
Three-dimensional coupled-wave theory for photonic-crystal surface-emitting lasers

*A dissertation submitted in fulfillment of the requirements
for the degree of Doctor of Philosophy*



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December 2013

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Chapter 1

Introduction

1.1 Background

Lasers have made a tremendous impact on modern science and technology, with widespread applications in areas such as communications, imaging, sensing, displays, medicine, materials processing, and optical physics. Since the the first demonstrations of the first laser in 1960 [1], five Nobel Prizes in Physics have been given to researches directly related to lasers, with the first one in 1964 to Charles H. Townes, Nicolay G. Basov and Aleksandr M. Prokhorov for their fundamental work leading to the constructions of lasers and the most recently one in 2000 to Zhores I. Alferov and Herbert Kroemer for developing semiconductor heterostructures which makes semiconductor lasers possible.

The word “laser” is the acronym for Light Amplification by the Stimulated Emission of Radiation, and its invention can be dated back to more than ninety years ago when Albert Einstein introduced the concept of the photon and predicted the phenomenon of the stimulated emission. The laser is a device that produces a coherent light beam with low-divergence at frequencies ranging from the infrared to ultra-violet region, and it has two essential components: a gain medium that amplifies light in the presence of an external pump, and a laser cavity that traps light and supplies the needed optical feedback. The early laser cavities are all of Fabry-Perot type (see Fig. 1.1(a)) where the light undergoes multiple reflections between two facing mirrors, one of 100% reflectivity and the other slightly less (about 95% in the first ruby laser [1]).

One shortcoming of Fabry-Perot lasers is that they cannot maintain stable single-mode operation particularly under high-speed modulation [2]. This is because the optical feedback is almost the same for the multiple closely-separated longitudinal modes located within the gain spectrum range. The advent of laser diodes with distributed optical

feedback [3–6] solves this problem. Depending on whether the diffraction grating is incorporated inside the gain region or outside, these lasers are classified as distributed feedback (DFB) lasers and distributed Bragg Reflector (DBR) lasers. The incorporated periodic gratings (index and/or gain) cause a wavelength selective feedback. Only wavelengths close to the Bragg wavelength experience maximum reflectivity and therefore only modes with these wavelengths are selected for lasing. In addition, the lasing wavelength in these lasers can be tuned precisely by varying the spatial period of the diffraction grating.

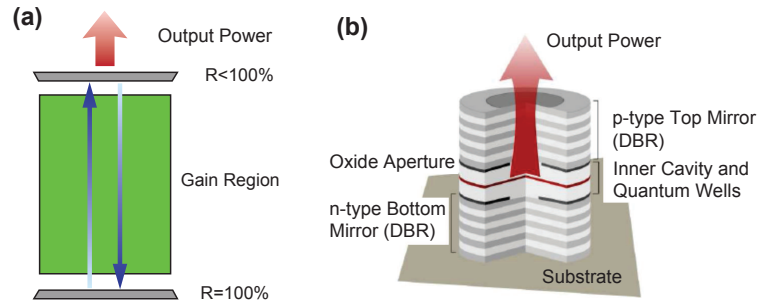


Figure 1.1: Schematic diagram of (a) a Fabry-Perot laser cavity and (b) a VCSEL device.

One important design of DFB lasers is the vertical cavity surface emitting laser (VCSEL) shown in Fig. 1.1(b). This novel type of semiconductor laser was suggested by Prof. Kenichi Iga in the the year 1977 [9, 10]. Due to their small sizes, the frequency spacing of the axial modes is large compared with the gain width and typically only one longitudinal mode is underneath the gain curve, which gives rise to more robust single-mode operation. More importantly, the surface-emitting properties provide a number of advantages compared to the conventional edge-emitting lasers, e.g., circular output beams (thus high coupling efficiency to optical fibers), high reliability without suffering from catastrophic optical damage (COD) at the output facets, efficient implementation of fabrication and simultaneous test on a wafer, low-cost two-dimensional array fabrication, etc. All these advantageous features have made them become the most versatile semiconductor laser diode and have enormous market growth potential [11]. Historically, VCSELs have been have been mostly confined to low-power applications (a few mW at most), such as fiber optics and high-speed data transmission. These VCSELs have been used as single devices or small addressable arrays. However, there are fundamental reasons why the VCSEL technology cannot extended to very high-power applications without fabricating large two-dimensional (2D) arrays of low-power single emitters. That is because the only mode selection mechanism in the transverse direction is due to the refractive index contrast and therefore there exists a limitation in increasing the device dimension for high power operation.

The rapid advance of micro- and nano- fabrication techniques over the past decade, along with the development of novel theoretical techniques, has led to the emergence of a number of new types of laser cavities, with dimensions and emission properties much different from those found in conventional lasers. Among them are dielectric micro-disk lasers [12–16], photonic crystal lasers [22, 23, 27, 29], photonic crystal VCSELs [17–21].

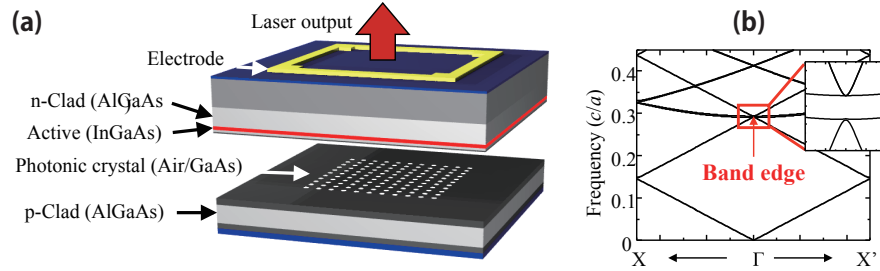


Figure 1.2: (a) Device structure of photonic crystal surface-emitting lasers (PCSELs). (b) Photonic band-structure. At the band edges (second-order Γ point), the group velocity of light becomes zero.

