isofrequency plot takes on a hyperbolic shape. From this, it is clear there are two types of hyperbolicity; Type I hyperbolicity where $\varepsilon_\perp > 0$ and $\varepsilon_\parallel < 0$ and Type II hyperbolicity where $\varepsilon_\perp < 0$ and $\varepsilon_\parallel > 0$.

Figure 2.7 Isofrequency Plots for (a) isotropic media (b) media with Type I hyperbolicity and (c) media with Type II hyperbolicity.

Hyperbolic materials and metamaterials have applications in hyperlens, nanolithography, spontaneous emission engineering, and thermal emission engineering. Hyperlens can be

engineered by curling flat hyperbolic materials into concentric cylinders. These cylindrical hyperlens magnify sub-wavelength objects inside the device to the outer layer boundary by the ratio R_{out}/R_{in} . Magnification is enabled by the high k-vector waves surviving transmission through the hyperbolic material and compression of the tangent wavevector component k_θ [50].

We define the region between the epsilon-near-zero and the epsilon-near-pole frequencies as the Reststrahlen band. In this region, media behave as a metal and strongly reflect incident light. Operation within the Reststrahlen band are typically forbidden, but hBN's phonon-polaritons allow engineers to access this region [51].

The permittivity equation for hBN is provided below [52].

$$\epsilon_m = \epsilon_{\infty,m} \left(1 + \frac{\omega_{LO,m}^2 + \omega_{TO,m}^2}{\omega_{TO,m}^2 - i\gamma_m\omega - \omega^2} \right) \quad 2.23$$

Table 1. Infrared dielectric properties for hBN. [52]

	$\mathbf{E} \perp \mathbf{c}$	$\mathbf{E} \parallel \mathbf{c}$
ϵ_∞	4.87	2.95
γ	5 cm^{-1}	4 cm^{-1}
ω_{TO}	1370 cm^{-1}	780 cm^{-1}
ω_{LO}	1610 cm^{-1}	830 cm^{-1}

The permittivity for hBN is shown in Figure 1-2, with the Type I (blue) and Type II (red) Reststrahlen bands highlighted.

Figure 2.8. Dielectric Function of hBN (a) Real part (b) Imaginary part

2.3.2 Gallium Nitride

In the wurtzite phase, GaN has lattice constants $a = 0.3112$ nm and $c = 0.4982$ nm. There have been increasing evidence of infrared and terahertz polariton activity in GaN systems, particularly in the form of ISB polaritons [53], surface plasmon polaritons [54], [55], magneto-plasmon-polaritons [56], and exciton polaritons [38].

Figure 2.9. Raman back-scattering spectra to determine the dielectric response for GaN with experimental set-up in inset. [57]

Our studies will use a wurtzite GaN structure, this uniaxial crystal has the dielectric function shown Equation 1.24. For the ionic crystal, the dielectric function is determined from the optical phonon modes. Davydov et al. performed Raman scattering and group analysis to determine the optical phonon modes and phonon dispersion. They identified six phonon modes; $A_1 + E_1 + 2E_2 + 2B_1$ [58]. The A_1 and E_1 modes are polarized and split into LO and TO branches. The constants for this equation are provided in Table 2, where $\epsilon_{0,m}$ and $\epsilon_{\infty,m}$ are the static and high frequency dielectric constants, respectively, γ_m are the damping constants, $\omega_{TO,m}$ and $\omega_{LO,m}$ are the frequencies for the TO and LO phonons, respectively. The A_1 and E_1 modes correspond to the parallel and perpendicular components, respectively.

$$\epsilon_m = \epsilon_{\infty,m} + \frac{(\epsilon_{0,m} - \epsilon_{\infty,m})\omega_{TO,m}^2}{\omega_{TO,m}^2 - i\gamma_m\omega - \omega^2} \quad 2.24$$

Table 2. Infrared dielectric properties of GaN. [57]

	$\mathbf{E} \perp \mathbf{c}$	$\mathbf{E} \parallel \mathbf{c}$
ϵ_0	9.22	10.32
ϵ_∞	5.35	5.35
γ	10.07 cm ⁻¹	10.07 cm ⁻¹
ω_{TO}	558.72 cm ⁻¹	531.67 cm ⁻¹
ω_{LO}	740.51 cm ⁻¹	734.17 cm ⁻¹

2.4 Self-Consistent Schrödinger-Poisson

In order to solve a two-way coupled system, the Schrödinger equation and Poisson's equations are iteratively solved until a self-consistent solution is found. The initial space charge density ρ is estimated from the Thomas-Fermi approximation. Next, Poisson's equation is solved for the electric potential V . This is used for the potential energy term V_e for the Schrödinger equation.

$$V_e = qV \quad 2.25$$

$$q = z_q e \quad 2.26$$

Where q is the charge of the carrier and e is the elementary charge. We solve the Schrödinger equation to get new eigenenergies E_i and normalized wave functions Ψ_i . The wave function Ψ_i is used to calculate the weighted sum of the probability densities for the new particle density profile n_{sum} .

