Fundamental electrical and optical properties of strained wurtzite InGaN/GaN-based quantum-well structures are calculated based on the Rashba-Sheka-Pikus (RSP) Hamiltonian in the vicinity of the Γ point since the simple parabolic model is very poor to fit the valence band structures of the nitride wurtzite materials. The model includes the spontaneous and the strain-induced piezoelectric polarization, as well as the crystal-field and the spin-orbit interactions and the strain effect that are already included in the RSP Hamiltonian. The propagation method is used for the QW structure calculation and the nitride parameters were optimized based on the up-to-date experimental results and the theoretical calculations. It is found that the strain-induced piezoelectric field significantly alters the subband structure and determines the output intensity of the nitride quantum well light emitting diodes. The calculations are compared with the available experimental data of the nitride light emitting diodes (LEDs) and a good match exists for low In composition LEDs. For the case with high In composition (> 0.2), the comparison between the calculations and the experiments supports the possibility of strain relaxation in the quantum well. The resulting model can accurately investigate the optoelectronic properties of nitride based QW LEDs over a wide range of In composition (< 0.5). Based on the understanding of the polarization fields, a design that uses AlInGaN as the quantum barrier is proposed to control the strain, and thus the piezoelectric polarization field. So an efficient red emission can be realized, which is hard to achieve if GaN is used as the barrier. In the proposed design, three different InGaN/AlInGaN QW structures emit red, green and blue light with similar intensities. Also, to achieve high efficiency, important factors related to the oscillator strength are discussed in detail.

Since the initial predictions, photonic crystals (PCs) have offered new opportunities for realizing photonic integrated circuits with many important applications including optical communication and display. The feasibility of an electrically programmable PC is investigated theoretically based on the metal-insulator transition of vanadium dioxide (VO$_2$). We propose a slab structure based on VO$_2$ whose dielectric properties can be modulated by selectively applying the bias on a lithographically defined array of gate electrodes to induce
the phase transition. So, unlike the ordinary PCs, wave propagation in the desired structure may be switched on/off or redirected as needed. To examine the idea, the optical properties of VO$_2$ in both the semiconducting and the metallic phase are investigated in the infra-red region. The photonic band structure and the wave guiding characteristics are studied by the iterative plane wave expansion (PWE) and the finite difference time domain (FDTD) methods. The results clearly indicate that the changes induced in the VO$_2$ dielectric properties via the phase transition can enable effective modulation of wave propagation at a high speed, offering a promising opportunity for a photonic circuit that can be programmed or reconfigured on demand.

The focusing effects in both ideal left-handed mediums (LHMs) and metallic photonic crystals (PCs) are investigated theoretically based on the finite difference time domain (FDTD) method. The analysis shows that the subwavelength resolution is possible in an ideal LHM system when the propagation loss is limited to $10^{-5}$ or smaller. However, image distortion may occur due to the interference effect. As for the metallic PC system, far-field images do appear at the opposite side to the source of the PC in the calculation. More importantly, the image location seems to follow the rule of geometric optics in respect to the changes in the source position as the direct proof of negative refraction in the PC-based system. The comparison between the ideal LHM and the metallic PC suggests that the focusing effect in the PC-based system is different from that of the ideal LHM system in many aspects due to the inhomogeneous nature of the PC. Also the effect may not be solely determined by the photonic band structure and may require a negative effective dielectric constant. Finally, the calculation also indicates that the effective index of $-1$ can be realized in both the ideal metallic PCs and the realistic copper/silicon PCs.
Electronic and Photonic Band Engineering for Novel Optoelectronic and Nanophotonic Devices

by

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To my wife Yi
Biography

After entering university in 1992, Dong Xiao received his B.S. degrees in Physics from University of Science and Technology in China (Hefei, Anhui, P. R. China) in 1997. In Spring 1998, he went to America for his graduate study in Physics and got his Master of Science degree in 2000 at Southern Illinois University at Carbondale, IL. In Fall 2001, he came to North Carolina State University for his PhD study in Electrical Engineering. His research interests are computational engineering, mathematical modeling, nano-optic and semiconductor device design and simulations.
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Chapter 1

Introduction

1.1 Nitride Optoelectronic Devices

Optoelectronics will undoubtedly play a major role in the applied sciences of the twenty-first century. This is due to the fact that optoelectronics holds the key to future communication developments that require high data transmission rates and extremely large bandwidths. For example, an optical fiber having a diameter of a few micrometers has a bandwidth of 50 THz, where an impressive number of channels having high bit data rates can be simultaneously propagated. Optoelectronics has advanced considerably due to the major development in the area of semiconductor nanotechnologies. Nanoscience and technology are advancing at a rapid pace and making revolutionary contributions in many fields including electronics, materials science, chemistry, biology, structures and mechanics, and optoelectronics. Among these scientific and technological fronts, the most impressive progress has been made in the area of semiconductor technology. Semiconductor nanostructures have been enabled by the advancements in epitaxial growth techniques, which are now capable of growing epilayers as thin as one atomic layer and with interface roughness that are mere fraction of a monolayer. Heterostructures at the nanometer scale such as quantum wells, quantum wires and quantum dots, have found robust applications in the generation, modulation, detection and processing of light.

Along with the major advances in the synthesis of wide bandgap III-nitride semi-
conductor compounds, these nitrides have attracted more and more interest in the opto-
electronic applications. The direct bandgap of III-nitride is one of their most beneficial
features for optoelectronic device applications. Moreover, the nitride alloys are particularly
attractive since the bandgaps of aluminum nitride (AlN), gallium nitride (GaN) and indium
nitride (InN) are 6.2 eV, 3.44 eV and 0.76 eV \[1\] at 300 K respectively and they cover the
entire visible wavelength spectrum. In addition, the wide bandgap found in GaN, AlN and
their compounds results in a low intrinsic carrier density which in turn leads to low voltage
and low dark current, especially important for photodetectors and high-temperature elec-
tronics. III-nitrides also have high melting points and mechanical strength. Adding to the
list, the infra-red resistance to radiation damage yields a material system suitable for high
frequency, high power and high temperature applications. In addition to optical devices,
many advances have taken place in the area of high-power, high-frequency power transis-
tors for radio-frequency transmission applications, due to the high thermal conductivity,
high melting point, low dielectric constant, and high breakdown voltage of III-nitrides. At
the same time, III-nitride alloys differ from the rest of III-V compound semiconductors in
many aspects. Their most thermodynamically stable structure is wurtzite; they exhibit
strong piezoelectric fields; they are chemically and physically strong, etc. In addition to
these inherent properties, there are many technical challenges associated with the growth
and processing of these materials. Most specifically, lack of commercially available native
substrates has forced the researchers to use substrates with mismatched lattice constants
and different thermal expansion coefficients. New ideas have had to be developed in order
to reduce the number of dislocations present in the resulting material grown atop these
substrates. Doping problems also, especially p-type doping, has plagued the development
of these materials for a long time.

Despite technology advances and commercial applications of III-nitrides, many of
the fundamental material properties are poorly understood and further experimental and
theoretical studies are required. Although the nitride materials are grown in both zinc-
blende (cubic) and wurtzite (hexagonal) structures, the wurtzite structure is predominant
for the device applications. As for these direct bandgap III-nitride compounds, many im-
portant optical and transport properties are determined by carriers in the small vicinity of
the \( \Gamma \) point. Conduction band states for small wave vector \( \vec{k} \) are doubly degenerate with
respect to spin and can be characterized by energy-independent electron effective masses.
The valence band spectrum near the \( \Gamma \) point is more complicated. Joint action of the
hexagonal component of crystal field and the spin orbit interaction in wurtzite crystals leads to the formation of three distinct levels $\Gamma_9$, upper $\Gamma_7$ and lower $\Gamma_7$ from the original sixfold degenerate $\Gamma_{15}$ state. [2] The separation between these levels, especially between the first two levels, is comparable to the thermal energy at room temperature. Therefore, the valence-band treatment in hexagonal nitride structures has to take into account interaction between all three levels, which results in a rather complicated dispersion relation and could not be simply fitted into the well-known parabolic model. So, due to the large deviation from the simple parabolic model, the effective hole mass parameters and also the single electron Schrodinger equation with effective mass approximation cannot accurately describe the valence band spectrum of these nitride compounds. Moreover, the strain also has an important effect on the band structure. The description of spectra and transitions in the vicinity of the $\Gamma$ point involving three doubly degenerate valence bands is conveniently achieved in an envelop-function formalism. The Hamiltonian for the valence band of wurtzite semiconductors was described by Rashba and Sheka [3]. Later, Pikus [4] included the effects of strain and presented the invariant form for the valence-band Hamiltonian. This Rashba-Sheka-Pikus (RSP) Hamiltonian [5], instead of the Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m_{eff}} \nabla^2$, is adopted for the calculation of the valence band structure for wurtzite nitrides.

Band engineering is the area that connects the physical principles with the technology applications and is most vital to analyze the properties of electronic and photonic devices. In Chapter 2, we investigate the III-nitride wurtzite semiconductors based on the RSP Hamiltonian in the vicinity of the $\Gamma$ point. The single quantum well (QW) model is adopted to calculate the oscillator strength in these nitride QW structures. The strain and its induced piezoelectric field are included in both the RSP Hamiltonian and the QW model. The nitride parameter database is optimized based on some recent experimental and theoretical studies. The simulation results are compared with experiments. Finally, based on the RSP Hamiltonian in the vicinity of the $\Gamma$ point, and taking into consideration of spontaneous and piezoelectric polarization, the optical intensity of nitride-based QW light emitting diodes (LEDs) has been calculated. A design that uses AlInGaN as the quantum barrier is proposed to realize the efficient red emission, which is hard to achieve if GaN is used as the barrier. In the proposed design, three different InGaN/AlInGaN QW structures emit red, green and blue light with similar intensity.
1.2 Novel Photonic Crystal Devices

Nanophotonics, defined by the fusion of nanotechnology and photonics, is an emerging frontier providing challenges for fundamental research and opportunities for new technologies. Nanophotonics is an exciting new frontier that has captured the imagination of people worldwide. In the last few years, research on photonic crystals (PCs) becomes one of the hottest areas in the field of nanophotonics. The concept of PCs is proposed by E. Yablonovitch [6] and S. John [7] in 1987. It is an optical material that has the refractive index periodic in space. In the similar way as the periodicity of solid state crystals determines the energy band structure, the periodic structuring of PCs at wavelength scales has turned out to be a viable approach to the control of the photons. The analogy between electron waves and electromagnetic waves is a consequence of the formal relation between the Schrödinger’s equation for electronic wavefunctions and Maxwell equations for electromagnetic waves.

The propagation of electromagnetic waves is determined by the Maxwell equations,

\[\nabla \cdot \vec{B} = 0; \quad \nabla \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = \vec{J}; \quad \nabla \cdot \vec{D} = \rho; \quad \nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0.\]

(1.1)

Where \(\vec{E}\) and \(\vec{H}\) are the macroscopic electric and magnetic fields, \(\vec{D}\) and \(\vec{B}\) are the displacement and magnetic induction fields, \(\rho\) and \(\vec{J}\) are the free charge density and the current density. Usually inside the PCs \(\rho = 0\) and the current density can be included by the use of the complex dielectric constant. For most materials, the magnetic permeability is very close to unity, \(\vec{B} = \vec{H}\), and for isotropic media, \(\vec{D} = \varepsilon(\vec{r})\vec{E}\). Then for a wave with frequency \(\omega\), Maxwell equations are simplified as:

\[\nabla \times \left[\frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H}\right] = \left(\frac{\omega}{c}\right)^2 \vec{H}(\vec{r});\]

\[\frac{1}{\varepsilon(\vec{r})} \nabla \times \left[\nabla \times \vec{E}\right] = \left(\frac{\omega}{c}\right)^2 \vec{E}(\vec{r}).\]

(1.2)

where \(\varepsilon(\vec{r})\) is equal to the dielectric constant of the inclusion medium \(\varepsilon_i\) when inside the inclusion medium and is equal to the dielectric constant of the host medium \(\varepsilon_h\) when inside the host medium. These two equations are the governing equations in the photonic band structure calculation. They are analogous to the equation ruling the wave function for an electron with mass \(m\) in a potential \(V\), i.e., the Schrödinger equation,

\[\nabla^2 \Psi(\vec{r}) = -\frac{2m}{\hbar^2} [E - V(\vec{r})] \Psi(\vec{r}).\]

(1.3)
In analogy with the electronic band gaps of semiconductors, a periodic dielectric function $\varepsilon(\vec{r})$ may result in the formation of photonic band gaps, a certain range of frequencies for which light cannot propagate. PCs are a revolution in optical technology and may become the "transistor" of this century. Photons will carry and store data like electrons do on classical computer chips. It is predicted that PCs will be involved with every bit of electronics from cell phones to supercomputers and make them smaller, faster and more energy efficient. When data moves on silicon chips, electrons are routed through electronic gates, or transistors. But electrons are charged particles that interact with each other when brought into close contact, producing excessive heat and limiting their movement. PCs promise to break this barrier through use of uncharged photons to carry data. PCs show promising applications for a lot of optical elements such as light emitters, resonators and filters, waveguides and fibers, prisms and polarizers, optical switches, antennas and nonlinear optical devices etc.

The photonic band structure is the most important tool to analyze the PCs. A detailed discussion is given in Chapter 3 on the subject of the numerical methods to analyze the PCs. Both the plane wave expansion (PWE) method [9, 10, 11] and the finite difference time domain (FDTD) method [8, 12, 13] are investigated for the photonic band structure calculations. An iterative PWE method is developed to analyze the metallic PCs, whose inclusions are metal. The feasibility of a novel type of PCs, the electrically programmable PCs, is explored based on the metal-insulator transition of vanadium dioxide (VO$_2$). Unlike the ordinary PCs, wave propagation in the desired structure may be switched on/off or redirected by applying an electrical bias on the selective electrodes by taking advantage of the electrically induced VO$_2$ phase transition and subsequent modulation of dielectric properties. The characteristics of the two-dimensional (2D) VO$_2$-based PCs with line defects are analyzed using the FDTD method. Particularly, the influence of the Drude relaxation on wave guiding is examined as the high rate typical for metallic VO$_2$ can lead to the signal loss. An optimized structure is proposed to minimize the loss and simplify the fabrication.

1.3 Negative Refraction Phenomena

Another potential application of the PCs is related to the negative refraction. Left-handed media (LHM) was first proposed by Veselago [14] in 1967 for media with both
negative \( \varepsilon \) and \( \mu \). This term is named so since for a plane wave, if \( \varepsilon > 0 \) and \( \mu > 0 \), then \( \vec{E} \), \( \vec{H} \) and \( \vec{k} \) form a right-handed set of vectors and on the other hand, if \( \varepsilon < 0 \) and \( \mu < 0 \), they are a left-handed set. A very interesting case about the negative refraction is the light propagation in a system in which a plate of LHM with thickness of \( W \) placed in the right-handed media whose impedance is matched to the LHM slab. A point source is located at a distance \( d_s (d_s < W) \) from the left side of the plate as treated by Veselago [14], the LHM plate can form an image at a plane located at \( W - d_s \) measured from the right side of the LHM. If such a LHM can be realized, a very promising feature of this flat lens is that it forms a three-dimensional (3D) image of an object, which makes it similar to a mirror. But in contrast to a mirror, it forms a real image. This feature may open new possibilities for 3D photography. Moreover, Pendry [15] pointed out that such a negative refractive index material has the power to focus all Fourier components of the image, even those that do not propagate in a radiative manner. So such a lens can overcome the conventional resolution limit of the wavelength. The scarcity of LHMs in the nature has triggered a search for an artificially structured counterpart.

Recently, Pendry et al. proposed that a periodic array of metallic split ring resonators can tune the effective permeability \( \mu \) to a negative value for electromagnetic waves of certain frequencies. [16] Combined with a periodic arrangement of thin wires providing a negative \( \varepsilon \), a medium is created whose effective index is negative (i.e., left-handed). The progress achieved through the periodic array of metallic elements stimulated significant interests in the photonic crystals (PCs) due to their obvious similarities. Following a theoretical study of light propagation in 2D dielectric PCs, [17] light bending in the opposite direction to the surface normal was predicted [18] and verified experimentally [19, 20] in the microwave regime. However, the issue of focusing due to the left handedness is far more complicated. Although the claims of as such have been made in both the simulations [21] and the experiments [22], the image formation occurred only very close to the PC slab. Ref. [23] pointed out that the observed image is due to a multi-scattering induced self-collimated effect and, consequently, strongly confined in the near-field region with little dependence of the image location (i.e., the distance from the PC to the image) on the source position change.

Very recently, some studies suggested the existence of far-field images in the metallic PCs. [24, 25, 26, 27] Clearly, detailed numerical analyses of wave propagation properties are necessary to clarify the imaging phenomenon in this promising PC system. In Chapter
4, we investigate comprehensively the light propagation and the focusing effects in both ideal LHMs and metallic PCs. Specifically, we examine such crucial issues as the image dependence on the source position and the width change, index mismatch, and propagation loss quantitatively based on the FDTD method. The similarities and differences of imaging characteristics in the ideal LHMs and PCs are compared. The calculation results suggest that the focusing effect in the PCs is very complicated and may not be solely determined by the photonic band structure.
Chapter 2

Analysis of Nitride LEDs

2.1 Rise of the Nitrides

Optoelectronics holds the key to future communication developments since it offers the great advantage of high data transmission rates and extremely large bandwidth compared to the traditional pure electronic communication. Optoelectronics has advanced considerably in the last few years due to the major developments in the area of semiconductors. Along with the major advances in the synthesis of wide bandgap III-nitride semiconductor compounds, these nitrides attracted more and more interest in the optoelectronic applications. The direct bandgap of III-nitrides is one of their most beneficial features for optoelectronic device applications. In addition, the wide bandgap of gallium nitride (GaN), aluminum nitride (AlN) and their compound results in a low intrinsic carrier density which in turn leads to low voltage and low dark current, especially important for photodetectors and high-temperature electronics. III-nitrides also have high melting points and mechanical strength. Adding to the list the ability to resist radiation damage yields a material system suitable for high frequency, high power and high temperature applications. Unlike conventional semiconductors such as silicon (Si) or gallium arsenide (GaAs) which have a diamond or zinc-blende structure with a cubic symmetry, III-nitride semiconductors crystallize in their most stable form into a wurtzite crystallographic structure. So III-nitrides are polar crystals since they do not have a center of symmetry and possess
piezoelectricity [28] pyroelectricity [29] and non-linear [30, 31] optical properties. Most importantly, AlN, GaN and InN have a direct band gap of 6.2 eV, 3.44 eV and 0.76 eV [1] at the room temperature respectively, which corresponds to a wavelength from 0.2 µm to 1.63 µm and thus covers the near ultraviolet (UV), visible and near infrared (IR) spectral bands.

The first AlN, GaN and InN compounds were synthesized as early as 1907 [32], 1910 [33] and 1932 [34], respectively. Thanks to the development of modern epitaxial growth techniques, Maruska and Tietjen succeeded in growing the first GaN single crystal on a sapphire substrate by hydride vapor phase epitaxy (HVPE) in 1969. [35] This was quickly followed in 1971 with the first metalorganic chemical vapor deposition (MOCVD) [36] and then the first molecular beam epitaxy (MBE) [37] of GaN in 1974. Also in the same period, Dingle [38] et al. demonstrated optically pumped UV stimulated emission from a GaN crystal at 2 K and the first LED having a metal-insulator-semiconductor (MIS) structure was developed by Pankove et al. in 1971 [39]. Ejder reported energy dispersion of the refractive index of GaN in 1971 [40] and Monemar reported the temperature dependence of exciton recombination energy in GaN grown by HVPE in 1974 [41]. An extremely high-quality GaN with a specular surface free from cracks on a sapphire substrate was achieved by Amano et al. in 1985 [42]. The essence of this method is to insert a slightly softer material between the epitaxial layer and the highly mismatched substrate in order to reduce the interfacial free energy. In 1989, for the first time, distinct p-type GaN with low resistivity was discovered in Mg-doped GaN with low-energy electron-beam irradiation (LEEBI) [43]. Immediately, the first p-n junction UV and violet LED were demonstrated. A p-type AlGaN and a p-type InGaN were also achieved in 1991 [44] and 1994 [45], respectively. In 1992, Nakamura succeeded in making p-type GaN by thermal annealing in a N₂ atmosphere of Mg-doped GaN using Cp₂Mg [46]. Regarding n-type doping, researchers succeeded in controlling the conductivity of n-type nitrides using high-quality GaN or AlGaN grown with the low temperature deposited (LT) buffer layer in combination with SiH₄ doping. The electron concentration could be linearly controlled from an undoped level to 10¹⁹ cm⁻³ without deterioration of surface morphology when the SiH₄ flow rate was varied.