PCs are optical materials with a periodic refractive index modulation. Photons within PCs are akin to electrons inside semiconductor, where the periodic atomic lattice is analogous to the periodic dielectric medium. Similar to electronic band structure for electrons, photonic-band structure is formed for photons. Two-dimensional photonic-crystal lasers can be divided in two families: defect mode lasers and band-edge mode lasers. The former operate at frequencies inside the band-gap by intentionally introducing a defect that supports localized modes [22–26]. Band-edge mode lasers instead operate in regions of energy-momentum space that have a high photonic density of states and a corresponding small group velocity. We implemented the latter device architecture in order to take advantage of the spatial delocalization of band-edge modes, which allows for improved power extraction. Since the first experimental demonstration performed by M. Imada, *et al.* and M. Meier, *et al.*, the band-edge photonic-crystal surface-emitting lasers (PCSELs) (see Fig. 1.2) are becoming increasingly important due to their much improved laser performance and functionality compared to the conventional semiconductor lasers [27–42]. A number of successful demonstrations over the past decade promise that PCSELs not only able to integrate almost all the advantages of VCSELs but meanwhile allow high-power operation.

By utilizing the band edge of the photonic band structure, single longitudinal and transverse mode oscillation in two dimensions has been achieved with a large lasing area, enabling high-power, single-mode operation [27, 34]. The output beam of such devices is emitted in the direction normal to the 2D PC plane and has a small beam divergence angle of less than 1° due to the large area of coherent oscillation [34, 35]. Furthermore, both the polarization and pattern of the output beam can be controlled by appropriate

design of the PC geometry [29, 35]. Recent developments of 2D PC lasers have allowed the lasing wavelength to be extended from the near-infrared regime to the mid-infrared [36], terahertz [37], and blue-violet regimes [40]. In addition, we have recently demonstrated the operation of a PC-SEL with entirely new functionality: on-chip dynamical control of the emitted beam direction, achieved by using a composite PC structure [42].

1.2 Unique features of photonic-crystal surface-emitting lasers

Although the configuration of PCSELS can be considered 2D versions of the second-order distributed-feedback (DFB) lasers [67], PCSELS are essentially different from the conventional DFB lasers. This is due not only to their ownership of the multidirectional coupling mechanisms [31] (which are unachievable in DFB lasers) but also to the remarkably high design freedoms of PC geometry including air-hole shapes [29, 35], 2D multiple phase-shift [35], unit cells [45, 52] lattice structures [42–44], etc. Both these multidirectional couplings and high structural design freedoms enables PCSELS to exhibit enhanced functionalities and improved performance compared to the conventional semiconductor lasers. In this section, we shall give a brief review of the unique features that have been demonstrated thus far.

1.2.1 Single-mode high-power operation over large area

One of the most important features of PCSELS is that they enable stable single-mode lasing over a large area. The large-area surface-emission further allows several advantages such as high output power, avoiding catastrophic optical damage (COD) at the output facet, and narrow divergence angle. This is all due to the notable feature of the two-dimensional band-edge effect [29, 31].

The large-area coherent lasing has been experimentally demonstrated in several previous publications [29, 31, 34]. Figure 1.3(a) shows a typical near-field pattern (NFP) of a junction-up PCSELS [34]. The lasing spectra were examined at different positions located within the broad lasing area ($> 100 \times 100 \mu\text{m}^2$). At each position, the lasing peak was observed at the same wavelength 958.2 nm. This is a strong evidence that the single-mode coherent lasing was indeed obtained over a large area. Figure 1.3(b) shows the corresponding far-field pattern (FFP), which features a small beam divergence angle of less than 1° . This small divergence angle reflects the large area coherent oscillation.

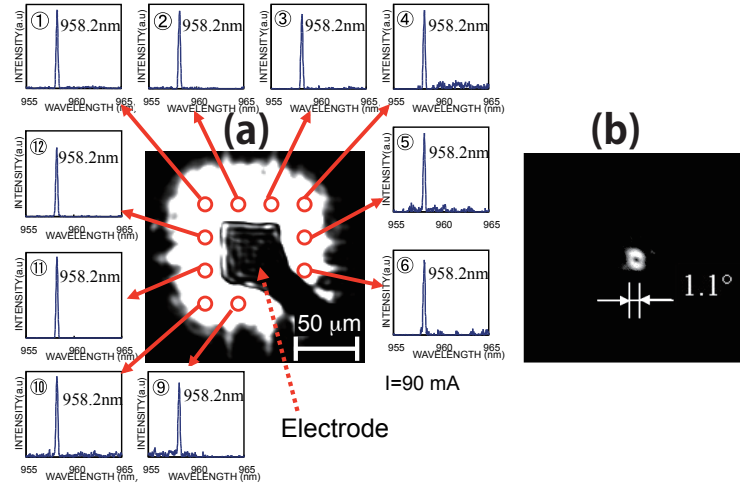


Figure 1.3: (a) Near-field pattern (NFP) and lasing spectra of a junction-up PCSEL. The side length of the electrode is $50\ \mu\text{m}$. (b) The obtained far-field pattern (FFP).

In general, the output power scales with the lasing area. Therefore, PCSELs are inherently suitable for high-power operation. Fig. 1.4(a) shows the measured light-current characteristic of a single PCSEL device under continuous-wave operation [54]. A highest output power of 780 mW was obtained at an injection current of $\sim 1.8\ \text{A}$. The slope efficiency is as high as $0.49\ \text{W/A}$, which is comparable to that of the conventional semiconductor lasers. The lasing spectrum measured at $1.8\ \text{A}$ is shown in Fig. 1.4(b), indicating that a single-peak lasing was obtained with a side mode suppression ratio (SMSR) over 20 dB. Even at this high power operation, the divergence angle of the almost single-lobed far-field pattern (FFP) is still within 1° , as shown in Fig. 1.4(c).