$$n_{\text{sum}} = \sum_i N_i |\Psi_i|^2 \quad 2.27$$

Here N_i is the weight calculated from the integral of the Fermi-Dirac distribution for a 1D system; where g_i is the valley degeneracy factor, E_f is the Fermi level, m_d is the density of state effective mass, k_B is the Boltzmann constant, T is the absolute temperature, and F_0 is the Fermi-Dirac integral.

$$N_i = g_i \frac{m_d}{\pi \hbar^2} k_B T F_0 \frac{E_f - E_i}{k_B T} \quad 2.28$$

We use the particle density profile n_{sum} to give us a better estimation for the space charge density ρ_{new} . This value is used to determine the new electric potential profile V with Poisson's equation. This new value is compared to the previous iteration's calculation and if it is within the tolerance level ϵ a self-consistent solution has been found. If not, the process is repeated until convergence. Figure 2.1 depicts a flow diagram for performing a self-consistent Schrödinger-Poisson process achieving convergence.

Figure 2.10. Flow diagram for a self-consistent Schrödinger-Poisson solver. [59], [60]

2.5 Rigorous Coupled Wave Analysis

Rigorous Coupled Wave Analysis (RCWA) or Fourier modal method (FMM) takes the constituent layers of the structure and expand the fields within each layer into eigenmodes. These eigenmodes have a simple $\exp(iqz)$ dependence. We determine a Fourier basis to represent the

fields and eigenmodes, with each basis related to the dielectric distribution. To satisfy boundary conditions, the modal expansion coefficients are related at the internal interfaces in the Fourier basis. The method described here was developed by Liu and Fan for implementation in their Stanford Stratified Structure Solver (S⁴) [61].

Figure 2.11. Schematic for RCWA formulation for a layered structure. Magnified cross-section depicts the propagation directions of forward and backward layer modes. [61]

We start with the time-harmonic Maxwell's equations

$$\nabla \times \mathbf{H} = -i\omega\epsilon_0\epsilon\mathbf{E} \quad 2.29$$

$$\nabla \times \mathbf{E} = i\omega\mu_0\mathbf{H} \quad 2.30$$

Switching to Lorentz-Heaviside units so that $Z_0 = \sqrt{\mu_0/\epsilon_0}$ and the speed of light c are both unity will simplify notation and bring the electric and magnetic fields onto the same scale. This is the same as starting with SI units and the letting $\sqrt{\mu_0\epsilon_0}\omega_{SI} \equiv \omega$, $\sqrt{\mu_0\epsilon_0}\mathbf{H}_{SI} \equiv \mathbf{H}$, and $\mathbf{E}_{SI} \equiv \mathbf{E}$.

$$\nabla \times \mathbf{H} = -i\omega\epsilon\mathbf{E} \quad 2.31$$

$$\nabla \times \mathbf{E} = i\omega\mathbf{H} \quad 2.32$$

We then take the spatial Fourier transform in the xy-plane. Due to the periodicity of the z-axis, the fields take the form of 2.9, with a similar equation for $\mathbf{E}$.

$$\mathbf{H}(\mathbf{r}, z) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{G}}(z) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad 2.33$$

Where $\mathbf{k}$ is the in-plane k-vector and $\mathbf{G}$ is the reciprocal lattice vector which typically takes the form of “circular truncation,” where all the $\mathbf{G}$ vectors in a circular region are used.

Now that the field vectors are taken care of, we move to the dielectric function for Fourier transformation.

$$\varepsilon_{\mathbf{G}} = \frac{1}{|L_r|} \int_{cell} \varepsilon(\mathbf{r}) e^{-\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} \quad 2.34$$

Assuming the z-axis is separable, ε is the permittivity tensor of the form in Equation 2.11. From here, each component of ε can be Fourier transformed individually, which will yield five sets of components for Equation 2.10; $\hat{\varepsilon}_{G,xx}$, $\hat{\varepsilon}_{G,xy}$, $\hat{\varepsilon}_{G,yx}$, $\hat{\varepsilon}_{G,yy}$, and $\hat{\varepsilon}_{G,z}$.

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{yx} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_z \end{bmatrix} \quad 2.35$$

These coefficients can be represented by Toeplitz matrices whose elements are defined by Equation 2.11. This means that the (m, n) entry of $\hat{\varepsilon}_{xx}$ is the Fourier coefficient of the reciprocal lattice vector $\mathbf{G}_m - \mathbf{G}_n$.

$$\hat{\varepsilon}_{xx,mn} = \varepsilon_{(\mathbf{G}_m - \mathbf{G}_n),xx} \quad 2.36$$