Thus, essential technologies for the realization of blue and green LEDs and laser diodes (LD) were established. Such components had long been desired in order to achieve bright full color electroluminescent displays, traffic lighting, automobile lighting, and higher density optical data storage. This impressive research and development work culminated
with the commercialization of candela class GaN-based blue LEDs in 1993. The first yellow/amber LED based on InGaN have been reported in 1995 [47]. Subsequently, the most commercially significant development since then has been the demonstration of a novel light source in 1996 in the form of a white LED that combined a blue LED and a phosphor coating [48]. The potential of this technology as a cheap, low energy consumption, more environmentally friendly solid-state light source has led to a large effort in the US called the "National Next Generation Lighting Initiative” that involves industry, universities and national laboratories. The first lasing operation with pulsed current injection was achieved in 1995 [49, 50] and a LD having continuous wave operation was announced in 1996 [51]. By 1998, an estimated lifetime of 104 hours had been achieved, which led to the successful commercialization room temperature continuous wave blue-violet laser diodes in 2001. One instrumental element in realizing long lifetime lasers was the development of lateral epitaxial overgrowth as a method to reduce dislocations in heteroepitaxially grown GaN [52, 53]. The performance and reliability of these lasers have been sufficient to allow mass production and start establishing the basic specifications of a standard for next generation high density optical disk video recordings. One of the leading standard format currently being developed, called Blue-ray Disc, is expected to make possible the recording, rewriting and playback of up to 27 GB of data on a single-sided, single layer 12 cm CD/DVD-size disc using a 405 nm blue-violet laser. These scientific and commercial successes in realizing blue LEDs and lasers, accomplished in such a short period of time, have since spurred a plethora of activity associated with III-nitrides.

A further area of research with growing interest is that of visible-blind and solar-blind ultraviolet (UV) photodetectors based on III-nitrides for use in many applications such as covert space-to-space communications, early missile threat warning, UV astronomy, chemical and biological agent detection, flame detection, engine and furnace monitoring. After the first report of a GaN ultraviolet photodetector in 1992 [54], that of GaN p-n junction photodiode in 1995 [55], and the demonstration of metal-semiconductor-metal GaN photodetectors [56], the entire range of AlGaN photodetectors has been demonstrated in 1996 with cut-off wavelengths from 200 to 365 nm, followed by the demonstration of AlGaN p-i-n photodiodes and by the realization of increasingly larger size focal plane arrays. With the recent report that the bandgap of InN is only around 0.7 eV, there is likely to be a growing interest in III-nitrides for high-efficiency solar cells.
2.2 General Formalism

Detailed understanding of the optical and electronic properties in III-nitrides is required with the growing interest in these III-V wurtzite nitrides. The detailed knowledge of electron and hole spectra near the Γ point is crucial for proper description of transport and optical properties of these materials. With the modern LED device with quantum well structures, the physical model has to be applied to guide the designs of these structures.

2.2.1 RSP Hamiltonian for a strained wurtzite semiconductor

The Hamiltonian for the valence band of wurtzite semiconductors was derived by Rashba and Sheka [3]. Later, Pikus [4] included the effects of strain and presented the invariant form for the valence-band Hamiltonian. By including terms to second order in the wave vector $\vec{k}$ and linear in the strain tensor $\varepsilon$, the RSP [5] Hamiltonian can be written in the following form independent of the choice of the basis functions:

$$
\hat{H} = I_i(\Delta_1 + \Delta_2 + A_1 k_z^2 + A_2 k_\perp^2 + D_1 \varepsilon_{zz} + D_2 \varepsilon_\perp) + \Delta_2 J_z \sigma_z + \sqrt{2} \Delta_3 (J_+ \sigma_+ + J_- \sigma_-) + D_5 (J_+^2 k_z^2 + J_-^2 k_\perp^2) - D_5 (J_+^2 \varepsilon_+ + J_-^2 \varepsilon_-) - 2i A_6 k_z ([J_z J_+] k_- - [J_z J_-] k_+) - 2i D_6 ([J_z J_+] \varepsilon_- - [J_z J_-] \varepsilon_+),
$$

where the following definitions are made:

$$
J_\pm = (J_z \pm i J_y) / \sqrt{2}, \quad 2[J_z J_\pm] = J_z J_\pm + J_\pm J_z,
$$

$$
k_\pm = k_x \pm i k_y, \quad k_\perp^2 = k_x^2 + k_y^2, \quad \sigma_\pm = (\sigma_x \pm i \sigma_y) / 2,
$$

$$
\varepsilon_{zz} = \varepsilon_{xx} + i \varepsilon_{yz}, \quad \varepsilon_\pm = \varepsilon_{xx} - \varepsilon_{yy} \pm 2i \varepsilon_{xy}, \quad \varepsilon_\perp = \varepsilon_{xx} + \varepsilon_{yy},
$$

and $m_0$ is the free electron mass. Here $z$ axis coincides with the [0001] hexagonal lattice direction, $I_i$ is the $i \times i$ unity matrix, $\sigma$s are Pauli matrices, and $J$s are components of the angular momentum operator $J$. The term $I_i(\Delta_1 + \Delta_2)$ is included in the Hamiltonian so that it fixes the energy position of the top band is equal to zero for $\vec{k} = 0$ in the bulk wurtzite materials and is used to set a energy reference point. The Hamiltonian depends on three splitting energies $\Delta_1$, $\Delta_2$ and $\Delta_3$, seven band-curvature parameters $A_1$ to $A_7$ with the last term linear in wave vector $k_\perp$ and six deformation potentials $D_1$ to $D_6$, altogether sixteen empirical constants. Since these parameters are impossible to be found from experiments, approximations have to be adopted in the calculation. we change both the band-curvature
parameters and deformation potentials according to:

\[
-A_1 = \gamma_{1z} + 4\gamma_{3z}, \quad -A_2 = \gamma_{1\perp} - 2\gamma_{3\perp}, \quad A_3 = 6\gamma_{3z},
-A_4 = 3\gamma_{3\perp}, \quad -A_5 = \gamma_{2\perp} + 2\gamma_{3\perp}, \quad -A_6 = \sqrt{2}(2\gamma_{2z} + \gamma_{3z})
\]  

(2.2)

and

\[
-D_1 = \delta_{1z} + 4\delta_{3z}, \quad -D_2 = \delta_{1\perp} - 2\delta_{3\perp}, \quad D_3 = 6\delta_{3z},
-D_4 = 3\delta_{3\perp}, \quad D_5 = \delta_{2\perp} + 2\delta_{3\perp}, \quad -D_6 = \sqrt{2}(2\delta_{2z} + \delta_{3z}).
\]  

(2.3)

To the special case of a strained-layer semiconductor pseudomorphically grown on a (0001)-oriented substrate, we can adopt the model of a biaxial strain:

\[
\varepsilon_{xx} = \varepsilon_{yy} = \frac{(a - a_0)}{a_0}, \quad \varepsilon_{zz} = -\left(\frac{2C_{13}}{C_{33}}\right)\varepsilon_{xx}, \quad \varepsilon_{xy} = \varepsilon_{yz} = \varepsilon_{zx} = 0.
\]  

(2.4)

Where \(a\) and \(a_0\) are the lattice constants of the substrate and the thin layer material, \(C_{13}\) and \(C_{33}\) are the elastic stiffness constants and \(\varepsilon_{ij}\)s are the components of the strain tensor.

So for the biaxial strain we can define \(\varepsilon_\perp = 2\varepsilon_{xx} = 2\varepsilon_{yy}\) and \(\varepsilon_\parallel = \varepsilon_{zz}\) as simplifications.

Following an approach described in Ref. [57], the \(6 \times 6\) RSP Hamiltonian can be transformed, by a unitary transformation, to the block diagonal form

\[
\hat{H} = \begin{pmatrix} \hat{H}_+ & 0 \\ 0 & \hat{H}_- \end{pmatrix},
\]  

(2.5)

where

\[
\hat{H}_\pm = -\begin{bmatrix} \frac{P + Q}{\sqrt{3}R} & \sqrt{3}R & \mp T \pm i\sqrt{1.5}S \\ \frac{P + Q + 2\Delta_2}{\sqrt{3}R} & P + Q + 2\Delta_2 & \sqrt{2}\Delta_3 \mp T \pm i\sqrt{1.5}S \\ \mp T \mp i\sqrt{15}S & \sqrt{2}\Delta_3 \mp T \mp i\sqrt{15}S & P - 2Q - 2\Delta_2 - 2\Delta_3 \end{bmatrix},
\]  

(2.6)

\[
P = (\Delta_1 + 2\Delta')/3 + \gamma_{1z}k_z^2 + \gamma_{1\perp}k_{\perp}^2 + \delta_{1z}\varepsilon_z + \delta_{1\perp}\varepsilon_\perp, \\
Q = -(\Delta_1 + 2\Delta')/3 - 2\gamma_{3z}k_z^2 + \gamma_{3\perp}k_{\perp}^2 - 2\delta_{3z}\varepsilon_z + \delta_{3\perp}\varepsilon_\perp, \\
R = (\gamma_{2\perp} + 2\gamma_{3\perp})k_{\perp}^2\sqrt{3}, \\
S = 2(2\gamma_{2z} + \gamma_{3z})k_zk_{\perp}\sqrt{3}, \\
T = \hbar^2k_zk_{\perp}/m_0.
\]

Quasicubic [5, 58, 59, 60] approximation is the well-known approximation that has been approved to be valid for the wurtzite nitrides. It stems from the fact that the nitride wurtzite structure could be approximated by a zinc-blende structure with a relatively small
stress applying on its [111] direction. Though it produces another symmetry group, a lot of physical quantities still show the cubic properties. Under the quasi-cubic approximation, corresponding to well-known Luttinger parameters for cubic structures, the seven valence band parameters also can be described by only three. The axial approximation [57, 61] simplifies the situation further by comparing the invariant Hamiltonian of both wurtzite and zinc-blende structures. These two approximations can be combined into the spherical cubic approximation. Under these approximations, \( \Delta' = \Delta_2 - \Delta_3 \) and \( T \) are approximated as zero, the longitudinal and transverse spin-orbit splitting parameters are equal and the longitudinal and transverse Luttinger-like parameters are equal. Similar approximations hold among deformation potential parameters. So

\[
\begin{align*}
\Delta_1 &= \Delta_{cr}, \\
\Delta_2 &\approx \Delta_3 \approx \Delta_{so}/3, \\
\gamma_{1z} &\approx \gamma_{1\perp}, \\
\gamma_{2z} &\approx \gamma_{2\perp} \approx \gamma_{3z} \approx \gamma_{3\perp}, \\
\delta_{1z} &\approx \delta_{1\perp} \approx \delta_a, \\
\delta_{2z} &\approx \delta_{2\perp} \approx \delta_{3z} \approx \delta_{3\perp} \approx -V_b/2.
\end{align*}
\] (2.7)

Here \( \delta_a \) is the hydrostatic deformation potential in the valence band and \( V_b \) is the shear deformation potential. Thus a reasonable description of valence bands in strained wurtzite crystal is achieved with a minimum of seven parameters: the hexagonal crystal field and the spin-orbit splitting energies \( \Delta_{cr} \) and \( \Delta_{so} \), Luttinger-like parameters \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) as well as the deformation potential constants \( \delta_a \) and \( V_b \).

### 2.2.2 Piezoelectric and Spontaneous Polarization

Noncentrosymmetric compound crystals exhibit two different sequences of the atomic laying in the two opposing directions parallel to certain crystallographic axes, and consequently crystallographic polarity along these axes can be observed. For binary A-B compounds with wurtzite structure, the sequence of the atomic layers of the constituents A and B is reversed along the [0001] and [000¯1] directions. Thus, in the case of GaN, a basal surface should be either Ga- or N-faced. The (0001) and (000¯1) surfaces of GaN are nonequivalent and differ in their chemical and physical properties. In the absence of external electric fields, the total macroscopic polarization \( \vec{P} \) is the sum of the spontaneous polarization \( \vec{P}_{sp} \) and the strain-induced piezoelectric polarization \( \vec{P}_{pz} \). The spontaneous polarization is \( \vec{P}_{sp} = P_{sp}\hat{z} \) and the piezoelectric polarization can be calculated as

\[
P_{pz} = e_{33}\varepsilon_z + e_{31}(\varepsilon_x + \varepsilon_y)
\]

for the biaxial strain and here \( es \) are the piezoelectric coefficients. In the case of GaN, for
Ga-faced wurtzite GaN crystals, the spontaneous polarization, as well as the piezoelectric polarization, are negative. For N-faced wurtzite GaN crystals, since the polarity is opposite, they become positive. Since the different faces of GaN have opposite signs for both the spontaneous polarization and piezoelectric polarization, it doesn’t affect the magnitude of the polarization-induced field. The amount of the piezoelectric polarization in the \( z \)-direction can be expressed by the piezoelectric tensor components \( d \) via the relation

\[
P_{pz} = \left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right)\varepsilon_{\perp} = d_{31}(C_{11} + C_{12} - 2\frac{C_{13}^2}{C_{33}})\varepsilon_{\perp}.
\]

The internal electric field due to the spontaneous and piezoelectric polarizations along the [0001]-direction for (0001)-oriented wurtzite structure is given by:

\[
\xi^W = \frac{(P_{sp}^W + P_{pz}^W - P_{pz}^B)L^B}{\epsilon^W L^B + \epsilon^B L^W}, \quad \xi^B = \frac{(P_{sp}^W - P_{pz}^W - P_{sp}^B)L^W}{\epsilon^W L^B + \epsilon^B L^W},
\]

where superscripts \( W \) and \( B \) mean the well and barrier region, respectively. \( L \) and \( \epsilon \) are the layer thickness and the static dielectric constant, respectively. We assume that the barrier is relaxed so that the piezoelectric polarization in the barrier is zero. In this case, the electric field is related with the spontaneous polarization difference between the well and the barrier, the well piezoelectric polarization.

### 2.2.3 Quantum Well and the Propagation Method

In a QW, the potential profile of the conduction and valence band can be described as

\[
V_{c,v}(z) = \begin{cases} 
-e\xi^W(z - z_l) & \text{in the well} \\
\Delta E_{c,v} - e\xi^B(z - z_l) & \text{in the barrier}
\end{cases},
\]

similar to the case in Fig. 2.1(b). And if the polarization is not included, it will become a square well, as shown in Fig. 2.1(a). Here \( e \) is the electric charge, which is equal to unit charge \( q \) for valence bands and \(-q\) for conduction bands, \( \xi \) is the internal field induced by the piezoelectric and the spontaneous polarization, and \( z_l \) is the position of the left interface between the barrier and the well. The screening by free carriers can be neglected due to the small carrier concentration in the well. A detailed calculation [62] showed that the sheet carrier concentration of AlGaN/GaN and InGaN/GaN QW is normally smaller than \( 10^{11} \text{cm}^{-2} \) if the QW width is less than 6 nm. This corresponds to an estimated field of less
than 0.02 MV/cm, which is much smaller than the induced field typically in the MV/cm range for nitride QWs.

While the conduction sub-bands can be characterized by a parabolic-band model as

$$\Psi_{n,k_\perp}^{c,j} = e^{i\vec{k}_c \cdot \vec{r}_\perp} \psi_{n}^{c,j} |s, \eta\rangle \quad (2.11)$$

where

$$\psi_{n}^{c,j} = A_n^{c,j} e^{ik_{c,n}^j(z-d_j)} + B_n^{c,j} e^{-ik_{c,n}^j(z-d_j)}. \quad (2.12)$$

Here we assume the wave function in the conduction sub-bands does not depend on the perpendicular wave vector $k_\perp$. The conduction sub-band energy is solved by the effective mass equation for electrons

$$\left[-\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2} + V_c(z)\right] \psi_c^j(z) = E_c^j(k_\perp = 0) \psi_c^j(z) \quad (2.13)$$

and

$$E_c^j(k_\perp) \approx E_c^j(k_\perp = 0) + \frac{\hbar^2 k_\perp^2}{2m_e^j}. \quad (2.14)$$

Under the quasicubic approximations, the upper and lower $3 \times 3$ Hamiltonian matrices have the identical eigenstates and can be transformed via the sign change of $k_z$. Since both Hamiltonians are symmetric to $k_z$, we know that these two Hamiltonians are in fact equivalent. The wave function of the $m$th valence sub-band in $j$th layer can be written as [63]

$$\Psi_{m,k_\perp}^{v,j} = e^{i\vec{k}_v \cdot \vec{r}_\perp} \sum_i \psi_{mi}^{v,j}(z, k_\perp) |u_i\rangle, \quad (2.15)$$

where

$$\psi_{mi}^{v,j}(z, k_\perp) = \sum_{s=1,2,3} \left(U_s F_s^+ e^{ik_z^j z} + V_s F_s^- e^{-ik_z^j z}\right). \quad (2.16)$$

Here $F_s$ are eigenfunction components for each layer, which satisfies the equation

$$\begin{bmatrix}
\hat{H}_+(\vec{k}) + V_v(z) \\
\hat{\Omega}_j 
\end{bmatrix}
\begin{bmatrix}
F_1^j \\
F_2^j \\
F_3^j 
\end{bmatrix} = E_m
\begin{bmatrix}
F_1^j \\
F_2^j \\
F_3^j 
\end{bmatrix} \quad (2.17)$$

and $U$, $V$s are coefficients determined by the boundary conditions at each interface, which can be written as

$$\begin{bmatrix}
\psi_1^j \\
\psi_2^j \\
\psi_3^j 
\end{bmatrix} = \begin{bmatrix}
\psi_1^{j+1} \\
\psi_2^{j+1} \\
\psi_3^{j+1} 
\end{bmatrix}, \quad \hat{\Omega}_j
\begin{bmatrix}
\psi_1^j \\
\psi_2^j \\
\psi_3^j 
\end{bmatrix} = \hat{\Omega}_{j+1}
\begin{bmatrix}
\psi_1^{j+1} \\
\psi_2^{j+1} \\
\psi_3^{j+1} 
\end{bmatrix}. \quad (2.18)$$
Here $\omega$ is the matrix representation of the differentiation of the Hamiltonian. For the
specified case, it can be obtained by a formal replacement $k_z^2 = -\partial^2/\partial z^2 \rightarrow -ik_z$, $k_z = -i\partial/\partial z \rightarrow -i$
and setting $k_z$ independent terms to zero:

$$\hat{\Omega}_\pm = \begin{pmatrix} -i(\gamma_1 z - 2\gamma_3 z)k_z & 0 & \mp\sqrt{2}(2\gamma_2 z + \gamma_3 z)k_\perp \\ 0 & -i(\gamma_1 z - 2\gamma_3 z)k_z & \mp\sqrt{2}(2\gamma_2 z + \gamma_3 z)k_\perp \\ \pm\sqrt{2}(2\gamma_2 z + \gamma_3 z)k_\perp & \pm\sqrt{2}(2\gamma_2 z + \gamma_3 z)k_\perp & -i(\gamma_1 z + 4\gamma_3 z)k_z \end{pmatrix}. \tag{2.19}$$

### 2.2.4 Optical Intensity Calculation

From a semiclassical treatment of the interaction between material particles and
electromagnetic radiation as described in most quantum mechanic books, the emission tran-
sition rate per unit volume from the interaction Hamiltonian $H_{vc}$ can be expressed by

$$W_{C \rightarrow V} = \frac{2}{V} \sum_{k_v} \sum_{k_c} \frac{2\pi}{\hbar} |H'_{vc}|^2 \delta(E_v - E_c + \hbar\omega)f_c(1 - f_v) \tag{2.20}$$

where

$$\hat{H}'_{vc} = \langle \Psi_v | \hat{H}'(\vec{r}) | \Psi_c \rangle \approx -\frac{eA_0}{2m_0} \hat{e} \cdot \langle \Psi_v | \hat{P} | \Psi_c \rangle \equiv -\frac{eA_0}{2m_0} \hat{e} \cdot \hat{P}_{vc} \tag{2.21}$$

and

$$f_{c,v} = \frac{1}{1 + e^{(E_{c,v} - E_f)/(k_B T)}} \tag{2.22}$$

is the possibility that the state is occupied. With a broad spectrum, the spontaneous
emission rate per unit volume per energy interval at an optical energy is given by

$$r^\delta_{sp}(\hbar\omega) = \frac{2C_0}{V} \sum_{k_v} \sum_{k_c} |\hat{e} \cdot \hat{P}_{vc}|^2 \delta(E_v - E_c + \hbar\omega)f_c(1 - f_v) \tag{2.23}$$

with the definition

$$C_0 \equiv \frac{\epsilon^2 n_{e\omega}}{\pi\epsilon_0 \hbar c^3 m_0^2}. \tag{2.24}$$

The total spontaneous emission rate per energy level per unit volume is given by

$$r_{sp}(\hbar\omega) = \left(2r^T_{sp} + r^T_{sp} \right)/3 \tag{2.25}$$

and the polarized spontaneous emission rate can be calculated including a Lorentzian line-
shape function [63]

$$r^\delta_{sp} = \frac{2C_0}{LW} \sum_{n,m} \int_{\eta=1,\perp} k_\perp dk_\perp \frac{3}{2\pi} \int \frac{d\varphi}{2\pi} \sum_{\sigma=1} I^{\eta\eta}_{nm} \left| u_i | \hat{e} \cdot \hat{P}_{vc} | S, \eta \right|^2 \int_{E_c}^{E_m} \left[ 1 - f^m_{v}(k_\perp) \right] \Gamma/2\pi (E_c - E_m - \hbar\omega)^2 + \Gamma/2)^2 \tag{2.26}$$
where \( m_0 \) is the electron rest mass, \( c \) and \( \epsilon_0 \) are the velocity of light and permittivity in free space, respectively. \( \eta \) is the electron spin, which can be either \( \uparrow \) or \( \downarrow \), \( \hat{e} \) is the polarization vector of the optical electric field, \( n^W \) is the refractive index, \( L^W \) is the QW width, \( \gamma \) is the line-width due to the scattering and \( I_{nm}^{\sigma\eta} \) is the overlap integral

\[
I_{nm}^{\sigma\eta} = \int dz [\psi_{mn}^j(z)]^* \psi_{n}^j(z).
\]

### 2.3 Parameter Database

To fully exploit the nitride properties and applications, a reliable and up-to-date band parameter database is necessary for the band calculation and device simulations. The most important and controversial parameters for nitrides include: (1) the crystal-field and spin-orbit splitting energies; (2) the Luttinger-like parameters; (3) the conduction and valence band deformation potentials that account for strain effects; (4) the piezoelectric and spontaneous polarization coefficients.