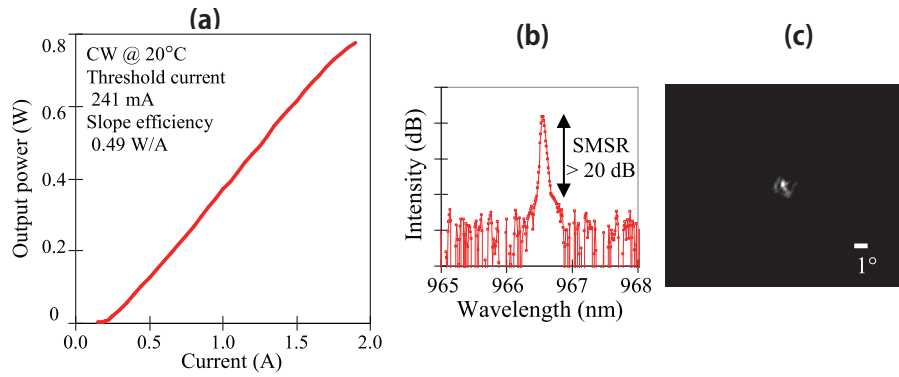


Figure 1.4: Measured lasing characteristic of a PCSEL under continuous-wave (CW) operation at 20°C : (a) Light-output characteristics, (b) lasing spectrum, and (c) far field pattern (FFP) operated at $1.8\ \text{A}$.

1.2.2 Beam pattern and polarization control

PCSELs is capable of producing diverse beam patterns on demand by appropriately designing photonic crystal geometries [35]. The beam pattern emitted by a semiconductor laser is determined by the Fourier transformation of the electromagnetic field distribution in its output plane. It is therefore important to alter the internal electromagnetic field of the resonant mode. This can be achieved by varying the air-hole shapes and/or introducing phase shift. Figure 1.5 shows a variety of beam patterns emitted from PCSELs, including single, twin and quadruplet doughnuts, either separated or touching, and single-lobed shapes.

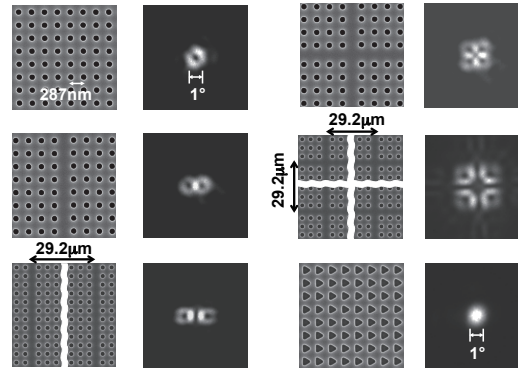


Figure 1.5: Various surface-emitted beam patterns produced by PCSELs with engineered air-hole shapes and/or lattice phases.

The polarization of the surface-emitted output beam from PCSELs is also closely related to the internal electromagnetic field of the resonant mode. By carefully engineering air-hole shapes and/or the lattice structures, various polarization profile can be realized. Figure 1.6 shows a range of polarization profile obtained from PCSELs. Within a square-lattice, a linear polarization is obtained by using an asymmetric triangular air-hole shape, whereas an azimuthal polarization can be obtained using a circular air-holes shape. On the other hand, more complicated polarization profile can be realized by using the triangular lattice or by using a fifth-order Γ -point mode of a square lattice [43]. The latter three polarizations are very useful in the field of vector beams, which are important in versatile applications such as high-resolution microscopy, advanced laser processing and optical trapping.

1.2.3 On-chip beam steering

As shown in Fig. 1.7(a), the output beam of PCSELs typically emits into the surface normal direction because the operating band-edge mode is located at the Γ point that has a zero in-plane wave vector. If an artificial lasing band-edge could be created

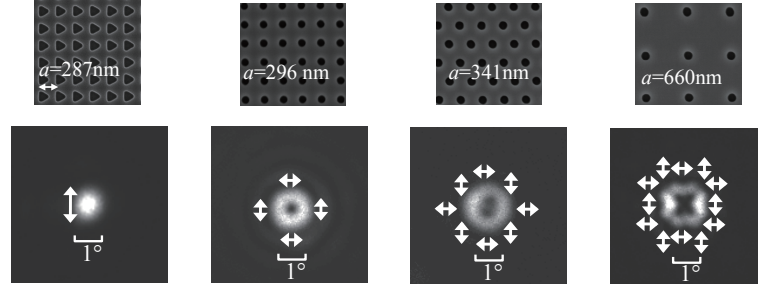


Figure 1.6: Various polarization profiles produced by PCSELs

deviated from the Γ point, the emitted laser beam would be deflected into an oblique direction. One possible method of realizing this artificial lasing band edge is to construct a composite photonic crystal composed of square and rectangular lattices as illustrated in Fig. 1.7(b). Lasers based on such composite photonic-crystal structures have been demonstrated to be able to emit beams over a range of directions of $\pm 30^\circ$ [42]. Moreover, the deflected laser beam can be scanned smoothly and continuously by on-chip integration. Recently, the beam-steering performance has experienced a remarkable progress. For maximum deflection angle have been extended to $\pm 45^\circ$ by using combination of triangular lattices, square lattice and rhombic lattice, and modulated photonic crystals. In addition, the beam-direction steering axis has been extended to 2D by using the square lattice and rhombic lattice, or modulated photonic crystals. Such on-chip controllability of the beam direction is important for a wide range of applications including mobile laser projection displays, advanced laser printers, and chip-to-chip optical communication.