Now we can use these equations to get the Fourier transform for Maxwell's equations for each component. Each component is shown in Equations 2.13-2.18. Here $\hat{k}_x$ is the diagonal matrix $(k_x + G_{1x}, k_x + G_{2x}, \dots)$ and similarly for $\hat{k}_y$. The values d_x and d_y are the Fourier coefficients of the displacement field $\mathbf{D}$, and e_x and e_y are the Fourier coefficients of the electric field $\mathbf{E}$.

$$i\hat{k}_y h_z(z) - h'_y(z) = -i\omega d_x(z) \quad 2.37$$

$$h'_x(z) - i\hat{k}_x h_z(z) = -i\omega d_y(z) \quad 2.38$$

$$i\hat{k}_x h_y(z) - i\hat{k}_y h_x(z) = -i\omega \hat{\epsilon}_z e_z(z) \quad 2.39$$

$$i\hat{k}_y e_z(z) - e'_y(z) = i\omega h_x(z) \quad 2.40$$

$$e'_x(z) - i\hat{k}_x e_z(z) = i\omega h_y(z) \quad 2.41$$

$$i\hat{k}_x e_y(z) - i\hat{k}_y e_x(z) = i\omega h_y(z) \quad 2.42$$

We need to relate the displacement and electric field via their components mentioned above to get a closed set of equations, so we let matrix $\mathcal{E}$ be the relational term.

$$\begin{bmatrix} -d_y(z) \\ d_x(z) \end{bmatrix} = \mathcal{E} \begin{bmatrix} -e_y(z) \\ e_x(z) \end{bmatrix} \quad 2.43$$

Using Equation 2.15 to eliminate the z components, Equations 2.16 and 2.17 become

$$-\hat{k}_y \hat{\epsilon}_z^{-1} \hat{k}_x h_y(z) + \hat{k}_y \hat{\epsilon}_z^{-1} \hat{k}_y h_x(z) + i\omega e'_y(z) = \omega^2 h_x(z) \quad 2.44$$

$$-i\omega e'_x(z) + \hat{k}_x \hat{\epsilon}_z^{-1} \hat{k}_x h_y(z) - \hat{k}_x \hat{\epsilon}_z^{-1} \hat{k}_y h_x(z) = \omega^2 h_y(z) \quad 2.45$$

Equations 2.20 and 2.21 show the previous equations in matrix form, where I is the identity matrix.

$$(\omega^2 I - \mathcal{K}) \begin{bmatrix} h_x(z) \\ h_y(z) \end{bmatrix} = -i\omega \begin{bmatrix} -e'_y(z) \\ e'_x(z) \end{bmatrix} \quad 2.46$$

$$\mathcal{K} = \begin{bmatrix} \hat{k}_y \hat{\epsilon}_z^{-1} \hat{k}_y & -\hat{k}_y \hat{\epsilon}_z^{-1} \hat{k}_x \\ -\hat{k}_x \hat{\epsilon}_z^{-1} \hat{k}_y & \hat{k}_x \hat{\epsilon}_z^{-1} \hat{k}_x \end{bmatrix} \quad 2.47$$

We can eliminate the z components from 2.13 and 2.14 with Equation 2.18.

$$-i\omega h'_x(z) + \hat{k}_x \hat{k}_x e_y(z) - \hat{k}_x \hat{k}_y e_x(z) = \omega^2 d_y(z) \quad 2.48$$

$$-\hat{k}_y \hat{k}_x e_y(z) + \hat{k}_y \hat{k}_y e_x(z) + i\omega h'_y(z) = \omega^2 d_x(z) \quad 2.49$$

Or in matrix form

$$(\omega^2 \mathcal{E} - K) \begin{bmatrix} -e_y(z) \\ e_x(z) \end{bmatrix} = -i\omega \begin{bmatrix} h'_x(z) \\ h'_y(z) \end{bmatrix} \quad 2.50$$

$$K = \begin{bmatrix} \hat{k}_x \hat{k}_x & \hat{k}_x \hat{k}_y \\ \hat{k}_y \hat{k}_x & \hat{k}_y \hat{k}_y \end{bmatrix} \quad 2.51$$

Now that we have the Fourier transforms for Maxwell's equations, we need to determine the layer eigenmodes.

We take the magnetic field eigenmode to be

$$\mathbf{H}(z) = \sum_{\mathbf{G}} \left[\phi_{\mathbf{G},x} \mathbf{x} + \phi_{\mathbf{G},y} \mathbf{y} - \frac{(k_x + G_x)\phi_{\mathbf{G},x} + (k_y + G_y)\phi_{\mathbf{G},y}}{q} \mathbf{z} \right] e^{i(\mathbf{k} + \mathbf{G}) \cdot \mathbf{r} + iqz} \quad 2.52$$

where $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ are the Cartesian unit vectors and $\phi_{\mathbf{G},x}$ and $\phi_{\mathbf{G},y}$ are the expansion coefficients that can be vectors of the form $\phi_x = [\phi_{G_1,x}, \phi_{G_2,x}, \dots]^T$. From $\mathbf{H}(z)$ we get the column vector $h(z)$ whose elements correspond to $\mathbf{G}$ vectors.