#### 2.3.1 Important Band Parameters

Early absorption studies reported a band gap of 1.8-2.0 eV [64] for InN at room temperature. Recent improvements in epitaxial growth techniques have lead to improved InN films and indicate the band gap energy is shown to be around 0.76 eV [1]. For the band gap of \( \text{In}_x\text{Ga}_{1-x}\text{N} \), it appears that \( \text{In}_x\text{Ga}_{1-x}\text{N} \) alloy’s bowing parameter is a strong function of In composition \( x \) and it decreases with increasing \( x \) [65]. Based on the results from these groups, we propose the following model of bowing parameter for \( \text{In}_x\text{Ga}_{1-x}\text{N} \) alloys with In composition \( x \leq 0.5 \):

\[
E_g(x) = \begin{cases} 
xE_g^{\text{InN}} + (1-x)E_g^{\text{GaN}} - 3.8x(1-x) & \text{if } x \leq 0.2 \\
xE_g^{\text{InN}} + (1-x)E_g^{\text{GaN}} - 2.4x(1-x) & \text{if } 0.2 < x \leq 0.3 \\
xE_g^{\text{InN}} + (1-x)E_g^{\text{GaN}} - 1.4x(1-x) & \text{if } 0.3 < x \leq 0.5 
\end{cases}
\]  

(2.28)

In contrast to zinc-blende materials, both the crystal-field and the spin-orbit interactions in wurtzite materials are responsible for the split between bands \( \Gamma_9 \), \( \Gamma_{7u} \) and band \( \Gamma_{7l} \). The recent contactless electro-reflectance study of Li [66] et al. shows three transitions of \( E_A = 3.484 \text{ eV} \), \( E_B = 3.49 \text{ eV} \) and \( E_C = 3.512 \text{ eV} \) in GaN at 15 K. The GaN
film was about 2-3 µm thick, and strain could be neglected. The transition line difference
\[ E_{AB} = E_B - E_A \] and \[ E_{BC} = E_C - E_B \] is 0.006 and 0.022 eV respectively. If we assume the
exciton broadening energies are same for all three bands, the difference of the three exciton
lines leads to the solutions of crystal-field splitting \( \Delta_{cr} \) and spin-orbit splitting \( \Delta_{so} \) from
RSP Hamiltonian through the following relations:

\[
\begin{align*}
E_{AB} &= \left[ (\Delta_{cr} + \Delta_{so}) - \sqrt{(\Delta_{cr} - \Delta_{so}/3)^2 + 8\Delta_{so}^2/9} \right]/2 = 0.006 \\
E_{BC} &= \sqrt{(\Delta_{cr} - \Delta_{so}/3)^2 + 8\Delta_{so}^2/9} = 0.022.
\end{align*}
\] (2.29)

We obtain \( \Delta_{cr} = 23 \text{ meV} \) and \( \Delta_{so} = 11 \text{ meV} \), which excellently agrees with Dugdale [67]
and Chen [68]. Table 2.1 lists the valence band curvature parameters \( A_1 \) to \( A_7 \) and the transformed
Luttinger-like parameters \( \gamma_1 \) to \( \gamma_3 \).

<table>
<thead>
<tr>
<th></th>
<th>GaN</th>
<th>InN</th>
<th>AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_1 )</td>
<td>7.24</td>
<td>7.71</td>
<td>7.22</td>
</tr>
<tr>
<td>( A_2 )</td>
<td>-0.51</td>
<td>-0.6</td>
<td>-0.51</td>
</tr>
<tr>
<td>( A_3 )</td>
<td>6.73</td>
<td>7.03</td>
<td>6.53</td>
</tr>
<tr>
<td>( A_4 )</td>
<td>-3.36</td>
<td>-3.08</td>
<td>-2.82</td>
</tr>
<tr>
<td>( A_5 )</td>
<td>-3.35</td>
<td>-3.05</td>
<td>-3.26</td>
</tr>
<tr>
<td>( A_6 )</td>
<td>-4.72</td>
<td>-4</td>
<td>-3.54</td>
</tr>
</tbody>
</table>

The strong nonparabolicity of the nitrides’ valence bands suggest that it is invalid
to use effective hole masses directly. Quasi-cubic and axial approximation requires \( \gamma_{1z} \approx \gamma_{1\perp} \) and \( \gamma_{2z} \approx \gamma_{2\perp} \approx \gamma_{3z} \approx \gamma_{3\perp} \). Table 2.1 lists the valence band parameters \( A_1 \) to \( A_7 \) and the
corresponding Luttinger-like parameters from several recent literatures. Since data from
Yeo [69] and Chen [68] satisfy the requirement better than other results, we will use Yeo et al.’s
valence band parameters for GaN and InN and Dugdale’s results [67] for AlN.

Under the quasi-cubic and axial approximations, six distinct valence band deformation potentials can be expressed in terms of the hydrostatic deformation potential $V_a$ and the shear deformation potential $V_b$. Under strain, based on the diagonalized Hamiltonian matrix we obtain:

$$
\begin{aligned}
E_A &= E_A(0) + (V_a + V_b)\varepsilon_z + (V_a - V_b/2)\varepsilon_\perp \\
E_{BC} &= E_B - E_C = \sqrt{[-\Delta_cr + \Delta so/3 + 3V_b\varepsilon_z - 3V_b\varepsilon_\perp/2]^2 + 8\Delta^2 c/9},
\end{aligned}
$$

(2.30)

where $\delta^c_\perp \approx \delta^c_\parallel = \delta^c$ and $\delta^c + \delta_a = V_a$ are applied. For GaN, Shikanai [72] et al. obtained $E_A = 3.478 + 15.4\varepsilon_z$ for exciton A’s energy. Deformation potentials are calculated from their original experiment data of ten samples shown in Table 2.2 and we obtain the hydrostatic deformation potential $V_a = -6.23$ eV and the shear deformation potential $V_b = -2.38$ eV. For InN, the calculated hydrostatic and shear deformation potentials of -2.8 [73] and -1.2 [74] eV are used, respectively.

Table 2.2: Original data of GaN from Shikanai [72] et al. and derived $V_a$ and $V_b$.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$E_A$</th>
<th>$E_B$</th>
<th>$E_C$</th>
<th>$\varepsilon_z$</th>
<th>$V_a$</th>
<th>$V_b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. 1</td>
<td>3.486</td>
<td>3.494</td>
<td>3.529</td>
<td>0.0005593</td>
<td>-6.11</td>
<td>-2.64</td>
</tr>
<tr>
<td>No. 2</td>
<td>3.484</td>
<td>3.492</td>
<td>3.521</td>
<td>0.0004822</td>
<td>-4.85</td>
<td>-1.78</td>
</tr>
<tr>
<td>No. 3</td>
<td>3.498</td>
<td>3.51</td>
<td>3.55</td>
<td>0.0011186</td>
<td>-6.27</td>
<td>-1.78</td>
</tr>
<tr>
<td>No. 4</td>
<td>3.5</td>
<td>3.51</td>
<td>3.549</td>
<td>0.0011572</td>
<td>-6.44</td>
<td>-1.63</td>
</tr>
<tr>
<td>No. 5</td>
<td>3.491</td>
<td>3.499</td>
<td>3.536</td>
<td>0.0009643</td>
<td>-5.09</td>
<td>-1.74</td>
</tr>
<tr>
<td>No. 8</td>
<td>3.488</td>
<td>3.496</td>
<td>3.531</td>
<td>0.0006557</td>
<td>-6.01</td>
<td>-2.25</td>
</tr>
<tr>
<td>No. 9</td>
<td>3.488</td>
<td>3.496</td>
<td>3.536</td>
<td>0.0005979</td>
<td>-7.35</td>
<td>-3.32</td>
</tr>
<tr>
<td>No. 10</td>
<td>3.488</td>
<td>3.495</td>
<td>3.539</td>
<td>0.0006172</td>
<td>-7.71</td>
<td>-3.87</td>
</tr>
<tr>
<td>Average</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>-6.23</td>
<td>-2.38</td>
</tr>
</tbody>
</table>

Note sample 6 and 7 are not listed since sample 6 lacks the third transition and 7 is abnormal.

Guy [75] et al. performed a careful study on the piezoelectric coefficients in GaN as shown in Table 2.3. They point out the difference between the coefficients in a bulk material versus a strained thin film. $d_{33} = 3.7$ pm/V and $d_{31} = -1.9$ pm/V were deduced for the bulk values. It has been found that the piezoelectric coefficient is strongly dependent on the strain and it causes the nonlinear polarization effect in III-V nitride alloy heterostructures. [75, 76, 77] In this calculation, we use Guy’s bulk value for GaN and derive the second order strain related coefficient from Fiorentini et al.’s calculations $d_{31}^{\text{GaN}} = d_{31}^{\text{GaN}}(1 + \frac{9.541}{0.918}\varepsilon_\perp)$ and $d_{31}^{\text{InN}} = d_{31}^{\text{InN}}(1 + \frac{7.559}{1.343}\varepsilon_\perp)$. The spontaneous polarizations are from Zoroddu [78] et al.
Table 2.3: Measurements of GaN piezoelectric polarization

<table>
<thead>
<tr>
<th></th>
<th>$d_{33}$ (pm/V)</th>
<th>$d_{13}$ (pm/V)</th>
<th>$\epsilon_{33}$ (C/m$^2$)</th>
<th>$\epsilon_{31}$ (C/m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk GaN measurement by Guy [75]</td>
<td>4.3</td>
<td>-2.2</td>
<td>1.31</td>
<td>-0.78</td>
</tr>
<tr>
<td>2.5 $\mu$m film GaN measurement by Guy [75]</td>
<td>3.7</td>
<td>-1.9</td>
<td>1.13</td>
<td>-0.68</td>
</tr>
<tr>
<td>1 $\mu$m poly GaN measurement by Guy [75]</td>
<td>2.8</td>
<td>-1.4</td>
<td>0.86</td>
<td>-0.5</td>
</tr>
<tr>
<td>0.14 epi GaN measurement by Lueng [79]</td>
<td>2.38</td>
<td>-1.19</td>
<td>0.73</td>
<td>-0.43</td>
</tr>
</tbody>
</table>

2.3.2 The Parameter Table

Apart from the band parameters and the well recognized values, we use elastic constant data from Deguchi [80] et al. for GaN and calculation results from Wright [81] for InN and AlN. The electron effective masses of these nitrides are discussed by Vurgaftman [82] et al. and notice due to the recent discovery of the narrow InN band gap, early measurements produced overestimated values [83]. Nitride parameters in Table 2.4 are used in the calculations.

2.4 Analysis of InGaN/GaN QW LEDs

As a specific example, we consider an In$_{0.16}$Ga$_{0.84}$N/GaN-based QW structure with $L^W = 3$ nm and $L^B = 7$ nm. The well is under compression and the barrier is relaxed. Figure 2.1(a) shows the potential profile without taking into account the internal field, while a more accurate calculation with the internal field is plotted in Fig. 2.1(b). The energy levels (solid lines) and the carrier distributions (dash lines) for the lowest sub-bands with the in-plane wave vector $k_\perp = 0$ are also provided. A large redshift ($\sim$0.3 eV) is clearly visible when the polarization induced field is considered compared to case (a). The piezoelectric field in the well is calculated to be -2.5 MV/cm, whereas the field due to the spontaneous polarization is 0.1 MV/cm. Under the total internal field of -2.4 MV/cm, the carriers accumulate at the interfaces between the barrier and the well region as expected. Figure 2.2 presents the valence sub-band dispersion spectrum for such a QW structure (a) without and (b) with the internal field. The internal field lifts up the valence sub-band energy levels and reduces the number of valence sub-bands in the QW. An interesting point is that the internal field seems to have only a weak influence on the dispersion curvature near
Table 2.4: GaN, InN and AlN parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>GaN</th>
<th>InN</th>
<th>AlN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice constant $a_0$ (Å)</td>
<td>3.189</td>
<td>3.538</td>
<td>3.112</td>
</tr>
<tr>
<td>Energy band gap $E_g$ (eV)</td>
<td>3.44</td>
<td>0.76</td>
<td>6.2</td>
</tr>
<tr>
<td>Relative dielectric constant $\epsilon$</td>
<td>9.38</td>
<td>15</td>
<td>8.5</td>
</tr>
<tr>
<td>Crystal-field splitting energy $\Delta_{cr}$ (eV)</td>
<td>0.023</td>
<td>0.037</td>
<td>-0.224</td>
</tr>
<tr>
<td>Spin-orbit splitting energy $\Delta_{so}$ (eV)</td>
<td>0.011</td>
<td>0.011</td>
<td>0.02</td>
</tr>
<tr>
<td>Valence band parameter $A_1$</td>
<td>-7.24</td>
<td>-9.28</td>
<td>-4.367</td>
</tr>
<tr>
<td>Valence band parameter $A_2$</td>
<td>-0.51</td>
<td>-0.6</td>
<td>-0.518</td>
</tr>
<tr>
<td>Valence band parameter $A_3$</td>
<td>6.73</td>
<td>8.68</td>
<td>3.854</td>
</tr>
<tr>
<td>Valence band parameter $A_4$</td>
<td>-3.36</td>
<td>-4.34</td>
<td>-1.549</td>
</tr>
<tr>
<td>Valence band parameter $A_5$</td>
<td>-3.35</td>
<td>-4.32</td>
<td>-1.68</td>
</tr>
<tr>
<td>Valence band parameter $A_6$</td>
<td>-4.72</td>
<td>-6.08</td>
<td>-2.103</td>
</tr>
<tr>
<td>Elastic stiffness constant $C_{11}$ (GPa)</td>
<td>373</td>
<td>223</td>
<td>396</td>
</tr>
<tr>
<td>Elastic stiffness constant $C_{12}$ (GPa)</td>
<td>141</td>
<td>115</td>
<td>137</td>
</tr>
<tr>
<td>Elastic stiffness constant $C_{13}$ (GPa)</td>
<td>80.4</td>
<td>92</td>
<td>108</td>
</tr>
<tr>
<td>Elastic stiffness constant $C_{33}$ (GPa)</td>
<td>387</td>
<td>224</td>
<td>373</td>
</tr>
<tr>
<td>Hydrostatic deformation potential $V_a$ (eV)</td>
<td>-6.23</td>
<td>-2.8</td>
<td>-</td>
</tr>
<tr>
<td>Shear deformation potential $V_b$ (eV)</td>
<td>-2.38</td>
<td>-1.2</td>
<td>-</td>
</tr>
<tr>
<td>Spontaneous polarization $P_{sp}$ (C/m²)</td>
<td>-0.034</td>
<td>-0.042</td>
<td>-0.09</td>
</tr>
<tr>
<td>Piezoelectric coefficient $d_{31}$ (pm/V)</td>
<td>-1.9</td>
<td>-2.6</td>
<td>-</td>
</tr>
<tr>
<td>Electron effective mass $m/m_0$</td>
<td>0.22</td>
<td>0.14</td>
<td>0.3</td>
</tr>
</tbody>
</table>

the zone center (for the first two valence sub-bands). This implies that the hole effective mass for these bands does not depend significantly on the internal field and/or the strain.

In Fig. 2.3, the hole distribution along $z$ axis is illustrated for the following four cases: (a) without internal field and wave vector $k_\perp = 0$; (b) without internal field and wave vector $k_\perp = 10^3 \mu m^{-1}$; (c) with internal field and wave vector $k_\perp = 0$; (d) with internal field and wave vector $k_\perp = 10^3 \mu m^{-1}$. Although the valence band mixing effect tends to produce different carrier distributions for different wave vector $k_\perp$, the internal field can suppress this effect by confining the carriers near one of the interfaces. The figure clearly confirms the latter scenario; the difference observed between cases (a) and (c) is no longer present in cases (b) and (d), which exhibit nearly identical distributions for different $k_\perp$. The effect
of strong polarization on the relative optical intensity spectra is studied in Fig. 2.4. The main emission peak is at 2.75 eV (451 nm) without the internal field and 2.43 eV (510 nm) when the field is considered, indicating a red shift of 0.32 eV. As anticipated, the strong polarization field greatly reduces the light emission and subsequently the LED efficiency by separating the electron and hole wave functions. When the internal field is accounted for, the intensity is about 400 times smaller than that without the field.

Since the amount of energy shift due the polarization field is also determined by the QW width, we examine its influence on the LED efficiency as well. In Fig. 2.5, the intensity spectra for an In$_{0.16}$Ga$_{0.84}$N/GaN QW are shown for different well thicknesses. The barrier width is fixed at 15 nm to simulate the results of Damilano et al. [84] The emission peaks are calculated to be 2.76 eV (450 nm), 2.33 eV (532 nm), and 1.9 eV (654 nm) corresponding to the InGaN well thickness of 1.5, 3, and 5 nm, respectively, which are in good agreement with the experimental result of 2.75 eV (451 nm), 2.33 eV (532 nm), and 1.89 eV (656 nm). [84] These three peaks give the blue, green and red light, respectively. As the well width increases, the internal potential drop becomes larger and changes the light emission from blue to red. At the same time, the electron and hole wave function separation becomes more significant and the oscillator strength decreases sharply with the increase of the well width. The calculation shows a ratio of 6.5 for blue to green and 850 for blue to red, similar to the photoluminescence data at 300 K.

Table 2.5: Comparison of calculated and experimental results for MQW emission peaks. Three emission peak columns are from: (a) experimental results; (b) Calculation results without strain relaxation model; (c) Calculation results with strain relaxation model.