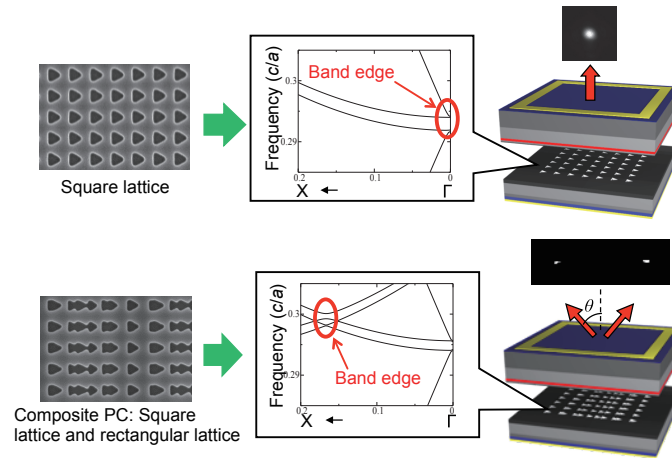


Figure 1.7: On-chip beam direction control of PCSELs

1.2.4 Extended wavelength regime

In the early stage of demonstrations, most experimental PCSEL works have been done using organic [28, 30], InP [27], and GaAs [34] material systems that operate at visible and near-infrared wavelengths (Fig. 1.8(b)). With the appealing features of PC cavity being widely noted, the PCSEL cavity design was later adopted in GaN-based materials [40, 41] for shorter wavelength operation, i.e., blue-to-ultraviolet region (Fig. 1.8(a)). Meanwhile, extensive researches have been devoted to the development of longer-wavelength PCSEL sources. For example, a mid-infrared PCSEL ($\lambda \approx 3.7\mu\text{m}$) was demonstrated by using antimonide (Sb) material [36] (Fig. 1.8(c)) and long-infrared terahertz (THz) PCSEL lasers ($\lambda \approx 110\mu\text{m}$) were demonstrated by operating by lithographically transferring PC patterns onto the top metallization of a metal-metal THz quantum cascade laser [38, 39] (Fig. 1.8(d)). As a result, the lasing wavelengths of PCSEL families have now spanned a wide range from near-infrared to blue-violet, mid-infrared, and terahertz regimes. These efforts for wavelength extension would open the door to a much broader range of blue-to-ultraviolet laser applications such as super-high-resolution laser source, optical tweezers for ultrafine manipulation, and promote the development of advanced quantum cascade laser for astronomy, environmental monitoring, and security.

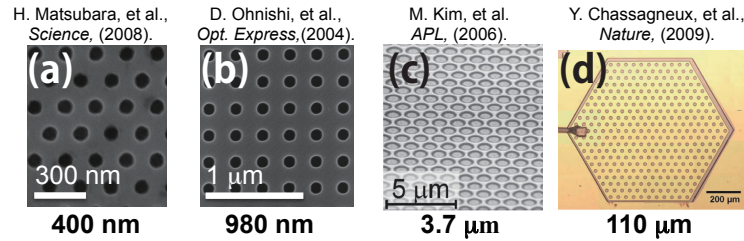


Figure 1.8: Extended wavelength regime of PCSELs. The lasing wavelength spans from blue-violet to terahertz regime.

1.3 Motivation

Despite the experimental advances that have recently been made in the field of 2D PCSELs, theoretical studies on these types of lasers have thus far been limited. An important but unresolved issue concerns the mechanisms by which the PC structure determines the output characteristics of the device, thereby limiting progress in optimizing the structural design of devices. Computer simulations based on the 2D plane-wave expansion method (PWEM) [31, 75, 76] or the finite-difference time-domain (FDTD) method [77–79], can provide valuable information about the lasing properties of the

PC laser cavity. However, there are some inherent limitations to these computational approaches. The 2D PWEM is only applicable to infinite structures, and the FDTD method requires substantial computational resources in order to model finite structures with realistically large areas. Moreover, neither simulation approach provides analytic insights into improving the design of devices. A group of alternative analytical methods [33, 61] have been developed, based on the concept of one-dimensional (1D) coupled-wave theory (CWT) [65]. However, these methods in their initial formulations consider only four basic waves in the coupled-wave model and disregard 2D optical coupling effects, which are important in 2D square-lattice PCs. Sakai *et al.* later derived a 2D CWT using an eight-wave model [62, 63] that incorporates both conventional 1D coupling and the more pertinent 2D coupling, allowing 2D coherent lasing action to be explained [34]. This more-detailed formulation of lasing underscored the importance of accurately modeling complicated coupling effects in PCSELs.

Because the previous theory [62, 63] is essentially a 2D model, it is accurate for 2D systems, while having inherent limitations when trying to model a full three-dimensional (3D) system. First, the device structure is assumed to be uniform in the vertical direction. However, realistic PCSELs require 3D analysis because the multi-layer nature of the device breaks the structural uniformity in the vertical direction. For example, light waves diffracted into the vertical direction (which are particularly important in the analysis of PCSELs) cannot be modeled explicitly without considering a 3D system. The second limitation is the difficulty in accurately modeling the 2D coupling effects. Light propagating within the PC is in principle a Bloch wave described by an infinite number of terms in a Fourier series expansion, and thus it is crucial to include as many wave orders as possible to model the PC cavity accurately. For example, it is becoming increasingly clear that the use of air holes with *asymmetric* shapes, such as equilateral triangles and right-angled isosceles triangles [51, 53], is often beneficial; these shapes are potentially important for improving the output power and slope efficiency of 2D PCSELs. However, analysis of these complicated PC geometries based on CWT model requires the inclusion of higher-order terms. Although it appears that the previous eight-wave model can be extended in a somewhat straightforward way to incorporate these higher-order terms, this still fails to accurately calculate the 2D coupling effects because of the essential difference between 2D and 3D systems. In 3D systems, the 2D coupling strength between individual waves is related to the overlap of their vertical field profiles. Therefore, the vertical field profile of the individual waves must be treated very carefully by considering a 3D system.

1.4 Objective

The main goal of this thesis is to develop a simple, efficient and accurate theory to analyze quantitatively the various lasing characteristics of the PCSEL cavity. We develop a 3D coupled-wave theory (CWT) for PCSELs in order to overcome the limitations discussed above. We present a generalized coupled-wave formulation for a 3D structure by extending the original coupled-wave approach developed by Streifer *et al.* and C. H. Henry *et al.* for 1D distributed feedback (DFB) lasers [66, 67]. Our 3D coupled-wave model not only incorporates a large number of high-order wave vectors, but also takes their individual vertical field profiles into account. This model accurately describes all the important coupling effects in 3D systems, and can also be generally applied to the analysis of PC structures with air holes of arbitrary shape in the PC plane. To develop a general theoretical tool for PCSELs, the basis of the 3D CWT framework will then be extended to treat 3D air-hole holes with arbitrary sidewalls in the vertical direction and a triangular lattice PC laser cavity. Therefore, our 3D CWT will be able to treat PC structures of arbitrary geometry. The accuracy and validity of our developed theory will be verified by comparing the theoretical results of 3D FDTD and further with experimental results. In the realistic experimental situations, the lasing properties will also be influenced by the interaction between photons and carriers, and the mode stability involves complex laser dynamics. Incorporate these effects is particularly important for designing high-power PCSELs. Therefore, we extend our linear 3D CWT model to the nonlinear above-threshold model. Our theory is intended to give a comprehensive description of the different design parameters and effects that determine the behavior of a PCSEL device. Emphasis is on the derivation of guidelines for their design. Since our developed theory in this thesis applies generally to the PC cavity with an arbitrary geometry, we believe that it provides an effective approach to systematically understanding the relation between the PC structures and the laser performance, and indicates a clear direction to optimize the device performance.