$$h(z) = \left[\phi_x \mathbf{x} + \phi_y \mathbf{y} - \frac{(\hat{k}_x + \phi_x) + (\hat{k}_y + \phi_y)}{q} \mathbf{z} \right] e^{-iqz} \quad 2.53$$

Maxwell's equations are then rewritten using the above and Equations 2.22 and 2.26

$$(\omega^2 I - \mathcal{K}) \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix} = \omega q \begin{bmatrix} -e_y \\ e_x \end{bmatrix} \quad 2.54$$

$$\omega q \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix} = (\omega^2 \mathcal{E} - K) \begin{bmatrix} -e_y \\ e_x \end{bmatrix} \quad 2.55$$

In the above equations, $e_x(z)$ and $e_y(z)$ lost their z dependence to represent a fixed mode. We eliminate the electric field and apply $\mathcal{K}K = 0$ to get

$$(\mathcal{E}(\omega^2 - \mathcal{K}) - K)\Phi = \Phi q^2 \quad 2.56$$

$$\Phi = \begin{bmatrix} \phi_x \\ \phi_y \end{bmatrix} \quad 2.57$$

where q^2 is the diagonal matrix whose diagonal elements are the eigenvalues q_n^2 . The matrix Φ contains the Fourier coefficients of the eigenmodes.

Next, we recover the field after layer propagation. The transverse magnetic field in layer i is

$$\begin{bmatrix} h_x(z) \\ h_y(z) \end{bmatrix} = \sum_n \begin{bmatrix} \phi_{x,n} \\ \phi_{y,n} \end{bmatrix} (a_n e^{iq_n z} + b_n e^{iq_n(d_i - z)}) \quad 2.58$$

where n are the eigenmode indexes, a_n is the coefficient of a forward propagating wave at $z = z_i$, and b_n is the coefficient of a backward propagating wave at $z = z_i + d_i$. We create a diagonal matrix operator $f(z)$ for the modal phase accumulation operator.

$$f(z)_{mn} = e^{iq_n z} \quad 2.59$$

The transverse field component vectors in the Fourier basis are defined as

$$h_t(z) = [h_x(z), h_y(z)]^T \quad 2.60$$

$$e_t(z) = [-e_y(z), e_x(z)]^T \quad 2.61$$

and the mode amplitude vectors for the forward and backward waves are

$$a = [a_1, a_2, \dots]^T \quad 2.62$$

$$b = [b_1, b_2, \dots]^T \quad 2.63$$

The mode amplitudes are related to the physical fields by Equation 2.40.

$$\begin{bmatrix} e_t(z) \\ h_t(z) \end{bmatrix} = \begin{bmatrix} (\omega^2 I - \mathcal{K})\Phi q^{-1} & -(\omega^2 I - \mathcal{K})\Phi q^{-1} \\ \Phi & \Phi \end{bmatrix} \times \begin{bmatrix} f(z)a \\ f(d - z)b \end{bmatrix} \quad 2.64$$

Now the Fourier components of the displacement field and electric field have been related via the matrix $\mathcal{E}$, however this is still an unknown value. This matrix is the scattering matrix and there are various ways to calculate its elements; closed-form Fourier transform, fast Fourier transform, subpixel anisotropic averaging, and vector-field-based formulations. We will take a closer look at closed-form Fourier transform and subpixel anisotropic averaging.

Rather than discretizing over a grid, closed-form method applies the dielectric profile of a layer over any closed polygon. This allows for vector paths rather than bitmaps. By evaluating simple polygons, arbitrary structures can be evaluated. Dielectric shapes must not intersect and fully contained within another shape. The dielectric constant is defined as the sum over all shapes plus the background dielectric. I_j is the indicator function and has a value of 1 for valid shapes.

$$\varepsilon(r) = \varepsilon_b + \sum_j (\varepsilon_j - \varepsilon_{\supset j}) I_j(\mathbf{r}) \quad 2.65$$

The simplest FMM form for the matrix $\mathcal{E}$ is shown below where $\hat{\varepsilon}$ is calculated with Equation 2.12.

$$\mathcal{E} = \begin{bmatrix} \hat{\varepsilon}_{xx} & \hat{\varepsilon}_{xy} \\ \hat{\varepsilon}_{yx} & \hat{\varepsilon}_{yy} \end{bmatrix} \quad 2.66$$

The dielectric function is averaged within each discretization pixel for calculating the anisotropic permittivity tensor. An FFT is applied to each layer to obtain the Fourier series coefficients of the dielectric function.

2.6 Transfer Matrix Method

Transfer matrix method (TMM) relates incident field to the reflected and transmitted electric fields of layer i of thickness d_i via a 4x4 matrix called the transfer matrix. As TMM is a frequency based reflection calculation, it starts with the frequency-domain Maxwell curl postulates [62]. Each structure consists of N layers with substrate layer $i = N + 1$.