<table>
<thead>
<tr>
<th>Group</th>
<th>In</th>
<th>Wells</th>
<th>$L^W / L^B$</th>
<th>Peak$^a$ (eV)</th>
<th>Peak$^b$ (eV)</th>
<th>Peak$^c$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chang[86] et al.</td>
<td>0.05</td>
<td>5</td>
<td>3/12</td>
<td>3.08</td>
<td>3.06</td>
<td>-</td>
</tr>
<tr>
<td>Damilano[84] et al.</td>
<td>0.16</td>
<td>1</td>
<td>1.5/15</td>
<td>2.75</td>
<td>2.77</td>
<td>-</td>
</tr>
<tr>
<td>Damilano[84] et al.</td>
<td>0.16</td>
<td>1</td>
<td>3/15</td>
<td>2.33</td>
<td>2.35</td>
<td>-</td>
</tr>
<tr>
<td>Damilano[84] et al.</td>
<td>0.16</td>
<td>1</td>
<td>5/15</td>
<td>1.89</td>
<td>1.91</td>
<td>-</td>
</tr>
<tr>
<td>Chuong[87] et al.</td>
<td>0.22</td>
<td>10</td>
<td>2/9</td>
<td>2.67</td>
<td>2.51</td>
<td>2.7</td>
</tr>
<tr>
<td>Lai[85] et al.</td>
<td>0.3</td>
<td>3</td>
<td>3/70</td>
<td>2.64</td>
<td>1.92</td>
<td>2.64</td>
</tr>
<tr>
<td>Chen[88] et al.</td>
<td>0.49</td>
<td>3</td>
<td>2.5/12</td>
<td>2.29</td>
<td>1.89</td>
<td>2.27</td>
</tr>
</tbody>
</table>

Table 2.5 summarizes the relevant InGaN/GaN experimental results available in the literature with the In composition ranging from 0.05 to 0.49. The number of QWs as well as the well/barrier dimensions are also provided in the table. The leftmost column on
the peak position (with the superscript \( a \)) records the experimental results of the emission peak positions, while the next one on the right (marked by \( b \)) represents our calculation results based on the model discussed earlier (i.e., the pseudomorphically strained QWs). From the comparison between these two data sets, it is clear that the calculation model fits only at the low In composition; the results deviate substantially when the In composition exceeds 0.3. For example, Lai [85] et al. grew a undoped In\(_{0.3}\)Ga\(_{0.7}\)N/GaN multiple quantum well LED structure with \( L^W = 3 \) nm and \( L^B = 7 \) nm, and observed a peak wavelength of 465 nm (2.64 eV). However, the calculation yields 1.92 eV. The inconsistency between the experimental and theoretical results indicates that the physical model used in the study is not complete.

One possibility concerns the description of strain inside the QW. According to Jahnen et al. [89], strain relaxation in the form of pinholes begins at a critical In composition of 0.14 for a 100 nm InGaN layer. Furthermore, high resolution x-ray diffraction measurements by Kim et al. [90] suggested that the critical thickness of In\(_{0.15}\)Ga\(_{0.85}\)N/GaN structure is about 60 nm. (The original article did not take the number of QWs into consideration, resulting in an erroneous estimation of 6 nm.) As is well-known, the critical thickness decreases sharply with the increase of strain. Hence, it is reasonable to assume that strain relaxation might have occurred in some of the LEDs listed in Table 2.5. Indeed, a very good correlation with the experiments was achieved when the calculation model assumes no strain in the QWs for high In composition (such as \( x \geq 0.3 \), for example) and partial strain relaxation exists for \( x > 0.2 \) (see the rightmost column denoted c in the table). This result strongly suggests that strain relaxation does occur in InGaN QW LEDs with high In composition. Perhaps the relaxation is only partial at the initial stage [the experimental result for \( x = 0.22 \) is between the strained (b) and fully relaxed (c) calculations], and becomes more significant with increasing In content. [91]

A potential issue with the assumption of strain relaxation is the subsequent defect formation in the QW LEDs. However, it is known that the defects in InGaN QWs are rather ineffective nonradiative recombination centers unlike those in pure GaN or AlGaN. At the same time, it should be pointed out when the number of defects is large enough to influence the LED efficiency, the increase of the In content will degrade the LED performance. Also, the electroluminescence spectra showed a spectral broadening and a blueshift with increasing forwarding currents. This is possibly because the number of carriers with higher energies increases with the increasing applied field. The emission occurs with a higher possibility at
nonzero wave vectors and higher valence sub-bands may also be more involved. The spectral broadening with high In content is potentially due to strain relaxation. As mentioned earlier, strain relaxation will decrease the energy separation between the valence sub-bands [see Fig. 2.2], thus permitting the higher sub-bands into play.

Another phenomenon that could further complicate our understanding is nonuniform strain relaxation leading to the localization effects [92] and/or the formation of the InN quantum dots [93]. In this case, the carriers are effectively localized in a certain potential minimum caused by the In composition fluctuation in the QWs to form quantized excitons. [94] The fluctuation in material composition is possibly due to a phase separation during the growth. However, there are several reports indicating that the phase separation only exists in relatively thick layers (300-400 nm) and/or layers with high In composition. [95, 96, 97] No phase separation has been observed in thin InGaN films, even with an In content of greater than 0.3. [95] Hence, our consideration of uniform strain distribution is justified for the structures under investigation.

2.5 White Nitride LED Design

Recently, tremendous progress has been achieved in GaN-based LEDs. [98, 99] Due to their long lifetime, small size, and low consumption of energy, they could advantageously replace incandescent bulbs or even fluorescent lamps. Basically, white light can be obtained by mixing different wavelengths with adequate intensity. [101] The most common method by which to achieve a white LED is to combine a phosphor wavelength converter with a GaN blue LED. The blue light from the LED is absorbed and then re-emitted at longer wavelength. However, additional packaging steps are needed to fabricate such phosphor-based white LEDs. Thus, it is of great interest to design an integrated one-chip white LED without use of a phosphor. [100] To achieve this, the LED must emit red, blue, and green light of adequate intensity. It is difficult to obtain efficient red emission from InGaN/GaN QW LEDs since a large internal field separates the wave functions of the holes and the electrons. The field is induced by piezoelectric and spontaneous polarization. The piezoelectric polarization is created by the lattice mismatch between the well and the barrier. The strain-induced piezoelectric field dramatically changes the dispersion spectrum of the QW structure as discussed in the last section, thus producing a large redshift and reducing
the LED efficiency.

In this section we propose a LED using an InGaN/AlInGaN QW structure. By using AlInGaN instead of GaN as the quantum barrier, we can control the internal field in the QW by adjusting the composition of the quaternary barrier. Thus, it is possible to obtain highly efficient red emission. As is well known, strain is very important in controlling the optical properties of QW LEDs. Depending on whether the material is in tension or compression, the strain decreases or increases the energy band gap, respectively. Figure 2.6 shows the energy of three valence bands and the energy band gap versus the lattice-mismatched strain for a relaxed In$_{0.2}$Ga$_{0.8}$N film. The zero energy point is set as the energy of the top valence subband when the bulk crystal is not strained. The in-plane strain $\varepsilon_x$ can be easily obtained by the lattice constants of the substrate $a_0$ and layer material $a$ using $\varepsilon_x = (a_0 - a)/a$. Positive strain means the bulk material is under biaxial tension and negative strain means the bulk is under biaxial compression. The top line represents the energy band gap of In$_{0.2}$Ga$_{0.8}$N versus the strain. It shows that the band gap of relaxed In$_{0.2}$Ga$_{0.8}$N is 2.55 eV. The band gap increases when the material is under compression and decreases sharply when it is under tension. When the in-plane strain is -0.021, which is equivalent to the compressive strain produced by an In$_{0.2}$Ga$_{0.8}$N/GaN structure, the band gap increases to 2.72 eV, which is in the blue range; when the strain is 0.021, which is equivalent to the tensile strain produced by an In$_{0.2}$Ga$_{0.8}$N/In$_{0.4}$Ga$_{0.6}$N structure, the band gap decreases to 2.2 eV, which is in the green range. The turning point of the band gap shown in Fig. 2.6 indicates that the energy of the light-hole (LH) band is equal to the energy of heavy-hole (HH) band. As seen in the figure, the HH band does not change much with the strain, but the LH band has a large shift of 0.2 eV under tension of 0.021.

Another important strain effect in the wurtzite nitride QW structure is the strain-induced piezoelectric field. The internal field is the sum of the strain-induced piezoelectric field and the field induced from spontaneous polarization. Normally the piezoelectric field is much stronger than the spontaneous field unless the QW nearly lattice matches the barrier layers. The piezoelectric field changes sign when the well material goes from tension to compression, although the spontaneous field remains negative all the time. If the polarity flips from Ga-face to N-face material, the piezoelectric as well as the spontaneous polarization changes sign. As we discussed earlier, the internal field redshifts the light emitted and, more importantly, reduces the efficiency of the light emitted because it separates the electron and hole wave functions. Figure 2.7 shows an optical intensity spectrum of a QW with different
In compositions. The well material is \( \text{In}_x\text{Ga}_{1-x}\text{N} \) and \( L^W = 3 \text{ nm} \). The barrier material is \( \text{Al}_{0.23}\text{In}_{0.2}\text{Ga}_{0.57}\text{N} \), which almost lattice matches \( \text{In}_{0.15}\text{Ga}_{0.85}\text{N} \), and \( L^B = 15 \text{ nm} \). At In composition \( x = 0.15 \), the well is relaxed and the piezoelectric field is almost zero. But the total internal field is not zero due to the existence of spontaneous polarization. The total internal field is close to zero when \( x = 0.1 \). At this point, the piezoelectric field cancels the field induced by spontaneous polarization and the oscillator strength reaches its maximum. From Fig. 2.7, we see that the optical intensity decreases sharply when \( x \) increases above 0.1. The intensity of an \( \text{In}_{0.35}\text{Ga}_{0.65}\text{N}/\text{Al}_{0.23}\text{In}_{0.2}\text{Ga}_{0.57}\text{N} \) QW LED is less than \( \frac{1}{30} \) that of an \( \text{In}_{0.1}\text{Ga}_{0.9}\text{N}/\text{Al}_{0.23}\text{In}_{0.2}\text{Ga}_{0.57}\text{N} \) QW LED.

To realize a one-chip white LED design with the same barrier, the barrier composition must be chosen carefully. Using the same barrier material requires that the red QW is in compression and that the blue QW is in tension. Also we need to avoid the strain relaxation so that the strain in all three wells should satisfy \( \varepsilon_x \leq 0.02 \). To achieve efficient red light emission, we need to minimize the internal field. But at the same time, it is difficult to process high quality InGaN film with In composition much beyond 0.5. Without the help of the internal field, it is impossible to emit red light (640 nm < \( \lambda < 680 \text{ nm} \)) even for a well In composition as high as 0.5. Thus, to achieve efficient red light emission, we have to use a well with In composition around 0.5 and keep a certain amount of internal field. Consequently, the barrier material has to lattice match \( \text{In}_x\text{Ga}_{1-x}\text{N} \) with \( x > 0.3 \). On the other hand, to realize blue light, we have to keep the light emitted within 420 nm < \( \lambda < 460 \text{ nm} \). It should be noted that both tensile strain and the piezoelectric field induce a large redshift. So it is not possible to use a low In composition for the well layer of the blue QW due to excessive tensile strain. The optical intensity from a one-chip white LED design is shown in Fig. 2.8 using the same barrier. The barrier is chosen to be \( \text{Al}_{0.23}\text{In}_{0.39}\text{Ga}_{0.38}\text{N} \) and \( L^B = 15 \text{ nm} \). The barrier almost lattice matches \( \text{In}_{0.34}\text{Ga}_{0.66}\text{N} \). Three different QW structures are chosen to emit red, green, and blue light of similar intensity. The three QW layers are 2 nm \( \text{In}_{0.53}\text{Ga}_{0.47}\text{N} \), 2.5 nm \( \text{In}_{0.38}\text{Ga}_{0.62}\text{N} \), and 1 nm \( \text{In}_{0.27}\text{Ga}_{0.73}\text{N} \) for red, green, and blue emission, respectively. The internal field in the three well layers is -3, -1.6, and -0.13 MV/cm. Their light-emitting wavelengths are 1.96 eV (632 nm), 2.27 eV (546 nm), and 2.76 eV (449 nm) for red, green, and blue, respectively. The line with closed circles is the calculated intensity for 1.5 nm \( \text{In}_{0.16}\text{Ga}_{0.84}\text{N}/\text{GaN} \) calculated in the last section. Compared with this design, the white LEDs intensity is three to four times stronger than that of 1.5 nm \( \text{In}_{0.16}\text{Ga}_{0.84}\text{N}/\text{GaN} \) blue LEDs.
The electron and hole distribution along the z axis is plotted in Fig. 2.9 at wave vector $k_{\perp} = 0$ for three QW structures for comparison: an In$_{0.53}$Ga$_{0.47}$N/Al$_{0.23}$In$_{0.39}$Ga$_{0.38}$N QW structure with $L^W = 2$ nm and $L^B = 15$ nm; an In$_{0.4}$Ga$_{0.9}$N/GaN QW structure with $L^W = 3$ nm and $L^B = 15$ nm; and an In$_{0.52}$Ga$_{0.47}$N/Al$_{0.23}$In$_{0.39}$Ga$_{0.38}$N QW structure with $L^W = 5$ nm and $L^B = 15$ nm. The first and third structures have an internal field of about -3.1 MV/cm and the second structure has an internal field of about -2.0 MV/cm. The graph clearly shows the wave function overlap in Fig. 2.9(a) is much larger than the overlap in Fig. 2.9(b) although the internal field in Fig. 2.9(a) is larger than the internal field in Fig. 2.9(b). The wave function overlap in Fig. 2.9(c) is extremely small since the QW width is large and the internal field dominates the optical properties. This implies that the oscillator strength not only depends on the magnitude of the internal field, but also on the QW width and the QW depth. To estimate whether the internal field plays an important role in LED efficiency or not, it is appropriate to compare the drop in internal potential, which is the product of the internal field and the QW width, with $\Delta E_g$, which determines the QW depth. For example, Fig. 2.9(a) will give an internal potential drop of 0.62 eV, which is much smaller than $\Delta E_g = 1.3$ eV. So the wave function overlap is quite large. In Fig. 2.9(b), the internal potential drop is 0.6 eV, which is comparable to $\Delta E_g = 0.7$ eV, and the wave function overlap is much smaller than in Fig. 2.9(a). In Fig. 2.9(c), the internal potential drop is 1.5 eV, which is larger than $\Delta E_g$ and the efficiency is very low.
Figure 2.1: Potential profile of In\(_{0.16}\)Ga\(_{0.84}\)N/GaN-based QW structure with \(L^W = 3\) nm and \(L^B = 7\) nm (a) Without the internal field (b) With the internal field.
Figure 2.2: Valence subband dispersion spectrum of $\text{In}_{0.16}\text{Ga}_{0.84}\text{N}/\text{GaN}$-based QW structure with $L^W = 3$ nm and $L^R = 7$ nm. (a) Without the internal field. (b) With the internal field.
Figure 2.3: Hole distribution of In$_{0.16}$Ga$_{0.84}$N/GaN-based QW structure with $L^W = 3$ nm and $L^B = 7$ nm for different wave vector (a) Without the internal field and $k_{\perp} = 0$ (b) With the internal field and $k_{\perp} = 0$ (c) Without the internal field and $k_{\perp} = 10^3$ $\mu$m (d) With the internal field and $k_{\perp} = 10^3$ $\mu$m.
Figure 2.4: Relative intensity spectrum of In$_{0.16}$Ga$_{0.84}$N/GaN-based QW structure with $L^W = 3$ nm and $L^B = 7$ nm (a) Without the internal field (b) With the internal field.
Figure 2.5: Intensity spectrum of In\textsubscript{0.16}Ga\textsubscript{0.84}N/GaN-based QW structure with $L^B = 15$ nm for different well width.
Figure 2.6: Three valence bands' energy positions and energy band gap as a function of the in-plane strain of a relaxed In$_{0.2}$Ga$_{0.8}$N film.
Figure 2.7: Intensity spectra of $\text{In}_x\text{Ga}_{1-x}\text{N}/\text{Al}_{0.23}\text{In}_{0.2}\text{Ga}_{0.57}\text{N}$ QWs with $L^W = 3$ nm and $L^B = 15$ nm for different In composition $x$. 
Figure 2.8: Intensity spectra of red (2 nm In$_{0.53}$Ga$_{0.47}$N as well layer), green (2.5 nm In$_{0.38}$Ga$_{0.62}$N as well layer) and blue (1 nm In$_{0.27}$Ga$_{0.73}$N as well layer) QWs in the white LED design using Al$_{0.23}$In$_{0.39}$Ga$_{0.38}$N as barrier with $L^B = 15$ nm. Solid dots represent spectrum for 3 nm In$_{0.16}$Ga$_{0.84}$N/GaN blue LED.
Figure 2.9: Electron and hole distributions along $z$ axis at $k_{\perp} = 0$ for three QW structures with $L^B = 15$ nm: (a) 2 nm In$_{0.53}$Ga$_{0.47}$N/Al$_{0.23}$In$_{0.39}$Ga$_{0.38}$N QW; (b) 3 nm In$_{0.1}$Ga$_{0.9}$N/GaN QW; (c) 5 nm In$_{0.53}$Ga$_{0.47}$N/Al$_{0.23}$In$_{0.39}$Ga$_{0.38}$N QW.
Chapter 3

Electromagnetic Theory and Photonic Crystals

3.1 Introduction to Photonic Crystals

Though multiple-layer dielectric mirrors such as those used for a high-Q laser cavity are examples of one-dimensional (1D) photonic crystals (PCs) and have already been widely used in optics for more than 70 years, they normally cannot count as the beginning of the research of PCs from the viewpoint of controlling light. The concept of PCs is proposed by E. Yablonovitch [6] and S. John [7] for the first time in 1987. They proposed the possibility of controlling the spontaneous emission of photons within the photonic bandgap (PBG). The propagation of light in this photonic energy range is inhibited in all directions in such a material, sometimes called as omnidirectional PBG. At almost the same time, John argued that light localization occurs in a uniform PC, when randomness is introduced in photonic atom arrangement, also described as doping by E. Yablonovitch [102]. PCs show promising applications on a lot of optical elements such as light emitters, resonators and filters, waveguides and fibers, prisms and polarizers, optical switches, antennas and nonlinear optical devices etc. [8] The following discusses some of its important applications.
3.1.1 Applications on Light Emitters

Due to their high efficiency, large bandwidth and compact size, semiconductor lasers have become indispensable for optical applications. For highly integrated optoelectronic circuits, today’s standard semiconductor lasers are clearly necessary for the miniaturation. One direct application is the use of PCs as the cavity mirrors. Ridge waveguide lasers with PC mirrors were first produced for GaAs based lasers [103] and later on for InP lasers at 1.55 \( \mu \)m wavelength. For the production of semiconductor lasers with two-dimensional (2D) PC mirrors, the combination of a ridge waveguide structure with PC mirrors has the advantage of relaxed requirements concerning the fabrication of the PC structures. To achieve single mode emitting lasers, another PC mirror inside the laser cavity can be introduced. The additional mirror results in the formation of two coupled cavities with a different mode spacing [104]. Also, as the first application discussed in Yablonovitch’s paper, the localized light at a defect induced into a PC exhibiting a PBG, which is acting as an ultra small laser cavity. The first lasing operation was demonstrated by photopumping at low temperature in 1999. [105] The simple defect is one missing element from a uniform PC. Thus far, a modified single point defect cavity recorded the lowest threshold of 0.2 mW. [106] In such laser, however, the internal quantum efficiency is restricted by surface recombination to less than 30% in a typical PC slab and the threshold pump power at low temperature is nearly 10 times higher than that of other microcavity lasers such as Vertical-cavity surface-emitting lasers (VCSELs) and microdisks at room temperature. Therefore, an effective surface treatment that suppresses the surface recombination is crucial in PC microcavity lasers.