1.5 Thesis outline

This thesis consists of seven Chapters including Introduction and Conclusions, as well as Appendices, Acknowledgments, and List of publications. The following gives a brief description of each Chapter.

- Chapter 1: Introduction

First, background is explained including the unique features and important functionalities of photonic-crystal surface-emitting lasers that have been experimentally

demonstrated so far. Next, we review the theoretical studies that have been devoted to PCSELS and emphasize the importance of developing a three-dimensional analytical model for the laser cavities. Finally objective of this thesis is presented.

- Chapter 2: Photonic crystal surface emitting lasers and modeling tools
As mentioned above, PCSEL is a new type of semiconductor lasers based on band-edge effect. To provide a basic understanding of PCSELS, in this Chapter, we first describe the basic laser structures used in the experiments. Then, we explain the formation of a 2D cavity mode based on the Bragg diffraction at the band-edge modes and the threshold conditions of the laser cavity. Moreover, we give an overview of theoretical methods that have been used for modeling PCSEL cavities, including 2D plane-wave expansion method, 3D finite-difference time-domain (FDTD) method, and 2D analytical coupled-wave theory (CWT) are described. Merit and limitation of each method is explained, and particularly the relevant part of the previous 2D CWT is presented in more detail. Finally, to circumvent the limitations of these methods, we suggest a 3D analytical method.
- Chapter 3: Three-dimensional modeling of wave interactions in PCSELS
The main body of the newly proposed 3D CWT is presented in this Chapter. To fully take into account of the complex wave interactions in a 3D laser structure, we propose a 3D coupled-wave model for the Γ -point band-edge modes and derive the analytical coupled-wave equations. In contrast to the previous 2D CWT model, the new 3D coupled-wave model incorporates a large number of high-order waves and the field profiles in the vertical direction, therefore capable of treating any arbitrarily shaped air holes. Next, to understand the radiation nature of all the modes at the band structure, the 3D coupled-wave model is extended for the non- Γ -point modes. Finally, to confirm the validity of the developed theory, the mode frequency and radiation constant for both band-edge and non- Γ -point modes are calculated and compared with 3D FDTD. The fundamental difference between the 2D and 3D systems is also discussed.
- Chapter 4: Finite-size analysis of lasing properties
Finite-size coupled-wave analysis results are presented, and comparisons with experiments are made. In the previous Chapter we assume a fully periodic structure in order to simplify our analysis and focus on the physical picture of wave interactions. However, the realistic PCSEL device necessitates a finite-size analysis. Therefore, we first derive a coupled-wave equation for finite-size structures by taking into account of the envelope functions of Bloch waves. We then use the derived coupled-wave equation to study various lasing properties including band structure, threshold gains, resonant mode frequency, near- and far-field patterns, polarization

profile, etc. These results are compared with experiments to confirm the validity of our analysis. Next, to understand the finite-size effect in more detail, we calculate the effects of cavity length on threshold gain and mode selectivity. The influence of the in-plane cavity losses will be discussed. Then, experimental demonstrations are performed to confirm the theoretical predictions, and meanwhile new PC unit cell structures are proposed and demonstrated to address the issues of the previous PC designs. Finally, towards single-mode high-power PCSELS, we study single-mode stability in large-area PCSELS. Key factors that affect the single-mode stability will be clarified.

- Chapter 5: Extended analysis towards a generalized photonic crystal geometry

This Chapter is intended to develop a more general theory that is able to treat a larger family of photonic crystal geometry. Two extensions are realized based on the framework obtained so far. The first, arbitrary sidewall shape in the vertical direction, presumes the cases where sidewalls of the fabricated PC air holes are tilted in the dry etching process or may have more complicated geometries if using the recently developed crystal regrowth techniques such as metal organic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE). In previous Chapters, for simplicity we assume perfectly vertical sidewalls for the PC air holes. Here, we extend the 3D coupled-wave equation by carefully incorporating the refractive index variation in the vertical direction and the reflections occurring at the interfaces of different semiconductor layers. The extended formulation is general because it is able to treat arbitrarily-shaped sidewalls. We then use the extended theory to study the radiation properties of several typical cases including tapered and tilted sidewalls. We conclude that introducing proper asymmetry into the sidewalls is beneficial for improving the radiation efficiency. Next a specific geometry that approximately represents the experimentally fabricated air holes using MBE is studied and good agreement with experimental results confirms our analysis. The second extension is intended for the analysis of triangular-lattice PCs which have also been widely adopted in many PCSEL devices. We extend the couple-wave model of square-lattice PC to triangular lattice by introducing six basic waves and carefully treating the direct 2D couplings. We then calculate the modal properties of interest including the band structure, radiation constant, threshold gain, far-field pattern etc. These calculated results are compared with experimental observations and good agreements are found. Finally the effect of air-hole size on mode selection is studied and is also demonstrated by experiment.

- Chapter 6: Above-threshold analysis

The coupled-wave analysis is further explored to model laser behavior in the above

threshold regime. For applications such as large-area high-power lasers, lasing behaviors at higher current injections levels (higher optical output power) are of particular interest. The coupled-wave theory described in previous Chapters basically applies to situations at or just above the laser threshold. Far above threshold, however, spatial hole burning effect resulted from the complex interaction between photons and carriers needs to be taken into account. This Chapter starts with a general description of the spatial hole burning effect and its effect on the spatial variation of refractive index and optical gain. Next we attempt to derive an above-threshold coupled-wave equation by incorporating the nonuniformity in both refractive index and spatial gain. Numerical algorithm for solving the derived coupled-wave equations is described. We then present the above-threshold analysis results of the photon and carrier densities, threshold gain, differential efficiency, and mode stability. Physical mechanisms that affect the above-threshold behaviors will be discussed and relevant findings on mode stability are found to well explain the unstable lasing observed in the experiment. Finally, to improve the single-mode stability in the above threshold regime, we propose several useful laser cavity designs. In particular, we experimentally demonstrate the single-mode stability can be improved by introducing an advanced double-hole design with suppressed spatial hole burning effect.