The transfer matrix of a layer is defined by satisfying the boundary conditions $\mathbf{A}_i$, for electric field propagation $\mathbf{P}_i$ in a system.

$$\mathbf{T}_i = \mathbf{A}_i \mathbf{P}_i \mathbf{A}_i^{-1} \quad 2.67$$

Where $\mathbf{P}_i$ is in the Yeh formalism and $\mathbf{A}_i$ is used to describe the relation between the forward and backward electric field components $\mathbf{A}_{i-1} \vec{E}_{i-1} = \mathbf{A}_i \vec{E}_i$, and is composed of the free singularities γ_{ijk} of the electric field vectors $\vec{\gamma}_{ij} = \begin{pmatrix} \gamma_{ij1} \\ \gamma_{ij2} \\ \gamma_{ij3} \end{pmatrix}$, which describe the material properties in terms of their permeability and permittivity. From this the transfer matrix for the entire system is $\mathbf{T}_{tot} = \prod_{i=1}^N \mathbf{T}_i$. However, $\mathbf{T}_{tot}$ does not accurately describe the incident and substrate layers, as only half of their transfer matrices are included in the total $\mathbf{T}_{tot}$ calculation. Thus, we form the full transfer matrix $\mathbf{\Gamma}_N$ where

$$\mathbf{\Gamma}_N = \mathbf{A}_0^{-1} \mathbf{T}_{tot} \mathbf{A}_{N+1} \quad 2.68$$

To keep with the Yeh formalism, a transformation of the transfer matrix is performed so that

$$\mathbf{\Gamma}_N^* = \Lambda_{1234}^{-1} \mathbf{\Gamma}_N \Lambda_{1234} \quad 2.69$$

The reflection and transmission coefficients for the total system are calculated from the elements of matrix $\mathbf{\Gamma}_N^*$, where each element describes an interface within the multilayered structure.

$$r_{pp} = \frac{\Gamma_{21}^* \Gamma_{33}^* - \Gamma_{23}^* \Gamma_{31}^*}{\Gamma_{11}^* \Gamma_{33}^* - \Gamma_{13}^* \Gamma_{31}^*} \quad 2.70$$

$$t_{pp} = \frac{\Gamma_{33}^*}{\Gamma_{11}^* \Gamma_{33}^* - \Gamma_{13}^* \Gamma_{31}^*} \quad 2.71$$

The reflectivity and transmittance are simply the square of the reflection and transmission coefficients.

The electric field of the total system is the sum of the transmitted and reflected components of each polarization which are functions of the interface $\mathbf{L}_i$ and propagation matrices $\mathbf{P}_i$. The interface matrices relate the electric field on either side of a layer interface, while the propagation matrices describe the electric field within a given layer i . As shown in Figure 2.12, $\mathbf{P}_i$ describes

the reflected waves, propagating towards the incident medium and the inverse $\mathbf{P}_{N+1}^{-1}$ matrix describes the transmitted waves, propagating towards the substrate [63].

$$\vec{E}_{i-1}^- = \mathbf{L}_i \vec{E}_i^+ \quad 2.72$$

$$\vec{E}_i(z) = \mathbf{P}_i(z) \vec{E}_i^- \quad 2.73$$

Figure 2.12. Electric field throughout a multilayer structure according to transfer matrix method. [63]

Chapter 3: Experiments

Here we describe the simulation environment for each experiment and their respective results. The structure in question is shown below in Figure 4.1(a) and the crystal lattice of materials are shown in Figure 4.1(b). A density functional theory study on hBN-AlN superlattice determined the relaxed states of the materials for three supercell geometries; $(hBN)_3(AlN)_4$, $(hBN)_6(AlN)_8$, $(hBN)_{12}(AlN)_{16}$, where the subscripts denote the hBN monolayers and AlN bilayers. It was shown that at larger, bulk sizes the AlN region relaxed into the wurtzite phase. From this, we expected our GaN region to similarly relax into the wurtzite phase for the wells. With an interlayer spacing of 0.33 nm, the hBN barriers correspond to 6 monolayers. Our lattice sizes were derived from similar studies on ISB and phonon polaritons in lattices.

Figure 3.1. (a) hBN/GaN heterostructure consisting of 4 nm GaN wells by 2 nm hBN barriers and capped by 40 nm hBN layers (b) crystal structure depicting a wurtzite GaN well region surrounded by AA' stacked hBN layers- gallium atoms are pink, boron atoms are green, and nitrogen atoms are silver.

3.1 Self-Consistent Schrödinger-Poisson

The Schrödinger-Poisson tool in COMSOL Multiphysics was used to determine the bound state wavefunctions of the superlattice. An eigenvalue study was selected with a 1 eV eigenvalue scale. COMSOL is a finite element method, meaning it discretizes the system to form a mesh. Once the structure was defined, a fine mesh setting was applied to the system. Since we were interested in the traveling waves, the left-hand boundary condition was set to incoming type and

the right-hand side was set to outgoing type; with the electric potential values pinned to the well value. The conduction band was a simplified model, only considering the electron affinities, χ_2 and χ_1 of the barrier and well materials.