VCSELs have been an attractive research subject due to their potential applications such as data transmission in optical network, optical interconnects, optical storage, and laser printing etc. Compared with the edge-emitting lasers, VCSEL design allows the chips to be manufactured and tested on a single wafer and large arrays of devices can be created. One of the attractive features about the VCSEL is its potential for low lasing threshold. [107] This potential stems directly from the ability to minimize the active volume using the short, low-loss vertical cavity. The potential for low threshold current, along with single spectral mode lasing, good beam characteristics, and surface normal emission, makes the VCSEL an important device for integrated optoelectronic applications. Recently the incorporation of PCs into VCSELs becomes an interesting direction because PC-VCSELs have
been demonstrated to be effective for the transverse mode control. \cite{108, 109, 110} 2D PC patterns etched into the top distributed Bragg reflectors (DBRs) of VCSELs have recently been demonstrated experimentally as a method of achieving single mode operation. \cite{108}

In addition, the polarization control of a triangular PC-VCSEL has also been reported by the modification of circular holes into elliptical air holes. \cite{111} Another attractive feature of PC-VCSEL structure is the enlargement of the emission area compared to that of oxide confined VCSEL with a small aperture which is typically less than 3 µm in diameter required by the single mode operation. Buried oxide apertures within VCSELs formed by selective oxidation of AlGaAs layers have enabled improved laser performance due to the reduction to the active volume of the lasers. However, as the laser diameter is decreased to 3 µm, the threshold current density increases and as the diameter is decreased further, the threshold current itself increases. \cite{112} This has been attributed to deterioration in both the optical and electrical characteristics of the lasers as the size decreases, with large diffraction losses from the oxide apertures and increased leakage current. Therefore we expect PC-VCSELs with an enlarged emission area to have the advantages of higher power output. This could be developed to solve the long existing problems in the fabrication and operation of the VCSEL design at high powers.

Group velocity close to zero can be obtained near the edges of the PBG as well as the Γ symmetry point of the Brillouin zone. Propagation modes presenting an almost flat dispersion curve over almost the entire Brillouin zone may also exist. The Band-edge laser is the expansion of a conventional DFB laser toward a 2D periodic structure. \cite{113} A unique advantage of this laser is the coherent lasing operation over the wide 2D area of a uniform PC. This laser is expected to be a high-power single-mode surface-emitting laser. It will be at a practical level by improving two general conditions: one is the threshold current or power due to the wide area current, and the other is the low light extraction efficiency due to the different directions of the resonance and light extraction.

Solid-state light emitting diodes (LEDs) with high external efficiency are currently in high demand for a variety of applications including flat panel displays, printers, optical interconnects in computers, and general lighting. However, while the internal quantum efficiency (QE) is close to 100%; most of the light is lost to guided modes in the semiconductor materials due to the strong refractive index of the semiconductor and only about \(\frac{1}{4n^2}\) of the light emitted radiates through the top and bottom. Several solutions have been devised in order to collect a larger number of photons such as the use of thick transparent layers and
placing it inside a planar cavity. \[114\] 2D PhCs are considered as suitable candidates for increasing the emission efficiency of LEDs beyond the limit values. An extraction of 100\% has been predicted for a 2D PC slab where the frequency lies either in the bandgap or in an allowed band of higher order. \[115\] The performance of the real device is disturbed by the surface recombination. \[116\] To avoid it, a structure with a PC pattern separated from the light-emitting area was studied. \[117\] In addition, the formation of metal electrodes for current injection is essentially difficult in these structures. Another simpler structure that may be useful is the surface grating 2D PC. The improvement of the efficiency by a factor 2 to 3 was confirmed. \[118\] It is attractive when considering the shallow etching process of 0.5 \(\mu\)m depth for the surface grating, a relatively large lattice constant of several \(\mu\)m, low wavelength sensitivity, robustness against structural imperfections and adaptability to arbitrary materials.

\section*{3.1.2 Applications on Waveguides and Optical fibers}

The line defect induced into a uniform PC acts as an optical waveguide. This is the so-called PC line-defect waveguide. A PC slab composed of hoels was employed in the experiment and the 2D PC of holes exhibits a wide PBG inside the 2D plane for TE-like polarization. \[119\] The biggest topic of the PC waveguide is the feasibility of ultra-compact waveguide elements such as sharp bends, small branches, and short directional couplers. The modal behavior is much more complex and the design window for efficient transmission is much narrower for these elements. To avoid these problems, various modified structures have been investigated. \[120\] To have an improvement on the PC waveguide, we may combine the high index contrast waveguide and the PC waveguide. Also, the unique ultralow group velocity at the band edge in PCs is attractive. Another important issue is the optical coupling between the waveguide and the single-mode fiber. Two methods are being studied; one is the mode size converter \[121\] and the other is a grating coupler \[122\].

Two kinds of PC fibers are pioneered by Russell \textit{et al.} \[123, 124\] and partly commercialized. They are fabricated by drawing a pure silica glass perform with many air holes. They have periodic structures in their cross sections and uniform structures along the optical axis. The first kind has a dielectric defect at the center of the PC as the fiber core and called a holey fiber. The principle of light propagation in the holey fiber is total internal reflection. Light is confined around the center silica core by the difference between the index
of the core and the effective index of the PC cladding. This fiber has unique features for the single-mode condition and related strong optical confinement, the dispersion characteristic, and the polarization characteristic. The second one has an air defect at the center of the PC as the fiber core. This fiber is based on reflection by the PBG, which can be controlled by the design of the lattice and the shape of holes. Therefore, single-mode propagation in a large size core and a small radius bend, which cannot be achieved in a holey fiber, are expected. Recently, the propagation loss was reduced to dB/km order. The remaining issue is the relative narrow transmission range dominated by the range of the PBG.

3.1.3 Applications on Resonators and filters

Resonators (cavities) and filters are the key components in wavelength division multiplexing (WDM) systems. PCs are expected to realize such ultra small functional components through the utilization of defects in PBG. A point defect in a PC can be an ultimately small cavity for sinusoidally oscillating light waves. So far, the combination of such a point defect and line-defect waveguides has been investigated. For the extraction of resonant light, the coupling to another waveguide [125] and the direct coupling to free space [126] were proposed and the latter was demonstrated as an add/drop filter. The wide range tenability of the resonant frequency is obtained by controlling the defect size. However, to get a target resonant frequency, the defect size must be controlled with nanometer order precision. Current interest for researchers is the improvement of the Q-factors and the efficiency. But in a real WDM system, the control of the filter function is necessary to obtain high efficiency. For this purpose, the design of coupled defects will be an important issue in future.

3.2 Analysis of Photonic Crystals

Development of the methods for analyzing photonic crystals has progressed rapidly. In particular, the foundation of photonic crystal analysis has been strengthened by the work of theoretical researchers of solid state physics, including research groups individually headed by Lueng [9], Zhang [10] and Ho [11]. They used the plane wave expansion (PWE) method to calculate energy bands, which is an optical version similar to the method used
in solid state physics. In 1990, using the PWE method, Ho et al. calculated the band configuration of a diamond structure, and first showed that it is possible to obtain a complete PBG. [11] In addition to providing a basic physical understanding of these phenomena, this technique is of general use in a wide range of application fields.

At around the same time, the scattering matrix method (SMM) appeared on the scene. [127, 128] This method has an inherent advantage in its ability to derive the spatial distribution of electromagnetic fields with a high degree of accuracy in a short time, even in the case of large scale nonperiodicity and defect introduction. However, the constraint on the structure of the photonic atom renders this method suitable for basic analysis only. The following limitations apply: (1) this method can only be applied to 2D crystals with circular shape inclusions or three-dimensional (3D) PCs formed by spherical inclusions because the calculation task is based on the analytical solutions induced for circular figures. (2) The objects must be isolated from each other. The same restriction is also applied on the multiple multipole method (MMP). [129, 130] These techniques generally require the natural basis of function for the inclusion scatters can preserve the symmetry of the lattice structure.

Since there are almost no limitations concerning the structures of photonic atoms, the finite-difference time-domain (FDTD) method is capable of computing photonic band structures for arbitrary frequency dependence and arbitrary geometry. [8, 12, 13] Additionally, the approach can observe the dynamics of the wave propagation in the PhCs and the corresponding transmission and reflection spectra. Another unbeatable advantage is the method is simple, stable and suitable for massive parallel computation. There are also other methods such as the finite element method (FEM) [131, 132], the finite difference method (FDM) [133, 134], the beam propagation method (BPM) [135] etc. Though they offer certain advantages under some specified situations, the PWE method and the FDTD method are considered to be the principle methods for analyzing PCs.

In this section, we describe the general formalism of the photonic band structure calculation for both dielectric and metallic 2D PCs. Here, the metallic PC is the PC whose inclusion is metal and the dielectric PC is the PC whose inclusion is dielectric medium. PWE method has been used extensively in the photonic band structure calculation extensively. In this method, the problem reduced to an eigenvalue problem. Unfortunately, the PWE method is only successful with frequency independent materials, and for the metallic PCs
where the metal’s dielectric function follows the Drude form of

$$\varepsilon_m(\omega) = \varepsilon_\infty \left[ 1 - \frac{\nu_p^2}{\nu(\nu + i\gamma)} \right], \quad (3.1)$$

where $\varepsilon_m$ is the dielectric function of the metallic inclusions, $\varepsilon_\infty$ is the dielectric constant of the metallic inclusions at high frequencies, $\nu_p$ is the plasma frequency, $\varepsilon_h$ denotes the dielectric constant of the host medium, the PWE method is only applicable under the condition of $\varepsilon_\infty = \varepsilon_h$ and the relaxation rate $\gamma = 0$. [136] Since the requirement $\varepsilon_\infty = \varepsilon_h$ is hard to be satisfied in the realistic design, the PWE method has never been used in the practical modeling of the metallic PCs. Here we develop an iterative PWE method to expand its capability to the general Drude form. Also, the popular FDTD method is included to calculate the photonic band structure and investigate the wave propagation in the metallic PCs. To avoid the surface waves located at the interface (i.e., the surface plasmon polaritons [12]) that appear in the H polarization, we consider only E polarization in the calculation and the TM source is always used in the metallic PC simulations.

### 3.2.1 PWE calculation for 2D dielectric PCs

The propagation of electro-magnetic waves is determined by the Maxwell equations,

$$\nabla \cdot \vec{B} = 0 ; \quad \nabla \times \vec{H} - \frac{\partial \vec{D}}{\partial t} = \vec{J} ;$$

$$\nabla \cdot \vec{D} = \rho ; \quad \nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0 . \quad (3.2)$$

Where $\vec{E}$ and $\vec{H}$ are the macroscopic electric and magnetic fields, $\vec{D}$ and $\vec{B}$ are the displacement and magnetic induction fields, $\rho$ and $\vec{J}$ are the free charge density and the current density. Usually inside the PCs $\rho = 0$ and the current density can be included by the use of the complex dielectric constant. For most materials, the magnetic permeability is very close to unity, $\vec{B} = \vec{H}$, while for isotropic media, $\vec{D} = \varepsilon(\vec{r})\vec{E}$. Then for a wave with frequency $\omega$, Maxwell equations are simplified as:

$$\nabla \times \left[ \frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H} \right] = \left( \frac{\omega}{c} \right)^2 \vec{H}(\vec{r}) ;$$

$$\frac{1}{\varepsilon(\vec{r})} \nabla \times \left[ \nabla \times \vec{E} \right] = \left( \frac{\omega}{c} \right)^2 \vec{E}(\vec{r}) . \quad (3.3)$$

where $\varepsilon(\vec{r})$ is equal to the dielectric constant of the inclusion medium $\varepsilon_i$ when inside the inclusion medium and is equal to the dielectric constant of the host medium $\varepsilon_h$ when inside
the host mediums. These two equations are the governing equations in the photonic band structure calculation.

Drilling periodic holes on a flat dielectric slab with infinite thickness can be a simple example of a 2D PC. Assume the electromagnetic wave propagates in the XY plane, there are two independent polarizations for this case: H polarization (the magnetic field in the Z direction) and E polarization (the electric field in the Z direction). We may transform the reciprocal of the dielectric constant $\varepsilon(\vec{r})$ into $\varepsilon^{-1}(\vec{r}) = \sum_{\vec{G}} \bar{\varepsilon}_{GG} e^{i\vec{G} \cdot \vec{r}}$ due to the periodicity of the dielectric constant, where $\vec{G}$ is the reciprocal lattice vector. Similarly, to satisfy the Bloch theorem, we expand electrical and magnetic field as $\vec{E}(\vec{r}) = \vec{E}_{G} e^{i(\vec{k} + \vec{G}) \cdot \vec{r}}$ and $\vec{H}(\vec{r}) = \vec{H}_{G} e^{i(\vec{k} + \vec{G}) \cdot \vec{r}}$ respectively, where $\vec{k}$ is the reduced wave vector. Then we derive the eigenvalue equations for H and E polarizations:

$$
\sum_{\vec{G'}} \bar{\varepsilon}_{GG'} \left[ (\vec{k} + \vec{G}) \cdot (\vec{k} + \vec{G}') \right] H_{G'} = \left( \frac{\omega}{c} \right)^2 H_{G};
\sum_{\vec{G'}} \bar{\varepsilon}_{GG'} \left| (\vec{k} + \vec{G}) \right| H_{G'} = \left( \frac{\omega}{c} \right)^2 E_{G},
$$

where $E_{G}^1 = \left| \vec{k} + \vec{G} \right| E_{G}$. Assume the inclusions are cylinder shapes as the stated example, the dielectric constant of the rods is $\varepsilon_i$ and the dielectric constant of the background is $\varepsilon_h$, $\bar{\varepsilon}_{GG'} = \left\{ \begin{array}{ll} 
\varepsilon_h^{-1} - f(\varepsilon_h^{-1} - \varepsilon_i^{-1}) & \text{if } \vec{G} = \vec{G}' \\
2f(\varepsilon_i^{-1} - \varepsilon_h^{-1})J_1(A) & \text{if } \vec{G} \neq \vec{G}'. 
\end{array} \right.$

Here $A = \left| \vec{G} - \vec{G}' \right| (r/a)$ and $r$ is the radius of the rods. $J_1$ is the Bessel function of the first order and $f$ is the filling fraction, which is the ratio of the inclusion area to the total area in the 2D case.

3.2.2 FDTD calculation for 2D metallic PCs

The standard differentiation is applied on the equation

$$\nabla \times [\nabla \times \vec{E}(\vec{r}, t)] + \mu \varepsilon \frac{\partial^2}{\partial t^2} \vec{E}(\vec{r}, t) = 0 \tag{3.6}
$$

and yields the scheme [13]

$$
\frac{\varepsilon_{ij} \delta_{tt} E_z^n}{(c\Delta t)^2} - \frac{\delta_{xx} E_z}{(\Delta x)^2} - \frac{\delta_{yy} E_z}{(\Delta y)^2} = 0 \tag{3.7}
$$

where

$$
\delta_{tt} E_z^n = E_{ij}^{n+1} + E_{ij}^{n-1} - 2E_{ij}^n ;
\delta_{xx} E_z = E_{i+1,j}^n + E_{i-1,j}^n - 2E_{ij}^n ;
\delta_{yy} E_z = E_{i,j+1}^n + E_{i,j-1}^n - 2E_{ij}^n ,
$$

(3.8)
and
\[ \varepsilon_{ij} = \begin{cases} \varepsilon_\infty \left[ 1 - \frac{\nu^2}{\nu^2 + \gamma^2} \right] & \text{inside the metallic inclusion} \\ \varepsilon_h & \text{inside the host medium.} \end{cases} \] (3.9)

The stability of the scheme is studied by Von Neumann Criteria: Express the field as 
\[ E_n = \lambda_n e^{i(k_1 x + k_2 y)h} \] and When \( |\lambda| \leq 1 \), the scheme is stable. Otherwise, it is unstable. Assume \( \Delta x = \Delta y = h \) and \( \gamma = 0 \), we obtain
\[ \varepsilon_{ij}(\lambda + \lambda^{-1} - 2) + \frac{4}{h^2} \left[ \sin^2 \left( \frac{k_h}{2} \right) + \sin^2 \left( \frac{k_h}{2} \right) \right] = 0. \] (3.10)

For \( \varepsilon > 0 \), with the definition of \( \alpha = \frac{2\pi \Delta t}{\sqrt{\gamma_0}}, \) \( \theta_1 = \frac{k_h}{2} \), and \( \theta_2 = \frac{k_h}{2} \), to satisfy \( |\lambda| \leq 1 \) requires \( \alpha^2 (\sin^2 \theta_1 + \sin^2 \theta_2) - 2 \leq 4 \) for arbitrary \( \theta_1 \) and \( \theta_2 \). This leads to the stability inequality of \( \frac{\alpha^2}{\alpha} \leq \sqrt{\frac{\pi}{2}} \); for \( \varepsilon_{ij} < 0 \), \( \left[ \alpha^2 (\sin^2 \theta_1 + \sin^2 \theta_2) + 2 \right] \leq 4 \) is required to be stable, which is impossible to be satisfied. So the scheme is unstable. Unfortunately, in our interested infrared region, the dielectric constant of the metal is negative, and calculation in the frequency domain will cause the stability problem. Here, we use the response function, which is the Fourier transform of the dielectric function in the band structure calculation:

\[ \Phi(\vec{r}, t) = \begin{cases} 0 & \text{for } t < 0 \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \varepsilon(\vec{r}, \omega) e^{-i\omega t} & \text{for } t \geq 0. \end{cases} \] (3.11)

Then, by combining the Maxwell’s equations and the Fourier transformed dielectric function \( \varepsilon_m(\vec{r}, \omega) \) as in Ref. [12], one can obtain
\[ \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial t^2} + \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial x^2} - \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial y^2} = 0 \] (metallic region),
\[ \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial t^2} + \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial x^2} - \frac{\varepsilon_m}{c^2} \frac{\partial^2 E_z(\vec{r}, t)}{\partial y^2} = 0 \] (non-metallic region),

where \( F(\vec{r}, t) = \frac{4\pi^2 \varepsilon_m c^2}{\alpha^2} \int_0^\infty e^{-\gamma t} \frac{\partial }{\partial t} E_z(\vec{r}, t') dt' \). The boundary condition satisfies the Bloch theorem \( \vec{E}(\vec{r} + \vec{R}, t) = e^{i\vec{k} \cdot \vec{R}} \vec{E}(\vec{r}, t) \); here, \( \vec{E} \) is the electric field, \( \vec{R} \) the lattice vector, and \( \vec{k} \) the reduced wave vector. The initial field distribution is set to satisfy the Bloch theorem as suggested by Chan et al. [137]

\[ E_z(\vec{r}) \big|_{t=0} = \sum G \frac{[\vec{k} + \vec{G}]}{\sqrt{\varepsilon_\infty}} e^{i(\vec{k} + \vec{G}) \cdot \vec{r}}, \]
\[ E_z(\vec{r}) \big|_{t=\Delta t} = \sum G \frac{[\vec{k} + \vec{G}]}{\sqrt{\varepsilon_\infty}} e^{i(\vec{k} + \vec{G}) \cdot \vec{r} - \frac{|\vec{G}|^2}{\sqrt{\varepsilon_\infty}} \Delta t}. \] (3.13)

Finally, the field is again transformed to the frequency space and the band structure is obtained by observing the peaks of the transformed field.
3.2.3 PWE calculation for 2D metallic PCs

Kuzmiak and his co-workers [136] move the dielectric function from the left side of the second equation of Eq. (3.2) to the right. Similarly expand the dielectric function and the field, for E polarization yield

\[ f \frac{\nu_p^2}{c^2} E_G + \frac{|\vec{k} + \vec{G}|^2}{4\pi^2\varepsilon_h} E_G + 2f \frac{\nu_p^2}{c^2} \sum_{\vec{G} \neq \vec{G}'} \frac{J_1(A)}{A} E_{G'} = \left(\frac{\nu}{c}\right)^2 E_G \]  

(3.14)

for the case of \( \varepsilon_\infty = \varepsilon_h \) and \( \gamma = 0 \). Now we eliminate these limits by iteration and consider the following two cases: (a) \( \varepsilon_\infty \neq \varepsilon_h \) and \( \gamma = 0 \) and (b) \( \varepsilon_h = \varepsilon_\infty \) and \( \gamma \neq 0 \). For simplicity the most general case of \( \varepsilon_\infty \neq \varepsilon_h \) and \( \gamma \neq 0 \) is not discussed here, which can be solved similarly as in case (b).