- Chapter 7: Conclusion and future directions

We summarize findings obtained in this thesis and present an outlook for further work.

Chapter 2

Photonic-crystal surface-emitting lasers and modeling tools

2.1 Introduction

This chapter introduces the fundamentals of photonic-crystal surface-emitting lasers (PCSELs) and the existing theoretical methods used for modeling. The essential part of the PCSEL device is the PC laser cavity. Therefore, first we illustrate how a 2D resonance is formed within the PC structures. To understand this 2D resonance in detail, we also describe the wave coupling diagram in the reciprocal space of PC. Finally, we describe the existing theoretical tools used for studying the lasing properties of PCSELs, including two-dimensional plane wave expansion method (2D PWEM), three dimensional (3D) finite-difference time-domain method (FDTD), and 2D coupled-wave model. The related formulation of each method will also be summarized, and limitations of these method will be mentioned. Finally, we shall point out the importance of developing a three-dimensional analytical model.

2.2 Device structures

In this section, we describe the device structure of PCSELs. A schematic of the PCSEL device investigated in this thesis is shown in Fig. 1(a). The laser structure is fabricated by using wafer-bonding technique [27, 34, 46] or metal organic chemical vapor deposition (MOCVD) method [49, 55–57]. Here, we briefly describe the wafer bonding process; in this case, two types of wafers (labeled A and B) are prepared. Wafer A consisted of an n-type GaAs layer for forming PC, (140 nm), carrier blocking layer ($\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$:

20 nm), $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{GaAs}$ (8 nm/20 nm) multiple quantum wells (MQWs), n-AlGaAs cladding layer (1500 nm) on an n-type GaAs substrate (150 μm). On the other hand, wafer B consisted of a GaAs separate confinement heterostructure (SCH) layer (20 nm), a p-type AlGaAs cladding layer (1500 nm), a GaAs contact layer (500 nm), and an AlGaAs etch stop layer on a p-type GaAs substrate. The photonic crystal air holes

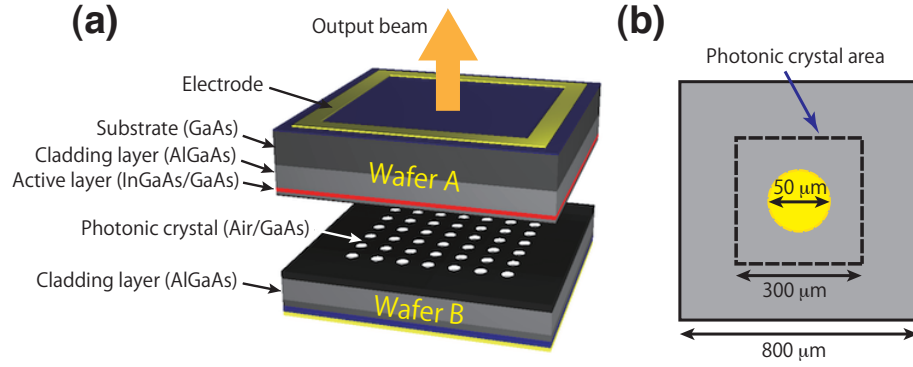


Figure 2.1: Schematic of (a) a PC-SEL device and (b) the top view of the in-plane dimension. The orange represents the output beam emitted into the vertical direction.

were formed on wafer A by electron beam lithography and inductively-coupled plasma etching. The air rods are arranged in a square lattice with a period of ~ 290 nm, which is approximately match the lasing wavelength within the semiconductor material. The typical depth of the air rods is ~ 100 nm. Both the depth and the size of the air holes within the photonic crystal determine the strength of optical feedback. After the formation of the photonic crystals, wafers A and B were stacked and fused at high temperature in a hydrogen atmosphere. The p-type GaAs substrate and the AlGaAs etch stop layer were removed by mechanical polishing and chemical etching. After that, insulating silicon nitride (SiN) was deposited on both the n-side and p-side device surfaces and then the n- and p- electrode patterns were defined on each surface by photolithography. After chemically etching the patterned SiN areas, a $800 \times 800 \mu\text{m}^2$ window electrode (Au/Ti/Au/Ni/Au/Ge: 500 nm/100 nm/200 nm/46 nm/72 nm/54 nm) and circular- (or square-) shaped electrode (Ti/Au) with a typical area of $50 \times 50 \mu\text{m}^2$ was formed on the surfaces of the exposed n-type substrate and p-type GaAs contact layer, respectively. Finally, the p side of sample was attached on an Au-coated heat sink (AlN) and Au wires were bonded to the electrodes for current injection. As the distance between the p-electrode and active layer is $\sim 2 \mu\text{m}$, the light emission area approximately corresponds to that of the p-side electrode. The lasing light from this area are diffracted through the n-side window electrode into free space.

2.3 Lasing principles: Intuitive description of two-dimensional cavity mode

Figure 2.2 shows a schematic diagram of a laser cavity composed of a 2D square lattice photonic crystal structure whose pitch in the both the x and y directions corresponds to the lasing wavelength, and in Fig. 2.2(a), one arrow corresponds to one wavelength. When the light wave propagating in the $+y$ direction (0°) is considered, the light wave is diffracted to the $-y$ direction (180°) by Bragg diffraction. The light wave is also diffracted into $\pm x$ directions ($\pm 90^\circ$) as shown in Fig. 2.2(a) because they also satisfy the Bragg diffraction condition. Consequently, light waves propagating in four directions are coupled with each other, and a 2D large area cavity is formed. In addition, the light wave is also diffracted toward the z vertical direction as the first-order Bragg diffraction is satisfied, as shown in Fig. 2(b). In this section, we describe the basic lasing principles of

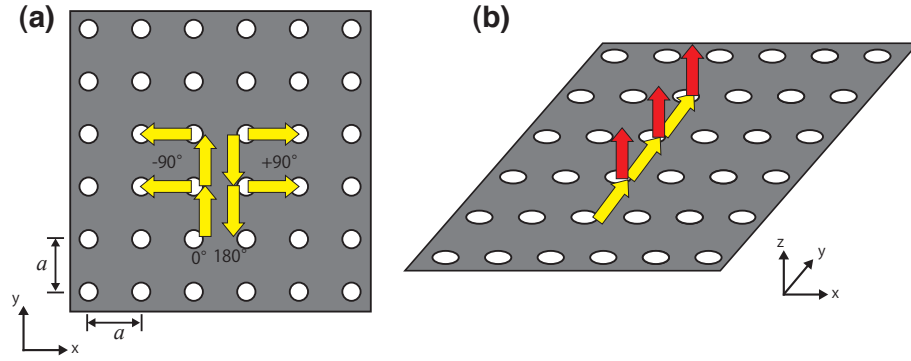


Figure 2.2: Schematic of light-wave diffraction (a) in and (b) out of the PC plane.