3.1.1 Schrödinger-Poisson Results

The results of the Self-Consistent Schrödinger-Poisson calculation is shown below. From this, we were able to show clear tunneling through the barrier layers and provide an estimate for the eigenenergies of the first few bound states.

The conduction bands below are square functions, indicating that the simulation did not consider any electric fields from the piezoelectric or spontaneous polarizations of the materials. If the model did consider these effects, the wells and barriers of the bands would have a slope related to the internal fields in their respective materials and would have a triangular potential profile. The wavefunctions would still be confined within the wells, as in Figure 4.2, however they would occupy a smaller region along the x-axis due to the smaller effective well area.

Figure 3.2. Conduction band diagram with moduli squared wave functions.

3.2 Fresnel Reflection

COMSOL Multiphysics offers a wide range of simulation capabilities. Here, it was used to determine the reflection coefficients of the structure while considering a non-reflective, continuous boundary conditions. However, the software requires user input of the Fresnel equations. The equations for multilayer Fresnel calculation [64] are shown below and were inserted in the results

GUI. The imaginary component of the reflection component from p-polarized light was plotted in frequency-momentum space.

$$r_{12p} = \frac{\frac{\varepsilon_{\perp,2}}{k_{z,2}} - \frac{\varepsilon_{\perp,1}}{k_{z,1}}}{\frac{\varepsilon_{\perp,2}}{k_{z,2}} + \frac{\varepsilon_{\perp,1}}{k_{z,1}}} \quad 3.1$$

$$k_z = \sqrt{\varepsilon_{\perp} k_0^2 - \varepsilon_{\perp} \frac{q^2}{\varepsilon_{||}}} \quad 3.2$$

$$r_{slab,p} = \frac{r_{12,p} + r_{23,p} \exp(2ik_{z2}d_2)}{1 + r_{12,p}r_{23,p} \exp(2ik_{z2}d_2)} \quad 3.3$$

3.2.1 Fresnel Results

The lower region, shown in Figure 4.3(a), only shows evidence of the in-plane LO GaN phonon. The in-plane hBN optical phonons are well separated from the other hBN and GaN phonon modes, so we expected to only see this mode, however we received the broad dispersion of Figure 4.3(b). This could be due to interference from between layers.

Figure 3.3. Dispersion Curves for phonon-polaritons in hBN/GaN heterostructure (a) depicts the lower (out-of-plane) Reststrahlen band (b) depicts the upper (in-plane) Reststrahlen band .

3.3 Rigorous Coupled Wave Analysis

The Stanford Stratified Structure Solver (S^4), a free RCWA system program from the Fan research group, was used to perform the RCWA calculations. The permittivity, permeability, and speed of light are all normalized in the software. Keeping with IR spectroscopy convention, the frequency units are inverse length and time is in units of length. The frequency dependent permittivity equations and corresponding get power flux commands were placed in a nested for loop over the incidence angle and frequency.

3.3.1 RCWA Results

The RCWA supports the interpretations of our Fresnel simulations. We see a single element at $\sim 800 \text{ cm}^{-1}$, this could be the ω_{TO} hBN phonon mode shifted due to interaction from the GaN phonons or the large device size [65]. In the upper Reststrahlen region we do not see defined phonon modes, likely due to the large number of layers.

(a)

(b)

3.4 Reflectivity calculated from RCWA software in the (a) lower and (b) upper frequency ranges.

3.4 Transfer Matrix Method

The TMM calculations were performed in MatLab with a function from Passler and Paarmann for anisotropic media. Their function takes in a range of frequency, an array containing the layers, an array of the layer sizes, and the step size for electric field calculations. The software simulated

reflection experiments performed in the Otto geometry, so that evanescent waves from a highly refractive prism ($n \approx 2.4$) irradiate the sample structure.

Figure 3.5. Otto geometry for multilayered reflection experiments. [63]

3.4.1 TMM Results

To identify any traces of phonon polariton modes within the structure, additional reflectivity and electric field measurements were performed. As shown in Figure 3.1, in the Otto geometry there is a space between the prism and sample called d_{gap} . Previous studies from Passler explained that not all phonon modes were visible at a static d_{gap} , and that by adjusting this parameter, other modes became visible [65]. Thus, in our experiments the reflectivity at various d_{gap} values at four incident angles were calculated at the upper hBN and lower hBN frequencies. From our TMM calculations, we were able to confirm the presence of the GaN and hBN phonon modes, even with a high number of layers. In Figure 4.6, we see electric field enhancement at the GaN phonon modes. In reference [63], localization along the z-axis is visible, this is due to fewer and larger layers in their structures compared to our superlattice.