For \( \varepsilon_\infty \neq \varepsilon_h \) and \( \gamma = 0 \), write the dielectric constant of the metal as

\[ \varepsilon_m(\nu) = \varepsilon_\infty \left(1 - \frac{\nu_p^2}{\nu^2}\right) = \varepsilon_h \left(1 - \frac{\nu_p^2}{\nu^2}\right) - \varepsilon', \]  

(3.15)

where \( \nu_p^2 = \frac{\varepsilon_\infty}{\varepsilon_h} \nu_p^2 \) and \( \varepsilon' = \varepsilon_h - \varepsilon_\infty \). Then the Fourier transform of the dielectric function becomes

\[ \bar{\varepsilon}_{GG'} = \begin{cases} \varepsilon_h - f \left(\varepsilon_h \frac{\nu_p^2}{\nu^2} + \varepsilon'\right) & \text{if } \vec{G} = \vec{G}' \\ -2f \left(\varepsilon_h \frac{\nu_p^2}{\nu^2} + \varepsilon'\right) \frac{J_1(A)}{A} & \text{if } \vec{G} \neq \vec{G}' \end{cases} \]  

(3.16)

and the eigenvalue equation modifies to

\[ f \left(\varepsilon_h \frac{\nu_p^2}{c^2} + \frac{\varepsilon'}{\varepsilon_h \nu^2}\right) E_G + \frac{|\vec{k} + \vec{G}|^2}{4\pi^2\varepsilon_h} E_G + 2f \left(\varepsilon_h \frac{\nu_p^2}{c^2} + \frac{\varepsilon'}{\varepsilon_h \nu^2}\right) \sum_{\vec{G} \neq \vec{G}'} \frac{J_1(A)}{A} E_{G'} = \left(\frac{\nu}{c}\right)^2 E_G . \]  

(3.17)

The initial solution is gotten by setting \( \varepsilon' = 0 \). After that, each iteration reevaluates the eigen-frequency with nonzero \( \varepsilon' \).

For the case of \( \varepsilon_h = \varepsilon_\infty \) and \( \gamma \neq 0 \),

\[ \bar{\varepsilon}_{GG'} = \begin{cases} \varepsilon_h - f \varepsilon_h \frac{\nu_p^2}{\nu(\nu+i\gamma)} \frac{\nu_p^2}{\nu^2} & \text{if } \vec{G} = \vec{G}' \\ -2f \varepsilon_h \nu(\nu+i\gamma) \frac{J_1(A)}{A} & \text{if } \vec{G} \neq \vec{G}' \end{cases} \]  

(3.18)

and the eigenvalue equation becomes

\[ \begin{pmatrix} M_1 & -M_2 \\ M_2 & M_1 \end{pmatrix} \begin{pmatrix} E_G' \\ E_G \end{pmatrix} = \left(\frac{\omega}{c}\right)^2 \begin{pmatrix} E_G' \\ E_G \end{pmatrix} , \]  

(3.19)
with sub-matrices
\[
M_1 = \frac{[k + G]^2}{4\pi^2\varepsilon_h} + f \nu^2 \text{Re}\left(\frac{\nu}{\nu + i\gamma}\right) + 2f \frac{\nu^2}{\varepsilon^2} \text{Re}\left(\frac{\nu}{\nu + i\gamma}\right) \sum_{G' \neq G} G' (A) \frac{J_1(A)}{A},
\]
\[
M_2 = f \nu^2 \text{Im}\left(\frac{\nu}{\nu + i\gamma}\right) + 2f \frac{\nu^2}{\varepsilon^2} \text{Im}\left(\frac{\nu}{\nu + i\gamma}\right) \sum_{G' \neq G} G' (A) \frac{J_1(A)}{A}.
\]  
(3.20)

Similarly, the initial solution is calculated by setting \(\gamma = 0\), followed by the reevaluation of \(M_1, M_2\) for nonzero \(\gamma\). As the matrix is not Hermitian and the eigenvalues are complex in general, it should be ensured that the imaginary part of the eigenfrequency be kept well within a preset small value and the real part shows convergence.

### 3.3 Tunable wave guiding in VO\(_2\)-based PCs

Photonic integrated circuits based on 2D PC slabs are promising candidates for optical communication, displays, data storage, and computer system devices. [8] While a number of useful elements have been demonstrated, most of them are for passive optical devices with their operation predetermined by fabrication steps. Clearly, a PC that can be programmed or reconfigured on demand by an external control will significantly increase its functionality and open drastically new possibilities. For example, if the control can be in the form of electrical bias, the resulting circuit can be readily integrated with electrical integrated circuits on a single chip for practical electro-optic systems. Thus far, various approaches (for example, via the strain, temperature and magnetic field, [138, 139, 140] etc.) have been adopted to tune the PBG or wavelength. As for the crucial tunable wave guiding, the use of the liquid crystal [141] was suggested by taking advantage of its orientation-dependent refractive index that can be controlled externally. However, the response time in the sub-millisecond range is a limiting factor for optical applications.

Since the first observation [142] of a metal-insulator (MI) transition at 340 K by Morin, VO\(_2\) has received much attention due to large changes in its electrical and optical properties. Recently, it was shown that the MI transition in this material can be initiated not only by a thermal excitation as almost all the early experiments did, but also by photonic excitation [143, 144] or a high electric field. [145, 146] While some groups argue that the electrically induced transition is due to the temperature increase brought about by the current (Joule heating), [147] Stefanovich et al. [145] pointed out that the switching mechanism is not thermal since their measurements give a negligible leakage current.
Moreover, Cavalleri et al. [143] used femtosecond x-ray and visible pulses to probe structural and electronic dynamics during an optically driven MI transition and found that the time scale of the transition is shorter than the typical internal thermalization time of a nonequilibrium phonon distribution. Thus, they also challenged the thermal model (i.e., the Peierls transition [148]) for the phase change in VO$_2$. Since the increase in carriers is the common link among all these excitation methods, it can be argued that the electron concentration, instead of temperature, is the controlling parameter for the MI transition in VO$_2$ and, consequently, it is a Mott-Hubbard transition. [149] This conclusion is further supported by fabrication of a rutile structured VO$_2$ in the semiconductor phase instead of the more common monoclinic structure. [150] Yet another group [151] reported that the monoclinic structure of the semiconductor phase does not change to the rutile structure during electronic excitation, providing direct evidence that the structural change does not induce the transition. The catastrophic situation is caused when the electrons near the Fermi surface delocalize the core electrons through the screening of the ionic potential and, thus, the number of electrons near the Fermi surface is further increased. As the applied electric field increases, more and more valence electrons tunnel through the potential barrier into the conduction band. Once the injected electron density reaches the critical value, the MI transition is triggered and a metallic state is formed. Chudnovskii et al. [146] estimated the threshold field of about 100-500 kV/cm and suggested strong dependence on the process. Since the phenomenon does not involve the Peierls transition, the intrinsic switching time is very fast (on the order of a picosecond [143, 144]). Clearly, VO$_2$ possesses the desired characteristics for fabricating the metallic PCs. Furthermore, the proposed structure is expected to be fully integrable with silicon integrated circuits. Experimental growth of thin film VO$_2$ on sapphire, metal, or silicon (followed by a layer of insulator, SiO$_2$ or Si$_3$N$_4$) has already been demonstrated. [145, 151]

Figure 3.1 shows the schematic illustration of the proposed device. The structure can be achieved straightforwardly by first drilling an appropriate hole pattern on a Si film, fill the holes with VO$_2$, and then form a 2D array of metal contacts through standard lithography and metallization techniques. Since the dielectric constants of Si and semiconductor phase VO$_2$ are similar, this structure is not expected to function much differently from the silicon film itself. However, when a suitable potential is applied to the electrodes, the VO$_2$ regions beneath the electrodes undergo the MI transition with a significant change in the dielectric properties. The resulting pattern of metallic VO$_2$ pillars within the silicon film
resembles the metallic PC slab. Once the desired photonic band structure is formed, various device elements can be defined electrically. For example, optical paths can be redefined to direct photons at a very high speed by turning off/on the bias at the chosen electrodes. In the 3rd dimension, SiO$_2$ can be used to reduce field penetration in the substrate and facilitate wave confinement inside the PC slab (in-plane wave propagation is assumed). If necessary, the top surface can also be covered with a layer of SiO$_2$. The height of the VO$_2$ pillars can be made sufficiently long (compared to the lattice period $a$) to realize a practical 2D PC structure. Alternatively, a metallic PC slab with an optimum thickness can be utilized. As discussed in Refs. [34] and [152], the slab structure is analogous to 2D PCs in many ways even though the gap is now defined, due to the finite thickness, as a range of frequencies in which no guided modes exist. The optimized slab thickness is normally on the same order of magnitude of $a$ and is related to the incident wavelength and the effective dielectric constant. Under the consideration of such parameters as the slab thickness, index contrast with the substrate and mirror symmetry, the PC slab will approximately have the same gap position and width as in the 2D PCs.

To examine the feasibility of the PC slab through a gate bias induced MI transition in VO$_2$, a 2D photonic band structure calculation is conducted. In our band calculations, the Z axis is chosen as the growth direction and the PC slab is in the XY plane. The radius of the metallic rods (i.e., VO$_2$ in the metallic phase) is $r$ and the lattice constant (the distance between the neighboring cylinders) is $a$. In the mid-infrared region (2.5 µm), the measurement of the optical constants of the VO$_2$ film gives the refractive index $n = 3.1$ and the extinction coefficient $k = 0.0$ for the semiconductor phase and $n = 1.9$, $k = 4.3$ for the metallic phase. [154] Assuming that the dielectric function of the metallic VO$_2$ follows the Drude form

$$
\varepsilon_m(\nu) = \varepsilon_\infty \left[ 1 - \frac{\nu_p^2}{\nu(\nu + i\gamma)} \right],
$$

(3.21)

we extract the plasma frequency $\nu_p = 0.768$ µm$^{-1}$ and the Drude relaxation rate $\gamma = 0.267$ µm$^{-1}$ with $\varepsilon_\infty = 9.61$. The resulting $n$ and $k$ calculation is plotted in Fig. 3.2 as a function of the wavelength. The figure also shows the results for a shorter wavelength of 0.6328 µm as comparison. [155]

Figure 3.3 shows the calculated photonic band structure for such a design with a square lattice of the period $a = 0.4$ µm and the radius $r = 0.176$ µm. The refractive index of Si is 3.4. The plasma frequency $\nu_p$ and the high frequency dielectric constant $\varepsilon_\infty$ of 0.768
µm⁻¹ and 9.61 are used for the metallic VO₂ inclusions. While the solid lines represent the results from the iterative PWE method with γ = 0, the triangular points denote those of the FDTD calculation. The first two bands also show the FDTD results with a nonzero relaxation rate (squares). From the figure, one can clearly see that the FDTD and PWE methods provide excellent agreement with each other. Moreover, it is interesting to note that the relaxation plays only a minor role in the band structure (triangles vs. squares) even with a large γ ( = 0.276 µm⁻¹). The calculated cut-off frequency is 0.5 µm⁻¹ and a large band gap appears between the first and the second band; i.e., between 0.61 µm⁻¹ (1.64 µm) and 0.738 µm⁻¹ (1.36 µm).

Once the PC structure is achieved, various device elements can be defined electrically. For example, a line defect can be formed by simply turning off the bias from a row/column of the electrodes as the VO₂ regions beneath the selected contacts experience the transition back to the semiconducting phase. Figure 3.4 shows the supercell of such a case along with the calculated band structure. Here, the solid circles represent the metallic VO₂ regions and the one in the center depicts the semiconductor VO₂ as the line defect. The grey background is Si. As indicated in the figure, one defect state exists below the cut-off frequency (near 0.383 µm⁻¹ or 2.61 µm in the Γ-X direction). The next one is found near 0.682 µm⁻¹ (1.47 µm). These defect states can be used to guide wave propagation in the PC.

To examine the feasibility of tunable wave guiding further, we investigate the structure with a L-shaped double line defect. Although this 90-degree bend is not very practical in the realistic design due to the potential complications, it nevertheless provides a clear indication on the wave guiding capabilities of the device. For numerical computation, the boundary condition of the perfectly matched layer is applied to a sample of 12×12 periods. It is also assumed that a continuous light source (with the communication wavelength of 1.55 µm) is placed at the bottom opening of the defect channel shown in Fig. 3.5(a). The corresponding plot of the calculated field pattern is provided in Fig. 3.5(b). As desired, the field is totally confined in the line defect composed of semiconducting phase VO₂ and the wave guiding is observed in spite of the presence of a sharp turn. This means that the wave propagation path can be defined on demand by an external control. However, the signal loss seems to be high as evident from Fig. 3.5(c); this is due partly to the large relaxation rate γ of metallic VO₂. The time-averaged intensity calculated from the field provides the wave guiding efficiency of about 12.6%.
The problem of large $\gamma$ may be circumvented if the use of the lossy medium (i.e., VO$_2$) is judiciously restricted. An alternative waveguide design is based on the Si/air hole PC with VO$_2$ filling only the selected holes for the desired line defects. As before, the electrodes are formed above the VO$_2$ regions. For tunable wave guiding, we consider a T-shaped line defect as shown in Fig. 3.6(a). The period $a$ and the radius $r$ of the Si/air hole PC are chosen to be 0.38 $\mu$m and 0.1672 $\mu$m, respectively, to ensure a bandgap near 1.55 $\mu$m. When no bias is applied (i.e., VO$_2$ in the semiconducting phase), the light of a proper wavelength will propagate through both the right and the left arms of the T line defect as the input enters from the bottom opening. Moreover, once the external control is employed to induce the VO$_2$ transition, this signal can be directed to the right or the left arm only, or the passage of the light can be blocked entirely. Fig. 3.6(a) shows the case when the inclusions in the left arm experience the bias-induced phase transition to the metallic VO$_2$. In this case, the wave propagates only to the right side and is generally well confined in the defect line as shown in Fig. 3.6(b); however, some penetration into the nearby region does occur due to the slight mismatch in the dielectric properties between the defect line (Si/VO$_2$) and the outside (Si/air hole) regions. It is also clearly seen that the propagation loss is substantially smaller than that of Fig. 3.5 since the signal is now exposed to the lossy medium only in the vicinity of the corner region where the metallic VO$_2$ exists. Figure 6(c) illustrates the output intensity distribution with respect to the input. The energy is mostly confined in the defect region and the peak intensity is comparable to the source intensity even under a 90-degree turn. The efficiency is calculated to be about 45.8%. However, a more meaningful assessment of the wave guiding capability is the comparison with the conventional Si/air PC (where the L-shaped double line defect is formed by the missing air holes). The calculation shows that the output intensity of the conventional Si/air PC produces a smaller but broader distribution with the efficiency of 42.4%. Hence, the result clearly indicates that the introduction of the VO$_2$ does not increase the propagation loss and can transfer a normal passive PC waveguide device into an electrically programmable PC waveguide.
Figure 3.1: Schematic diagrams of the proposed PC slab design utilizing VO$_2$. Silicon is used as the PC host medium. The radius is $r$ and the lattice constant is $a$. The corresponding gate electrodes and a back gate are not shown for the simplicity of illustration.
Figure 3.2: Optical constants $n$ and $k$ of metallic phase VO$_2$ in the near-infrared frequency region. A Drude form is assumed. The solid (hollow) square data points are from Ref. [154] and Ref. [155].
Figure 3.3: Calculated photonic band structure of the VO$_2$-based PC with a square lattice for E polarization. The host medium is Si. The triangles represent the results from the FDTD method with $\gamma = 0$ and the squares are the first two bands from the FDTD method with $\gamma = 0.276$ $\mu$m$^{-1}$. The iterative PWE results with $\gamma = 0$ are illustrated by the solid lines.
Figure 3.4: Calculated photonic band structure of the VO$_2$-based PC with a straight line defect. The schematic provides a top view of the supercell. The solid circles represent the metallic VO$_2$ regions, while the center circle symbolizes the defect (i.e., VO$_2$ in the semiconducting phase). The host medium is Si.
Figure 3.5: (a) Schematic drawing of the VO$_2$-based PC with a L-shaped double line defect. The black background is silicon. The white and grey circles represent semiconducting and metallic phase VO$_2$, respectively. (b) Calculated field pattern with the light source placed at the bottom opening of the defect waveguide. (c) Time averaged source (solid line) and output (dashed line) intensity distribution.
Figure 3.6: (a) Alternative waveguide design based on the Si/air hole PC with VO$_2$ filling only the selected areas for the T-shaped double line defect. The black background is silicon. The white circles represent air. The dark grey circles indicate VO$_2$ in the semiconducting phase comprising the wave guiding portion of the T-shape, while the light grey ones in the left branch are VO$_2$ in the metallic phase due to the applied bias. (b) Calculated field pattern with the light source placed at the bottom opening of the defect waveguide. (c) Time averaged intensity distribution. The thin solid line is the source intensity distribution at the bottom opening of the defect waveguide, while the thick dashed line represents the output intensity at the waveguide exit of the proposed VO$_2$-based Si/air PC. The output intensity of a conventional Si/air PC is also shown for comparison (thick solid line).
Chapter 4

Left-handed Media and Negative Refraction

4.1 Introduction to negative refraction

The concept "left-handed media" (LHM) was first proposed by Veselago [14] in 1967 for media with a negative refractive index. This is named since for a plane wave, if \( \varepsilon > 0 \) and \( \mu > 0 \), then \( \vec{E} \), \( \vec{H} \) and \( \vec{k} \) form a right-handed set of vectors and on the other hand, if \( \varepsilon < 0 \) and \( \mu < 0 \), they are a left-handed set. So not surprisingly, the Poynting vector \( \vec{S} = \frac{c}{4\pi} \vec{E} \times \vec{H} \) and the wave vector \( \vec{k} \) are in the opposite directions in the LHM. Since the wave vector \( \vec{k} \) is in the direction of the phase velocity \( \vec{v}_p \) and the group velocity \( \vec{v}_g \) coincides with the Poynting vector \( \vec{S} \), we also recognize that in the LHM \( \vec{v}_p \cdot \vec{v}_g < 0 \).

4.1.1 negative refraction in LHM

Since the established physics is based on the right-handed media (RHM), modifications need to be done for some basic physics. For example, as Veselago [14] has pointed out, instead of writing the index refraction as \( n = \sqrt{\varepsilon \mu} \), we have to write \( n^2 = \varepsilon \mu \) and then \( n = \sqrt{\varepsilon \mu} \) for RHM and \( n = -\sqrt{\varepsilon \mu} \) for LHM.
The LHM leads to negative refraction at the boundary between two media with different rightness. When a ray of light incidents to a media with different rightness, it is determined from the two boundary conditions: \( \varepsilon_1 E_{\perp 1} = \varepsilon_2 E_{\perp 2} \) and \( \mu_1 H_{\perp 1} = \mu_2 H_{\perp 2} \) and \( E_{\perp} (H_{\perp}) \) are the electric (magnetic) field components perpendicular to the interface. Thus the normal components of the fields \( \vec{E} \) and \( \vec{H} \) change the sign and the tangential components remains the same. If the first media is a RHM and the second one is a LHM, the tangential component of the wave vector \( k \) remains the same and the normal component changes its sign as shown in Fig. 4.1. An interesting case about the negative refraction is the light propagation in a system that is a plate of LHM with thickness of \( W \) placed in the RHM whose impedance is matched to the LHM slab. A point source is located at distance \( d_s < W \) from the left side of the plate as illustrated by Veselago. [14] The LHM plate can form an image at a plane located at \( W - d_s \) measured from the right side of the LHM as shown in Fig. 4.2. If such kind of LHM can be realized, a very promising feature of this flat lens is that it forms a three-dimensional (3D) image of an object, which makes it similar to a mirror. But in contrast to a mirror, it forms a real image. This feature may open new possibilities for 3D photography. As promising as it is, this flat lens also has a certain drawback: for an object to be imaged, it must be placed sufficiently close (i.e. less than the thickness of the lens) to the surface of the lens.

This novel phenomenon of negative refraction is questioned directly by some researchers. [156] In 2002, a paper entitled "Wave refraction in negative-index media: always positive and very inhomogeneous" is published and claim that negative refraction contradicts the causality principle. The idea is very simple with the help of Fig. 4.3. Let a wave packet be incident on an interface of the vacuum and a LHM with line AB represent its wave front at time \( t_1 \). After the ray is transmitted into the LHM, if the negative refraction happens, then the ray should have a wave front AD at time \( t_2 > t_1 \). This means that the outer ray should travel along the path BCD with infinite speed and thus violates the causality principle. Ref. [18] found from the simulation that the incident beam is eventually refracted in the negative direction. Also, they found out that each ray does not refract in the final direction immediately upon hitting the surface of the LHM. Instead, the whole wave front is trapped in the surface region for a relatively long time (of the order of a few tens of the wave period \( T \) in their simulation); and then gradually after this transit time, the wave recognizes itself and starts propagating in the negative direction as expected from the steady state solution. This provides an explanation for the occurrence of negative
refraction without violating causality.