PCSELs. Figure 2.3(a) shows a schematic of the coupling diagram the reciprocal lattice space. When the resonant wavelength equals to the PC pitch, the resonant states are primarily made up of fields of four wavevectors with in-plane wave numbers: $(\pm\beta_0, 0)$ and $(0, \pm\beta_0)$ (the shortest light arrows), as illustrated in Fig. 2.3(a). Hereafter, we refer to these waves as basic waves. In the case of TE polarization, the counter-propagating basic waves couple directly due to the 2nd-order Bragg diffraction (orange arrow), and the basic waves propagating in orthogonal directions couple indirectly (dashed red arrows) via the high-order wave vectors (blue arrows). This indirect 2D optical coupling via high-order waves is critical for forming 2D resonance in PC-SELs. Simultaneously, the in-plane light waves in resonance are also diffracted in the direction normal to the PC surface (purple arrow) due to first-order Bragg diffraction (dashed purple arrow), as illustrated in Fig. 2.3(b). The vertically radiated light waves constitute the laser output (i.e., surface emission) and significantly affect the threshold gain of the laser cavity.

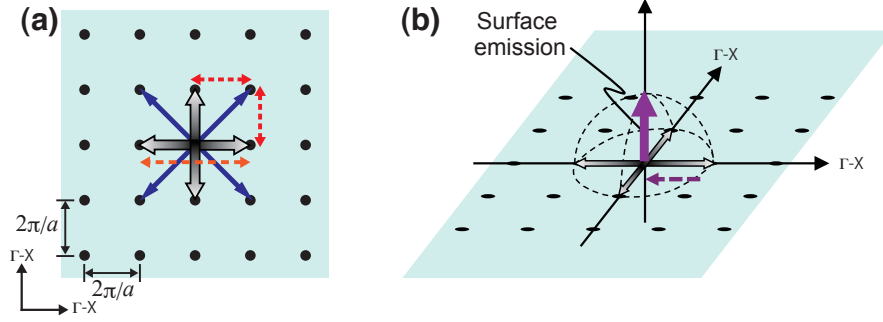


Figure 2.3: Coupling diagram illustrated in the reciprocal space of a square-lattice PC: (a) in-plane coupling and (b) out-of-plane coupling.

2.4 Theoretical methods

In this section, we describe several theoretical methods that have been used to study of PCSELs. These methods include the 2D plane-wave expansion method (PWEM) and the Finite-difference time-domain (FDTD) method, and the earlier 2D coupled-wave theory.

2.4.1 Plane-wave expansion method

The 2D plane-wave expansion method (PWEM) [75, 76] is particularly useful and powerful method for the calculating the photonic band structure and modal pattern within a 2D PC structure. By assuming a specific polarization, the Maxwell's equations can be reduced to a standard eigenvalue problem. In this section, we present the derivation process and the calculated band structures and modal patterns for a typical PCSEL structure.

In a region with no charges ($\rho = 0$) and no currents ($J = 0$), Maxwell's equations reduce to

$$\nabla \times \mathbf{E}(\mathbf{r}) = -i\omega\mu_0\mathbf{H}(\mathbf{r}), \quad (2.1)$$

$$\nabla \times \mathbf{H}(\mathbf{r}) = i\omega\varepsilon_0\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}), \quad (2.2)$$

where we have assumed an $e^{i\omega t}$ time dependence for electromagnetic waves. Then, we obtain the following equations for $\mathbf{E}(\mathbf{r})$ or $\mathbf{H}(\mathbf{r})$,

$$\frac{1}{\varepsilon(\mathbf{r})}\nabla \times \nabla \times \mathbf{H}(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{E}(\mathbf{r}), \quad (2.3)$$

$$\nabla \times \left\{ \frac{1}{\varepsilon(\mathbf{r})}\nabla \times \mathbf{H}(\mathbf{r}) \right\} = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(\mathbf{r}). \quad (2.4)$$

Within a two-dimensionally periodic structure, the $\varepsilon^{-1}(\mathbf{r})$, $\mathbf{E}(\mathbf{r})$, and $\mathbf{H}(\mathbf{r})$ can be expanded as follows according to Bloch's theorem

$$\varepsilon^{-1}(\mathbf{r}) = \sum_{\mathbf{G}} \varepsilon^{-1}(\mathbf{G}) e^{i\mathbf{G}\mathbf{r}}, \quad (2.5)$$

$$\mathbf{E}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{E}_{\mathbf{G}} \cdot e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad (2.6)$$

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{G}} \cdot e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad (2.7)$$

where $\mathbf{k}$ is the wave vector and $\mathbf{G}_{m,n}$ is the reciprocal lattice vector that is given by

$$\mathbf{G}_{m,n} = m\mathbf{b}_1 + n\mathbf{b}_2. \quad (2.8)$$

Here, $\mathbf{b}_1$ and $\mathbf{b}_2$ are the primitive reciprocal lattice vectors.