Figure 3.6 Frequency and gap dependence of reflectivity measurements of the hBN-GaN structure in the (a) lower and (b) upper frequencies

(a)

(b)

Figure 3.7. Electric field plots of the hBN-GaN structure in the (a) lower and (b) upper frequencies.

Chapter 4: Conclusion and Future Work

From our studies, we were able to identify a GaN phonon mode in the reflection plots of our heterostructure. From the TMM study, we were able to verify the presence of all $E \perp c$ phonon modes, with strong reflectivity for the upper hBN mode. In the electric field plots from the TMM calculations, we saw large field enhancement at the phonon modes throughout the structure. Through structure optimization, such as removal of the cap layers and altering the well/barrier ratio, the enhancement could be localized for second harmonic generation [65].

Our simulations did not consider the internal structure dynamics and their effects on the optical phonon frequencies, affecting the conduction band, minibands, and reflection. Because of this, computational analysis on the structure dynamics and phonon perturbations should be performed for determining the properties of an hBN GaN heterostructure with greater accuracy. In the following section, we review the experiments and their respective results and a plan for improving each study is presented.

From the Schrödinger-Poisson study, the conduction band and square wave functions of the hBN GaN structure were calculated without considering strain or internal fields. The lattice mismatch between hBN and GaN will produce interfacial strain which will alter the conduction band, shifting the finite wells' eigenenergies and minibands [66]. DFT is an essential tool in materials science and has been used for many projects such as chemical manufacturing, metallurgy, and even describing planet formation. However, DFT is primarily used for predicting semiconductor properties as when utilized by Spataru et al. for a hBN-AlN superlattice. In this study standard DFT in the localized density approximation was used to optimize the atomic structure and determine how the bulk material stabilizes, while the hybrid-DFT eigenvalues were used to determine the band offsets and the interfacial macroscopic electric potential drop. The hybrid DFT was a long range separated hybrid functional that in the slowly decaying range, the Fock exchange interaction was replaced with the corresponding PBE functional. We suggest a similar project to calculate the stress within our proposed structure. In the following section we describe how DFT is performed.

Density functional theory is the leading method to calculate an approximate solution for the Schrödinger equation for a many body system due to being sufficiently accurate and

computationally simple in comparison to the Hartree-Fock theory [67]. The first step is to reduce the number of degrees of freedom as much as possible by applying the Born-Oppenheimer (BO) approximation. While the ions and electrons in a system experience the same magnitude of force, the nuclei are magnitudes larger than electrons and have a significantly smaller kinetic energy. In the BO approximation, the large atomic nuclei are considered static [67], [68]. From this approximation we get the following time independent, non-relativistic Schrödinger equation.

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad 4.1$$

Where the Hamiltonian consists of the kinetic energy, the interaction with the external potential, and the electron-electron interaction. The external potential is the interaction of the electrons with the nuclei. In Equation 2.2, $\mathbf{p}_i$ and $\mathbf{r}_i$ are the position and momenta with mass m .

$$\hat{H} = \hat{T} + \hat{V}_{ext} + \hat{U} = \frac{1}{2} \sum_i^M \frac{\mathbf{p}_i^2}{m} + \sum_i^M v(\mathbf{r}_i) + \sum_{i < j}^M u(|\mathbf{r}_i - \mathbf{r}_j|) \quad 4.2$$

The potential $v(\mathbf{r})$ is measured from an arbitrary origin, so we set it as the convenient value of the chemical potential and set it at 0; $\mu = 0$, and $u(r)$ is the simple pair potential.

In the grand-canonical ensemble, we have the grand potential

$$\Omega(\mu, T, V) = -T \log \Xi \quad 4.3$$

With the grand partition function

$$\Xi(\mu, T, V) = \sum_{M=0}^{\infty} \frac{1}{M!} \text{Tr} \exp\left(-\frac{\mathcal{H}_{MB} - \mu M}{T}\right) \quad 4.4$$

Tr is the classical trace and represents the 6M-dimensional phase-space integral.

The Hohenberg-Kohn energy $F_{HK}[n(r)]$ is equal to the total energy minus the potential, i.e. the internal energy; and is given by the density distribution $n(\mathbf{r}) = \langle \rho(r) \rangle = \frac{\delta \Omega}{\delta v(\mathbf{r})}$

$$F_{HK}[n(r)] = \Omega[v(r)] - \int dr n(\mathbf{r})v(\mathbf{r}) \quad 4.5$$

Once the free energy functional is minimized we get Equation 2.6. A functional of $n(\mathbf{r})$ is necessary for DFT analysis.

$$\frac{\delta F_{HK}}{\delta n(r)} = -v(r) \quad 4.6$$

Application of DFT to electron processes require an explicit construction of $F_{HK}[n]$ for interacting electrons and can take the form of Equation 2.5. This is a sum of the noninteracting kinetic energy $F_{ni}[n]$ and two interaction terms; the electrostatic energy $E_{es}[n]$ and exchange-correlation energy $E_{xc}[n]$.

$$F_{HK}[n(\mathbf{r})] = F_{ni}[n(\mathbf{r})] + E_{es}[n(\mathbf{r})] + E_{xc}[n(\mathbf{r})] \quad 4.7$$

All three terms must be evaluated, however $E_{es}[n(\mathbf{r})]$ is the only term easily found.

$$E_{es}[n(\mathbf{r})] = \frac{e^2}{2} \int \frac{d\mathbf{r} d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} n(\mathbf{r})n(\mathbf{r}') \quad 4.8$$

There are two possible ways to determine the noninteracting kinetic energy and the exchange correlation energy: determining the explicit approximations for both terms or using the Kohn and Sham orbital equations.