4.1.2 A perfect lens

It has been known that no matter how lens is well made it can not focus light onto an area smaller than square wavelength. In year 2000 Pendry [15] pointed out that such a negative refractive index material has the power to focus all Fourier components of the image, even those that do not propagate in a radiative manner. Such lens can overcome the conventional resolution limit of the wavelength. Consider a LHM imaging system as shown in Fig. 4.2 and a source object emits electromagnetic wave of frequency $\omega$. In the system, the space is divided into three regions: vacuum region ($z < 0$), where the point source is located; LHM region ($0 < z \leq W$), where is the LHM slab; vacuum region ($z > W$), where the image is located. Consider the E polarization case, where the electric field has only y component, and the magnetic components is inside the XZ plane. Then the electric field in the three regions can be written in the following form of

$$
\begin{align*}
E_1(x, z) &= e^{ik_x x} \left[ A_1 e^{ik_z z} + B_1 e^{-ik_z z} \right] \\
E_2(x, z) &= e^{ik_x x} \left[ A_2 e^{ik'_z z} + B_2 e^{-ik'_z z} \right] \\
E_3(x, z) &= e^{ik_x x} A_3 e^{ik_z (z-W)}.
\end{align*}
$$

(4.1)

where $k_x$ and $k_z$ are the $x$ and $z$ component of the wave vector in the vacuum region respectively and $k_z'$ is the $z$ component of the wave vector in the LHM slab. For propagating wave, $k_z = \sqrt{\frac{\omega^2}{c^2} - k_x^2}$ and the wave vector in the LHM has $k_z' = -\sqrt{\frac{\omega^2}{c^2} - k_x^2}$. The boundary condition gives $B_1 = 0$ and $B_2 = 0$. For evanescent wave, $k_x \leq \frac{\omega}{c}$, $k_z = i\sqrt{k_x^2 - \frac{\omega^2}{c^2}}$ in the vacuum and $k_z = -i\sqrt{k_x^2 - \frac{\omega^2}{c^2}}$ in the LHM slab. Instead, the boundary condition gives $B_1 = 0$ and $B_2 = 0$. The transfer function of the system at the imaging plane is $H(k_x) = \frac{E_3(x,W+d_f)}{E_1(-d_s)} = \frac{A_3}{A_1} e^{ik_x d_f}$ and yields 1 for all $k_x$. This means the imaging system is perfect. Numerical simulations [157, 160] based on the two-dimensional (2D) finite difference time domain (FDTD) method verified the focusing effect in the hypothetical homogeneous LHM slabs. However, the claim of subwavelength imaging is still an unsettled issue since the subwavelength resolution is only verified in the lateral (X) direction. [160]
4.1.3 Recent Progress

The scarcity of LHMs in the nature has triggered a search for an artificially structured counterpart. Recently, Pendry et al. proposed that a periodic array of metallic split ring resonators can tune the effective permeability $\mu$ to a negative value for electromagnetic waves of certain frequencies. [16] Combined with a periodic arrangement of thin wires providing a negative $\varepsilon$, a medium is created whose effective index is negative (i.e., left-handed). Subsequently, the dispersion curves of this composite medium were simulated numerically and the negative group velocity observed. [158] Transmission experiments were also performed detecting a transmission region centered at $\sim 11$ GHz. [159] As stated in Ref. [159], the lattice constant $a$ is 5 mm and the ratio of $a$ to the source wavelength $\lambda$ is about 0.2, justifying its treatment as a homogenous metamaterial. Comparison with the numerical result of the hypothetical LHM supports that this composite medium does exhibit the left-handedness in a specific frequency range. [160]

The progress achieved through the periodic array of metallic elements stimulated significant interests in the photonic crystals (PCs) due to their obvious similarities. Furthermore, the PCs are more readily scalable toward the smaller dimensions necessary for the technologically important infra-red and visible wavelengths. Following a theoretical study of light propagation in 2D dielectric PCs, [17] light bending in the opposite direction to the surface normal was predicted [18] and verified experimentally [19, 20] in the microwave regime. However, the issue of focusing due to the left handedness is far more complicated. Although the claims of as such have been made in both the simulations [21] and the experiments [22], the image formation occurred only very close to the PC slab. Ref. [23] pointed out that the observed image is due to a multi-scattering induced self-collimated effect and, consequently, strongly confined in the near-field region with little dependence of the image location (i.e., the distance from the PC to the image) on the source position change. A further investigation conducted in the triangular dielectric PC system [161] also generated the images only the near-field region. So far, no dielectric PC has overcome this particular limitation.

Very recently, some studies suggested the existence of far-field images in the metallic PCs. [24, 25, 26, 27] Clearly, detailed numerical analyses of wave propagation properties are necessary to clarify the imaging phenomenon in this promising PC system. In the present paper, we investigate comprehensively the light propagation and the focusing ef-
fects in both ideal LHMs and metallic PCs. Specifically, we examine such crucial issues as the image dependence on the source position and the width change, index mismatch, and propagation loss quantitatively based on the FDTD method. The similarities and differences of imaging characteristics in the ideal LHMs and PCs are compared. The calculation results suggest that the focusing effect in the PCs is very complicated and may not be solely determined by the photonic band structure.

4.2 Imaging in an ideal LHM system

The dielectric properties of an ideal LHM can be expressed as:

\[
\begin{align*}
\varepsilon &= 1 - \frac{K_\varepsilon^2}{\nu(\nu + i\gamma_\varepsilon)} \\
\mu &= 1 - \frac{K_\mu^2}{\nu(\nu + i\gamma_\mu)}
\end{align*}
\]  

(4.2)

where \(K_\varepsilon, \gamma_\varepsilon, K_\mu, \gamma_\mu\) are the constants specific to a given material and \(\nu\) is the source wave frequency. For example, when we set constants \(K_\varepsilon = K_\mu = \sqrt{2} \mu m^{-1}\) and the source wavelength \(\lambda = 1 \mu m\) (i.e., \(\nu = 1 \mu m^{-1}\)), both \(\varepsilon\) and \(\mu\) become \(-1\) if \(\gamma_\varepsilon\) and \(\gamma_\mu\) are negligibly small. Assuming that the background is vacuum, this LHM will have the negative refraction phenomenon as schematically illustrated in Fig. 4.2. A typical field distribution of such a system is provided in Fig. 4.4(a). Specifically, the simulation is carried out on the 2D \(XZ\) plane for a LHM of \(L = 60 \mu m\) and \(W = 13 \mu m\) along with \(\gamma_\varepsilon = \gamma_\mu = 10^{-8} \mu m^{-1}\). A TM (i.e., the electric field is perpendicular to the \(XZ\) plane) point source is placed at a distance of 6.5 \(\mu m\) from the left of the LHM, exactly half of the LHM width. The perfect matched layer (PML) absorbing boundaries are assume surrounding the whole structure. Outside the LHM material, the vacuum background gives an impedance match with the LHM with the extremely small \(\gamma\). The time step of \(c\Delta t = 0.025 \mu m\) is adopted to satisfy the stability requirement. As expected, two foci appear in the field pattern [Fig. 4.4(a)]; one inside and the other outside the LHM. The first focus is located at 6.75 \(\mu m\) (\(= d_1\)) away from the left edge of the LHM, while the second is at 6.4 \(\mu m\) (\(= d_f\)) from the right edge. The sum of \(d_s = 6.5 \mu m\) and \(d_f = 6.4 \mu m\) is very close to the width of the LHM \(W = 13 \mu m\) following the rule of geometric optics. Also, the first focus position \(d_1 = 6.75 \mu m\) matches with the anticipated value of 6.5 \(\mu m\). Accordingly the calculated field pattern and the foci positions provide a clear indication of the negative refraction phenomenon.
To examine the feasibility as a superlens, [15] the field intensity distribution of the image (i.e., the second focus) is plotted along the propagation (Z) direction and the lateral (X) direction in Figs. 4.4(b) and 4.4(c), respectively. The analysis in both directions is essential to clearly demonstrate the subwavelength resolution. Unlike an earlier study, [160] in the Z direction, the calculation shows a prominent peak as the image; its intensity is more than two times of that of its neighboring peaks. The resolution represented by the full width at the half maximum (FWHM) is about 0.34 µm (i.e., 0.34λ) in the Z direction, independent of the neighboring peaks. In the lateral direction, the image is also well focused with a resolution of 0.4λ, as the intensity of the neighboring peaks is much smaller than that of the center peak. Consequently, the FDTD simulation results suggest a subwavelength resolution for both directions in an ideal LHM. It should be noted that the subwavelength resolution is possible only when the size of the lens (i.e., the length L of the slab) is much larger than the wavelength. The requirement to achieve the subwavelength resolution in the propagation (Z) direction here is \( L \geq 60 \lambda \). Furthermore, one must wait long enough for the image to be fully developed. (Here we use the time range \( 10^4 c \Delta t = 250 \lambda \). In the simulation, at that time, the peak intensity of the first focus is very close to that of the second focus.) This also means that the ideal LHM may not work as a superlens when the source signal changes rapidly beyond a certain limit.

The case with a different wavelength is studied next. As Pendry predicts the LHM plate as the perfect lens, [15] the size of the focus (i.e., FWHM) would not be dependant on the source frequency. Figure 4.5 provide the results for \( \lambda = \sqrt{2} \mu m \). Here, \( K_\varepsilon = K_\mu = 1 \mu m^{-1} \) are used to satisfy \( \varepsilon = \mu \approx -1 \). Due to the longer wavelength, the slab length is increased to 100 µm and the time step to \( c \Delta t = \frac{0.05}{\sqrt{2}} \mu m \). Other parameters (including the width W of 13 µm) remain the same as in Fig. 4.4. Figure 4.5(a) shows the field distribution after 250 time cycles, while Figs. 4.5(b) and 2(c) illustrated the field intensity of the second focus along Z and X direction, respectively. Two foci appear at the position of \( d_1 = 6.9 \mu m \) and \( d_f = 6.3 \mu m \). Resolution of 0.48 µm (i.e., 0.34λ) and 0.53 µm (i.e., 0.37λ) are obtained for the second focus along the propagation and lateral direction, respectively. The subwavelength resolution in both directions is realized. At the same time, we note that the resolution depends on the source wavelength contrary to the expectation. A resolution of 0.3-0.4λ is obtained for both the present case of \( \lambda = \sqrt{2} \mu m \) and the previous case of \( \lambda = 1 \mu m \). This resolution dependence is possibly due to the finite length of the slab and/or some rays does not propagate into the LHM slab since some of them propagate along the
We also investigate the case with a different LHM width $W$. When the LHM width is reduced to 6.5 µm as shown in Figs. 4.6(a) ($d_s = 2$ µm) and 4.6(b) ($d_s = 4.5$ µm). In case (a), two foci appear at $d_1 = 2.3$ µm and $d_f = 4.35$ µm and correspondingly, in case (b) $d_1 = 4.75$ µm and $d_f = 1.85$ µm. The calculated resolution worsens to 0.46λ and 0.5λ along the propagation and lateral direction, respectively. This trend continues and the focusing effect disappears once the LHM width is smaller than the source wavelength. A similar phenomenon of unstable focus was observed in Ref. [157] for $W = \lambda$. Hence it seems that the subwavelength resolution in an ideal LHM may require the condition $W >> \lambda$. However, if the loss is large enough and/or the index of the LHM has a mismatch with the background media, the subwavelength resolution is strongly restricted by the LHM width and it is only possible when the LHM width is very small in these cases. [162]

To further explore subwavelength imaging, we consider the case of two point sources separated by the distance of one wavelength along the propagation ($Z$) direction. Figure 4.7(a) shows the field distribution of such a case after 250 time cycles in a structure as described in Fig. 4.2 ($\lambda = 1$ µm); Figs. 4.7(b) and 4.7(c) provide a magnified view of the sources and the images, respectively. The point sources are placed at $d_{s1} = 7$ µm and $d_{s2} = 6$ µm. As expected, two foci form, each with two peaks. The two peaks of the first focus, which are inside the LHM, are located at 6.4 µm and 7.15 µm away from the left edge of the LHM, while those of the second focus are at $d_{f1} = 6$ µm and $d_{f2} = 6.75$ µm revealing an excellent match with the rule of geometric optics. Moreover, the fact that the two peaks can be clearly identified at the opposite side of the LHM slab verifies the subwavelength resolution of far-field images. However, Fig. 4.7(c) also shows uneven intensity of the two peaks due to the interference effect causing image distortion.

Finally, we examine the effects of the loss and the index mismatch on the LHM system. Although this issue has been investigated before through the transfer function and the wave vector component, it is still unclear what the critical conditions or the acceptable ranges are to have the focusing effect. Here we try to answer these questions through the simulations. With the consideration that the loss is now a significant part and an assumption of $\gamma_\varepsilon = \gamma_\mu = \gamma$, we choose $K_\varepsilon = K_\mu = \sqrt{2(\nu^2 + \gamma^2)}$ µm$^{-1}$. Then, the real part of $\varepsilon$ and $\mu$ is $-1$ and the imaginary part, which is the loss, becomes $2\gamma/\nu$. For $\nu = 1$ µm$^{-1}$, that is $\varepsilon = \mu = -1 + 2\gamma i$. Figure 4.8(a) shows the field distribution with $\gamma = 10^{-2}$ µm$^{-1}$. Other parameters still remain the same as used in Fig. 4.4. The focusing effect is strongly
degraded and the foci become very weak. The second focus is not distinguishable from the
graph due to the high loss. Figure 4.8(b) shows the relationship between the intensities of
the second focus and the Drude relaxation rate. From the graph, the focusing effect is not
influenced much when the relaxation rate is smaller than $10^{-5}$.

Along with the loss, the index mismatch also has a large influence on the imaging.
Figure 4.9 shows the field distribution with the LHM index of $n = -1.1$. We use $K_\varepsilon = K_\mu = \sqrt{2.1} \, \mu m^{-1}$ in this case. The graph shows that even for such a small index mismatch, the focusing effect is degraded since light ray with different angles refracts differently and
does not have a common focus. This can also be explained by the imaging mechanism
shown in Fig. 4.2. The foci expanded in the $Z$ direction and the peaks appear at $d_1 = 7.95$
$\mu m$ and $d_f = 4.1 \mu m$, both have a obvious deviation from the ideal value of $6.5 \mu m$. The
distortion of the foci and the large deviation on the position suggest that a small index
mismatch of several percent will have a serious impact on the imaging phenomenon in a
system composed of the ideal LHM.

4.3 Imaging in a metallic PC system

In this section we investigate the negative refraction and the imaging phenomenon
in the metallic PCs. We use a PC structure that consists of a triangular array of metallic
rods in a dielectric host medium of $\varepsilon = 6$. The radius of the metallic rods is chosen to be
$0.25 \mu m$ and the lattice constant $a$ of the PC is $1 \mu m$. The dielectric constant of the metal
follows the Drude form
\[ \varepsilon = 1 - \frac{\nu_p^2}{\nu(\nu + i\gamma)} \] (4.3)
and the permeability $\mu = 1$. Here $\nu_p$ is the plasma frequency of the metal and $\gamma$ is the
Drude relaxation rate. The photonic band structure of this PC is shown in Fig. 4.10(a)
for E polarization. In the simulation, the plasma frequency $\nu_p$ is set to be $1 \mu m^{-1}$ and
the relaxation rate is $10^{-6} \mu m^{-1}$. As suggested by Notomi [17], the negative band slope
may induce the negative effective index. We hope the fictious PC can become a LHM in
a certain frequency. So the PC is placed in a vacuum background with the lattice $\Gamma M$
direction oriented parallel to the $Z$ axis and $\Gamma K$ to the $X$ axis as shown in Fig. 4.10(b).
The PC has a length $L$ of 41 layers ($62 \sqrt{3} \mu m$) and a width $W$ of 9 layers ($13 \sqrt{3} \mu m$). The
PMLs are applied outside the system. A point source is placed at the exactly half PC width
away from the left side of the PC. The source wavelength is 2.755 \( \mu m \), corresponding to \( \frac{\lambda}{\chi} = 0.363 \) (\( a = 1 \mu m \)) and somewhere in the lower-half of the second photonic band in Fig. 4.10(a). The time step is chosen as \( c \Delta t = \frac{\lambda h}{6a} \).

Figure 4.11(a) shows a snapshot of the calculated field distribution after 20 time cycles. Clearly, a focus appears at \( 2.1\sqrt{3} \mu m \) away from the right side of the PC. The existence of the far field image indicates the existence of the negative refraction as anticipated from the negative slope of the band structure. Moreover, compared with the PC width of \( \frac{13\sqrt{3}}{3} \mu m \), the sum of \( d_s \) and \( d_f \) is \( 4.26\sqrt{3} \mu m \) and satisfies the negative refraction criteria \( d_s + d_f \approx W \). However, the issue of superlens imaging is far more complicated if we take a careful look at the field intensity distribution along the propagation (Z) direction. Figures 4.11(b) and 4.11(c) analyze the field intensity near the focus along the Z and X directions, respectively. In the lateral (X) direction, a very high peak exists at \( X = 0 \) with a subwavelength resolution of 1.54 \( \mu m \) (i.e., 0.56\( \lambda \)) as in the ideal LHM case. As for the Z direction, however, two large peaks of similar intensities are observed. The separation of these peaks is comparable to the half wavelength, suggesting that the subwavelength resolution cannot be achieved in the PC system; the earlier studies claiming otherwise [10, 25, 26, 27] reached their conclusion based only on the analysis in the lateral direction. At the same time, the peak intensity of the far field image produced by the PC is about 10 times smaller than that in the ideal LHM case with the identical source intensity. No clear focus forms inside the PCs either, contrary to the ideal LHM case.

To observe whether the image will make the corresponding move with the source position change is an important method to determine the focusing mechanism. When the source position is moved to \( d_s = \frac{\sqrt{3}}{3} \mu m \) and \( d_s = \frac{4\sqrt{3}}{3} \mu m \), the image moves to \( d_f = 3.93\sqrt{3} \mu m \) and \( d_f = 2.93\sqrt{3} \mu m \) as shown in Fig. 4.12(a) \( (d_s = \frac{\sqrt{3}}{3} \mu m) \) and 4.12(b) \( (d_s = \frac{4\sqrt{3}}{3}) \mu m \), respectively. [163] The fact that \( d_s + d_f = 4.26\sqrt{3} \mu m \approx W \) in all three cases strengthens the idea of negative refraction with an estimated effective index of \(-1\) for the PC at the selected frequency.

As many practical applications would involve a non-monochromatic source, we also consider the cases with different source frequencies. It is natural that the PC will exhibit a different effective index for different frequencies since the band slope is different. The model of the effective index dependance with the source frequency is extremely important in the lens applications and unfortunately no accurate model has been given. Figures 4.13(a) and 4.13(b) show the snapshots of field distributions with \( \frac{\lambda}{\chi} = 0.355 \), while Figs. 4.13(c) and
4.13(d) are for $\alpha / \lambda = 0.375$. Both cases (a) and (c) assume the vacuum background with the index $n_b = 1$. Since the effective index of refraction for the metallic PC is frequency dependent, the location of the image may no longer satisfy the relationship $d_s + d_f \approx W$ as the source frequency changes. Clearly, the figures show that the sum of $d_s$ and $d_f$ in case (a) is substantially smaller than the PC width $W$, while it is longer for case (c). This indicates that the effective PC index for (a) [(c)] is larger (smaller) than 1, respectively. The new value for the effective index can be estimated by searching for $n_b$ that restores the stipulated simple relationship. Figures 4.13(b) and 4.13(d) achieve this scenario when the index of the background is assumed to be 1.12 and 0.85, respectively. Two interesting points can be observed from the figures. Firstly, the focusing seems possible even with a large index mismatch (of more than 10%) in the PC-based structures. It is in contrast to results in the ideal LHM systems, where even a small mismatch can degrade the far-field image. Secondly, the frequency dependence of the effective index change is rather strong; only a 2–3% shift affects the effective index by more than 10%. Subsequently, the location of the focal point is frequency sensitive, leading to the image broadening and/or distortion in practical applications. The crucial effective index change as a function of the frequency can be estimated more systematically by utilizing the dispersion relation $\omega = \pm k c / n$, where $\omega$ is the frequency, $k$ is the wave number, $c$ is the light speed, and the $\pm$ sign corresponds to the positive/negative index, respectively. As

$$\frac{d\omega}{dk} = \pm \frac{c}{n} - \omega \frac{dn}{d\omega} \frac{d\omega}{dk} = \pm \frac{c}{n + \omega \frac{dn}{d\omega}}$$

(4.4)

and $\frac{d\omega}{dk}$ can also be calculated from the photonic band structure, $\frac{dn}{d\omega}$ is readily obtained for the given frequency once the effective index is known (e.g., $n \approx -1$ at $\alpha / \lambda = 0.363$). Then, $n$ for the neighboring frequencies can be estimated by assuming that the slope does not change appreciably. The calculation results are plotted in Fig. 4.13(c) along with two data points from the simulation of Figs. 4.13(b) and 4.13(d) ($n \approx -1.12$ at $\alpha / \lambda = 0.355$ and $n \approx -0.85$ at $\alpha / \lambda = 0.375$). The excellent match verifies the validity of the effective index model given in Eq. (3).

However, the concept of effective index based on the photonic band structure may be of limited use in predicting the imaging properties. This seems to be due to the fact that the band calculation assumes an infinitely periodic 2D array, while the realistic PC "lens" has a finite length $L$ and even smaller width $W$ (which is typically on the order of a few $\lambda$). As such, the imaging properties are strongly influence by the geometrical
parameters, which are not reflected in the band structure. Figure 4.14 shows the snapshots of field distribution with a PC width of 17 layers with two source distances of (a) \( d_s = \frac{5\sqrt{3}}{6} \mu \text{m} \) and (b) \( d_s = \frac{13\sqrt{3}}{6} \mu \text{m} \). The terminating surface of the PC does not change from the earlier calculation [i.e., Fig. 4.10(b)]; 8 layers are simply inserted into the original PC of 9 layers. The image exists at \( \frac{15\sqrt{3}}{6} \mu \text{m} \) from the PC in case (a) and at \( \frac{23\sqrt{3}}{6} \mu \text{m} \) in case (b). While the sum of \( d_s \) and \( d_f \) is a constant \( \frac{14\sqrt{3}}{3} \mu \text{m} \), it is very different from the total PC width of \( \frac{25\sqrt{3}}{3} \mu \text{m} \). Obviously this does not match with the properties of the \( n \approx -1 \) case. In other words, the effective index is modified even though the band structure calculation provides the same answer. Another interesting parameter is the terminating surface of the PC. When this surface is somewhat into the dielectric layer as shown in Fig. 4.15(a), the focal position moves very close to the PC and the distance is only \( 1.27\sqrt{3} \mu \text{m} \) compared with \( 2.1\sqrt{3} \mu \text{m} \) of Fig. 4.11(a).

Now we found that the focusing effect in the PCs is very complicated and may not be solely determined by the photonic band structure. In the following we suggest that the negative band slope may not necessarily have a negative index. This may helps to explain why only near-field images found in the dielectric PCs. [21, 22, 23] We use the Drude from

\[
\varepsilon = 6 - \frac{\nu_p^2}{\nu(\nu + i\gamma)}
\]  

(4.5)

instead of Eq. (2) as the metal’s dielectric function. Other parameters remain the same as used in Fig. 4.11. Figure 4.16(a) shows the calculated band structure of such a PC. \( \varepsilon_{\infty} = 1 \) is also shown here represented by the squares for the comparison. The snapshot of field distribution after 20 time cycles is shown in Fig. 4.16(b). Interestingly, though their second bands do not differ much, there is no focus observed no matter what frequency is chosen and the wave front is continuous inside the PCs. That infers to us that in addition to the band structure, other factors determine the negative refraction phenomena in the PC system. We suggest that a negative effective dielectric constant is necessary for the negative refraction to happen in PC-based system.

Here we use a one-dimensional (1D) example to verify the statement. A composite medium is placed in XZ plane. We assume the media can be treated as homogeneous and it has a negative effective dielectric constant. A plane wave with frequency \( \omega \) propagates in
such a media along the \( z \) direction and the field can be expressed as

\[
\begin{align*}
\vec{E} &= E_0 e^{i(k_z z - \omega t)} \hat{x} \\
\vec{H} &= H_0 e^{i(k_z z - \omega t)} \hat{y}.
\end{align*}
\] (4.6)

The Maxwell equation leads to

\[
\begin{align*}
k_z H_0 &= \varepsilon_{\text{eff}} \omega E_0 \\
k_z E_0 &= \mu_{\text{eff}} \omega H_0.
\end{align*}
\] (4.7)

\( \varepsilon_{\text{eff}} < 0 \) suggests \( \mu_{\text{eff}} \) has to be smaller than 0. Then \( (\vec{E} \times \vec{H}) \cdot \vec{k} = \varepsilon_{\text{eff}} \omega |\vec{E}|^2 = \mu_{\text{eff}} \omega |\vec{H}|^2 \) is smaller than zero and the media is LHM.

### 4.4 Discussion

The results presented above indicate that the metallic PC system in a certain frequency range can exhibit the imaging effect similar to that in an ideal LHM system. The existence of a far-field focus is clearly observed from the field pattern. More interestingly, the focus will change its position with the change of the source position correspondingly. Thus, the results provide a clear demonstration of the negative refraction phenomena in the PCs.

However, the comparison between the results of the ideal LHM and the PCs reveals many interesting differences. (1) The wave front in an ideal LHM is continuous, while it is broken in PCs as illustrated in Figs. 4.11-4.15. A careful comparison of the structure and the field distribution shows that due to the presence of the metal, the electric field is located outside the metallic inclusions of the PC at the specified frequency. This means that the metallic PC is an inhomogeneous medium to the electromagnetic wave. Also consequently, the focus inside the ideal LHM cannot be observed in the metallic PC based system. (2) The peak intensity of the focus is much smaller in the PC-based system compared to the ideal LHM system as mentioned before. Moreover, from the field intensity distribution in the propagation (Z) direction, the peak intensity of the focus is comparable with that of the neighboring peaks. Hence, the subwavelength imaging in the propagation (Z) direction is not observed. This is because the light rays in the metallic PCs are scattered by the metallic region such that not all paths converge to the same point unlike the ideal homogeneous LHM system that all light rays with different directions focuses onto one point. (3) The
imaging effect is possible in PCs even when the background has a large index mismatch with the effective index of the PCs. The disadvantage discussed in (2) also works here in this regard; i.e., the index mismatch doesn’t influence the image significantly since the light rays already do not focus onto one point due to the inhomogeneity-related multi-scattering. So we suggest that both the internal spacing (i.e., the lattice constant) and the size of the metallic inclusion used in these simulations are too big for the specified source wavelengths so that the PC cannot be treated as homogeneous.

Next we discuss the influence of the PC’s geometrical parameters such as the PC width \( W \) and the terminating surfaces of the PCs. First, we notice that all the photonic band structures we have calculated is for 2D infinite PCs. (i.e., we suppose the periodicity extends infinitely in the 2D plane, which is of course not the realistic case.) It is worthy to point out that the effective index of the PC is related with the band slope instead of the band itself. So the sensitivity of these PC geometrical parameters to the effective index is very high. This is beyond what the band structure for the infinite PC can explain and has not been addressed very well in the earlier works. (4) The change of the PC width may affect the wave propagation pattern significantly. This may be due to the finite number of PC period considered in the study (i.e., 9 vs. 17 layers). We suggest a PC width of several layers will alter the band structure and dramatically change the band slope (i.e., the effective index) from that of infinite 2D PCs. (5) The terminating surface also has a strong influence on the PC properties. The abrupt termination of the periodicity will produce the surface states and different terminating surfaces may produce different states due to the inhomogeneous nature of these PCs. This in turn changes the band structure and the effective index.

Finally, a realistic PC structure is proposed to realize the negative refraction as shown in Fig. 4.17. The host medium is silicon \((\varepsilon = 12)\) and the rods are made of copper. We have \(\varepsilon_\infty = 1\), \(\mu_p = 6.38 \ \mu m^{-1}\) and \(\gamma = 0.0278 \ \mu m^{-1}\) for the copper [164] and the background is vacuum of \(n_b = 1\). The band structure is drawn as in Fig. 10(a) and the snapshot of field distribution with \(\lambda = 0.275\) in Fig. 4.17(b). The source is placed \(d_s = \frac{13}{6}\sqrt{3} \ \mu m\) and a clear focus appears at \(d_f = 2.35\sqrt{3} \ \mu m\), close to the half PC width \(\frac{13}{6}\sqrt{3} \ \mu m\).
Figure 4.1: Light propagation from a RHM to a LHM. Light makes a negative angle with the normal. Note the normal component of the wave vector $\vec{k}$ in the LHM changes to the opposite direction of the normal component of $\vec{k}$ in the RHM.
Figure 4.2: Schematic diagram of lensing by an ideal LHM slab due to negative refraction. Light from a point source in a RHM propagates into the LHM slab whose index is lattice matched to the RHM background.
Figure 4.3: Wave front passes from a RHM to a LHM. At time $t_1$, it hits line AB and at time $t_2 > t_1$, the front becomes line AD.
Figure 4.4: The snapshot of the field distribution of such a system after 250 time cycles with a source wavelength of 1 µm. The field distributions of the second focus along the propagation direction (Z direction) and the lateral direction (X direction) is shown in (b) and (c), respectively.
Figure 4.5: (a) The snapshot of the field distribution with a source wavelength of $\sqrt{2}$ $\mu$m. The field distributions of the second focus along the propagation (Z) direction and the lateral (X) direction is shown in (b) and (c), respectively.
Figure 4.6: The snapshot of the field distribution with the LHM width $W = 6.5 \, \mu m$ and the source distance (a) $d_s = 2 \, \mu m$ and (b) $d_s = 4.5 \, \mu m$. 
Figure 4.7: (a) The snapshot of the field distribution with two identical sources both in axis $X = 0$ and with a separation of one wavelength. (b),(c) Corresponding field intensity of the source and the second focus, respectively.
Figure 4.8: (a) The snapshot of the field distribution with $\gamma = 10^{-2} \, \mu m^{-1}$. (b) The intensities of the second focus peak as a function of loss determined from drude relaxation constant $\gamma$. 
Figure 4.9: The snapshot of the field distribution with the LHM has an index of -1.1.
Figure 4.10: (a) The photonic band structure of a metal whose dielectric constant follows the Drude form and the plasma frequency $\nu_p = 1 \text{ } \mu\text{m}^{-1}$, the relaxation rate $\gamma = 10^{-5} \text{ } \mu\text{m}^{-1}$. The lattice constant of the PC $a = 1 \text{ } \mu\text{m}$ and the radius of the metallic rod $r = 0.25 \text{ } \mu\text{m}$. The dielectric host medium has a dielectric constant $\varepsilon = 6$. (b) The schematic drawing of a system composed of a metallic PC with a triangular lattice placed in vacuum with $\Gamma M$ as its horizontal $Z$ direction and $\Gamma K$ as its lateral $X$ direction. The dark area is the background and only part of the PC structure is shown in the graph.
Figure 4.11: (a) The snapshot of the field distribution of such a system after 20 time cycles with a source wavelength of 2.755 µm. The field distributions of the focus along the propagation (Z) and the lateral (X) direction are shown in (b) and (c), respectively.
Figure 4.12: The snapshots of the field distributions with $d_s = \frac{\sqrt{3}}{3} \mu$m and $d_s = \frac{4\sqrt{3}}{3} \mu$m are shown in (a) and (b), respectively.
Figure 4.13: The snapshots of the field distributions when the source frequency $a/\lambda = 0.355$ and the background index (a) $n_b = 1$; (b) $n_b = 1.1$. The snapshots of the field distributions when $a/\lambda = 0.375$ with (c) $n_b = 1$ and (d) $n_b = 0.9$. (e) Effective index model of the specified PC as a function of the source frequency.
Figure 4.14: The snapshots of the field distributions after 30 time cycles when PC width \( W \) is increased to 17 layers with (a) \( d_s = \frac{5\sqrt{3}}{6} \) \( \mu \text{m} \) and (b) \( d_s = \frac{13\sqrt{3}}{6} \) \( \mu \text{m} \).
Figure 4.15: (a) Schematic drawing of a system composed of a metallic PC in vacuum. Only part of the structure is shown and the PC has a different terminating surface compared with the one in Fig. 4.10(b). (b) The snapshot of the field distributions for such a system.
Figure 4.16: (a) Calculated photonic band structure with $\varepsilon_\infty = 6$ for E polarization. The triangles represent the result with $\varepsilon_\infty = 1$ for comparison. (b) The snapshot of the field distribution with $\varepsilon_\infty = 6$. 
Figure 4.17: (a) Calculated photonic band structure of a PC with Si as the host medium and Cu as the inclusion rods for E polarization. (b) The snapshot of the field distribution of such a system.
**Chapter 5**

Conclusions and Future Work

5.1 Nitride Light Emitting Diode Design

Significant advancements have been taken place in group-III wurtzite nitride semiconductors in the past few years. [47, 50, 98, 99] InGaN-based blue light emitting diodes (LEDs) have found their market in full color displays and white lighting; blue laser diodes will be used in the next generation high-capacity CD/DVD read/write systems; Ultraviolet (UV) LEDs and photodetectors have seen tremendous improvements in their properties and can be used for detection of biochemical agents, early missile threat warning, air/water purification, or even higher quality white lighting. Also, these materials have been successfully utilized to constitute high-frequency high-power transistors for radio frequency (RF) transmission purposes. In Chapter 2, we presented a detailed study of band structure calculation of nitride compounds based on the Rashba-Sheka-Pikus (RSP) Hamiltonian [3, 4, 5] in the vicinity of the Γ point. Clearly, the parabolic model does not fit the band structure of the nitride wurtzite materials. In the analysis of InGaN/GaN quantum well (QW) structures, the propagation method is used with the consideration of the huge internal polarization fields inside the QW. It is found that the strain and strain-induced piezoelectric field significantly alter the subband structure and determine the output intensity of the nitride QW LEDs. The band parameters of nitride alloys were discussed and an optimized parameter set was established. For high In composition InGaN/GaN QW LEDs, the recombination
mechanism was discussed and a guideline for elastic strain relaxation was proposed based on the comparison between the theoretical calculations and the experimental data. The resulting model can accurately investigate the optoelectronic properties of nitride based QW LEDs with a wide range of In compositions. Based on the calculation results, a design that uses AlInGaN as the quantum barrier was proposed to realize efficient red emission, which is hard to achieve if GaN is used as the barrier. In the proposed design, three different InGaN/AlInGaN quantum-well structures can emit red, green, and blue light of similar intensity. Also, to achieve high efficiency, important factors related to the oscillator strength were discussed in detail.

There is pretty much opportunities for future work. First, a lot of nitride parameters are not very accurately determined and should be verified from experiments. Our envelop function based on the RSP Hamiltonian can help to derive these important band parameters, which is hard to directly derive from experiments. Then, a detailed LED structure design is needed so that the red, green and blue QWs will not interfere with each other during transition. Also, light with different color should be mixed very well and become uniformly white. In the numerical simulation, since the effective mass is not a constant and can be approximately expressed as a function of the carrier concentration, a model that can establish the relationship of the effective mass of the nitrides and the carrier concentration is very important. While it is till the most accurate to analyze the transport properties with the RSP Hamiltonian, another feasible way is to apply our results of nitride effective hole mass parameters in the available commercial software to realize the structure.

5.2 VO$_2$-based Photonic Crystal Devices

Since the initial prediction, [6, 7] photonic crystals (PCs) have offered new opportunities for realizing photonic integrated circuits with many important applications including optical communication and display. While significant progress have been made, most is for passive optical elements with their device operation predetermined by fabrication steps. Clearly, a PC that can be programmed or reconfigured on demand by an external control will significantly increase the functionality. Thus far, various approaches (for example, via the strain, [138] temperature, [139] magnetic field, [140] etc.) have been adopted to tune the PC bandgap or wavelength. As for the crucial wave guiding, the use of the liquid crys-
tal [141] was suggested by taking advantage of its orientation-dependent refractive index that can be controlled externally. The foundation of photonic crystal analysis has been strengthened by the work of theoretical researchers of solid state physics, including research groups individually headed by Lueng [9], Zhang [10] and Ho [11]. They used the plane wave expansion (PWE) method to calculate energy bands, which is an optical version similar to the method used in solid state physics. Since there are almost no limitations concerning the structures of photonic atoms, the finite-difference time-domain (FDTD) method is capable of computing photonic band structures for arbitrary frequency dependence and arbitrary geometry. [8, 12, 13] The feasibility of electrically programmable wave guiding in a PC was explored based on the metal-insulator transition of vanadium dioxide (VO$_2$). Unlike the ordinary PCs, wave propagation in the desired structure may be switched on/off or redirected by applying an electrical bias on the selective electrodes by taking advantage of the electrically induced VO$_2$ phase transition and subsequent modulation of dielectric properties. The characteristics of the 2D VO$_2$-based PCs with line defects were analyzed using the iterative PWE and FDTD methods. Particularly, the influence of the Drude relaxation on wave guiding was examined as the high rate typical for metallic VO$_2$ can lead to the signal loss. An optimized structure was proposed to minimize the loss and simplify the fabrication.

In the next step, the most important research should be the experimental verification. The process of putting vanadium dioxide into holes surrounding with dielectric media such as silicon has not been realized experimentally. The data of the critical electrical field needed for the metal-insulator (MI) transition of vanadium dioxide with thickness of around the micrometer order is unknown or not accurate. For the device design, a lot of attention should be paid on the third dimension of the device. How to minimize the influence of the metal contacts to the guiding wave is one critical research direction. Also the determination of the optimum thickness of the PC slab is important. Three-dimensional (3D) modeling is essential for studying the features of realistic PC waveguides. The defects should be designed appropriately for a maximum propagation.
5.3 Negative Refraction by metallic PCs

In Chapter 4, the light propagations and the focusing phenomenon in both the ideal LHM and the metallic PC systems were investigated by the FDTD method. For the first time, the investigation of the image along the propagation (Z) direction was conducted. The existence of two foci was verified in the ideal LHM system and the subwavelength resolution was realized not only in the lateral (X) direction, but also in the propagation (Z) direction. Certain important factors such as the LHM width, the source frequency, the loss and the index mismatch are discussed through the simulations. To achieve high quality subwavelength images, we should have a loss less than $10^{-5}$ and an index mismatch much less than a few percent in the ideal LHM system.

Far-field images are possible in the metallic PC system. The corresponding change in image position with the different source positions was observed. The sum of $d_s$ and $d_f$ remains a constant during the source position change, which is a direct proof that negative refraction does happen in metallic PC system. The similarities and differences of imaging properties in both systems are compared quantitatively. Though the negative refraction exists in metallic PC system, the multi-scattering makes the system very different from the ideal LHM system. The effective index model as a function of source frequency has been established for the specified metallic PC. Critical factors such as the PC width and the terminating surface were discussed to develop a clearer picture of the negative refraction that occurs in the metallic PC-based system. We suggest that the focusing effect of the PCs may not be solely determined by the photonic band structure. The effective index of -1 under certain frequencies have been realized in both a metallic PC following an ideal Drude form and a realistic copper/silicon PC.

For the continuing work, more simulations are necessary to be conducted for the lens application in the metallic PC system. Though the negative refraction in metallic PC system has been verified in the simulation, the difference with an ideal LHM system is obvious. To reduce the multi-scattering effect, one possible way is to decrease the radius of the metallic inclusion $r$. If the condition $\lambda \gg r$ is satisfied, the wave will not be scattered by these metallic inclusions. At the same time, care should be taken to ensure the slab shows a negative effective dielectric constant of the PC. Another possible solution is to decrease the dimensionless frequency $a_{\lambda}$. That could be realized either by increasing the dielectric constant of the host medium, or decreasing the plasma frequency of the metallic inclusion.
Still, we need to retain a negative effective dielectric constant of the PC.
Bibliography


The shear deformation potential of wurtzite InN is referred to the value of zinc-blende structure due to the lack of the data.


In these cases, the location of the image is determined not by the peak intensity but by the shape and the field pattern. As the main peak and the neighboring peaks have comparable intensities, it is not possible to differentiate them based only on the intensities.