We were unable to determine the dispersion of phonon-polaritons in the proposed hBN-GaN heterostructure. We aimed to do so by projecting the reflectivity onto frequency- wavevector space to view the phonon-polariton dispersion. First, this was attempted from an iterative calculation of the Fresnel reflection coefficients, from which we detected one of the GaN phonon modes but did not notice any anti-crossing points indicating Rabi splitting or strong coupling. Similar results were found from the RCWA calculations where we plotted the reflectivity in frequency-wavevector space rather than the reflection coefficients. This could be due to two possible issues; (i) the multiple layers in our structure cause errors due to broadening (ii) improper targeting of the phonon mode. The multiple modes within our structure could cause broadening of the modes, making it difficult to identify Rabi splitting. And it has been shown that when broadening is the main contribution, only the principle modes are visible [69], this could be why we only see notes of the GaN phonon mode.

As for as the second issue, the well and barrier dimensions were determined from similar experiments on ISB and exciton polaritons. The well and barrier sizes of our structure may not be optimized for coupling the photon and phonon modes in the structure. In the electrically pumped phonon polariton laser presented by Ohtani, the AlInAs barriers were significantly thinner (sub-nanometer scale) than our hBN barriers. Our hBN barrier sizes were determined from the practicality of fabrication, as a lattice consisting of bulk GaN and monolayer hBN would exert a large amount of strain on the hBN layer and could lead to interfacial separation.

Even with optimization of the lattice design through DFT calculation, the equations describing the material may produce inaccurate results in comparison to a fabricated structure. A recent study showed that in superlattices consisting of atomic scale layers, the dispersion of the structure is not an explicit function of the component permittivities, but rather a new dielectric function is produced as the phonon modes are dramatically shifted due to interfacial chemical bonding and strain. Such superlattices were deemed crystalline hybrids (XH). The dielectric function of the superlattice was determined by collecting IR ellipsometry data to measure the phonon modes and placing the values in the parametrized form of the dielectric function for a polar semiconductor. This function was then used in the same TMM algorithm used in our project, utilizing the Otto geometry for launching modes into the superlattice via evanescent waves to calculate the dispersion. The dielectric function derived from the IR ellipsometry experiments agreed with the dielectric function predicted by density function perturbation theory (DFPT) [70]. Thus, DFPT could be used to derive the permittivity of other crystalline hybrids and TMM algorithm could be employed in reflection measurements for dispersion plotting.

4.1 Application in a Phonon Polariton Laser

The structure presented here was just to determine if phonon-polariton can be found in the hBN GaN heterostructure. For hBN and GaN to be employed as a coherent source of phonon polaritons, an active region would need to be designed so that the E_{21} transition energy is near the upper or Type-II hBN phonons. An injector region allowing for the tunneling to the next active region would then be included. The bias voltage for this III-Nitride QCL would be less than that of GaAs based lasers due to its large spontaneous polarizations and internal field [71]. These devices could then be fabricated and tested with Raman spectroscopy.

Without fabricated devices, it is impossible to probe the tripartite nature of phonon-polaritons coupled with ISB transitions. In Chapter 2, it was mentioned that by solving equations 2.3 and 2.4, one can determine the polariton dispersion. However, in the literature, some of the variables, including n_g and n_{eff} are approximated from the QCL and Fabry-Pérot reference devices.

In hBN fabrication mechanical exfoliation produces fewer defects, but chemical vapor deposition (CVD) and metal organic vapor phase epitaxy (MOVPE) allows for greater accuracy in atomically thin layers. While hBN has been placed in superlattice structures, they were used in conjunction with other 2D materials, as the similar structure allow for simple construction [72] and for application in Moiré pattern formation [73]. Thus far, only preliminary calculations for hBN in superlattices with III-V nitrides have been performed for hBN/AlN crystal lattice formation using DFT. Though in following the process laid out by GaN or AlN on hBN as a substrate or transfer layer, a multistep MOVPE growth process should be applied. Triethylboron (TEB) can be used as a boron source [74], [75] and triethylgallium can supply gallium to the system [76], both can use a hydrogen carrier gas. While there have been issues of “self-separation” of GaN deposited on hBN, this was on largely due to rough surface morphology [77], where as thin hBN ($d_{hBN} < 10\text{ nm}$) exhibits smoother surface morphologies [75]

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