For a 2D PC structure that has periodicity in the xy plane and uniform in the z direction, there exist a pair of orthogonal modes. The mode that has only (E_x, E_y, H_z) components is called transverse-electric (TE) mode, and the one that has only (H_x, H_y, E_z) is called transverse-magnetic (TM) mode. We are interested in the TE mode, because our PCSELs mainly operate at TE mode (or TE-like mode). In this case,

$$\mathbf{E}_{\mathbf{r}} = (E_x, E_y, 0), \quad (2.9)$$

$$\mathbf{H}_{\mathbf{r}} = (0, 0, H_z), \quad (2.10)$$

Then, Eq. (2.4) reduces to

$$\frac{\partial}{\partial x} \left\{ \frac{1}{\varepsilon(\mathbf{r})} \frac{\partial H_z}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ \frac{1}{\varepsilon(\mathbf{r})} \frac{\partial H_z}{\partial y} \right\} + \frac{\omega^2}{c^2} H_z = 0 \quad (2.11)$$

By substituting Eqs. (2.12), (2.7), and (2.10) into Eq. (2.11), we obtain

$$\sum_{\mathbf{G}'} (\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') \varepsilon_{\mathbf{G}-\mathbf{G}'}^{-1} H_{\mathbf{G}'} = \frac{\omega^2}{c^2} H_{\mathbf{G}}. \quad (2.12)$$

This equation can now be solved as a simple linear-matrix, eigenvalue problem. The $\varepsilon_{\mathbf{G}-\mathbf{G}'}^{-1}$ can be approximated via the Discrete Fourier Transform of $\varepsilon(\mathbf{r})$ or can be explicitly derived by taking the Fourier Transform of $\varepsilon(\mathbf{r})$ based on the following equation

$$\varepsilon_{\mathbf{G}}^{-1} = \frac{1}{\Omega} \int_{\Omega} \varepsilon^{-1}(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}, \quad (2.13)$$

$$= \frac{1}{\varepsilon_b} \delta_{\mathbf{G},0} + \left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b} \right) \frac{1}{\Omega} \int_{\Omega} S(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}, \quad (2.14)$$

where Ω is area of the unit cell, ε_a and ε_b are the dielectric constants inside and outside the lattice point, respectively; and $S(\mathbf{r}) = 1$ for $\mathbf{r} \in R$ and $S(\mathbf{r}) = 0$ for $\mathbf{r} \notin R$ (R : area of the lattice point).

When we employ the 2D plane-wave expansion method to calculate the band structure, we need to use the modified dielectric constants instead of the actual ones (e.g., $n_{\text{air}} = 1.0$ and $n_{\text{GaAs}} = 12.25$) [31]. This is because this method unrealistically assumes the structure has an infinite depth. The air holes in the actual device have finite depth and only a small fraction of light is confined in the air holes. In order to compensate for these differences, we use a small dielectric-constant difference in the calculation [31]. The two dielectric constants, ε_a and ε_b , are calculated as follows. The distribution of the electric field in the vertical direction of the device is calculated for nonperiodic structure using the transfer-matrix method (TMM). From the result, we estimate the effective refractive index of the fundamental mode, n_{eff} , and the confinement factor for the photonic crystal layer Γ_g . Modified dielectric constants of the air holes $\tilde{\varepsilon}_a$ and the background $\tilde{\varepsilon}_b$ are determined using the following two relations

$$n_{\text{eff}}^2 = f\tilde{\varepsilon}_a + (1 - f)\tilde{\varepsilon}_b, \quad (2.15)$$

$$\tilde{\varepsilon}_b - \tilde{\varepsilon}_a = \Gamma_g(\varepsilon_b - \varepsilon_a). \quad (2.16)$$

Here, f is the air-hole filling fraction.

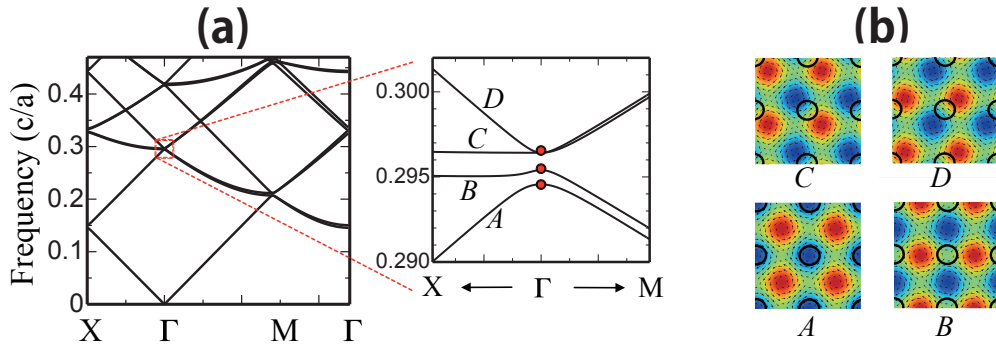


Figure 2.4: (a) TE band structure calculated for a square-lattice photonic crystal with circular air holes. (b) Field distributions around the air hole at the band-edge modes A, B, C, and D. Magnified structure at the Γ point.

As an example, we show in Fig. 2.4(a) a typical band structure calculated by using the above described PWEM. In the calculation, we considered a circular-shape air hole shape with a filling fraction of 12%. The square-lattice PC has two specific directions, $\Gamma - X$ and $\Gamma - M$. In the band structure, it is expected that lasing occurs at specific points on the Brillouin zone boundary and at points of band crossing and splitting when optical gain is supplied. The specific Γ point enclosed in the red dashed square is particularly interesting, whose enlarged image is shown on the right hand side. There

are four bands, resulting from the four coupling waves. At the Γ point, there are two singly-degenerate bands and one pair of degenerate bands. We will call these bands A , B , C , and D , as indicated in Fig. 2.4(a). Bands A and B are nondegenerate and bands C and D are doubly degenerate. The electromagnetic field distribution in the plane of the photonic crystal plane calculated for each mode is shown in Fig. 2.4(b). The amplitudes of magnetic fields in the direction perpendicular to the plane are indicated by the red and blue areas, corresponding to positive and negative amplitudes, respectively. The arrows indicate the electric-field vectors in the plane, and the black circles indicate the locations of lattice points. It can be clearly seen from the figure that the different modes are characterized by different magnetic patterns, which is useful for classifying the lasing modes. These field patterns calculated by the 2D PWEM represent in-plane electromagnetic (EM) fields. However, the property of interest observed experimentally is the surface-emitting component of these EM fields. These theoretical results can, therefore, not be compared directly to the experimental results. To make a valid comparison, we need to calculate the surface-emitting components of each lasing mode using a 3D method. In the next section, we shall briefly introduce a widely used 3D simulation tool called 3D Finite-difference time-domain (FDTD) method.

2.4.2 3D finite-difference time-domain method

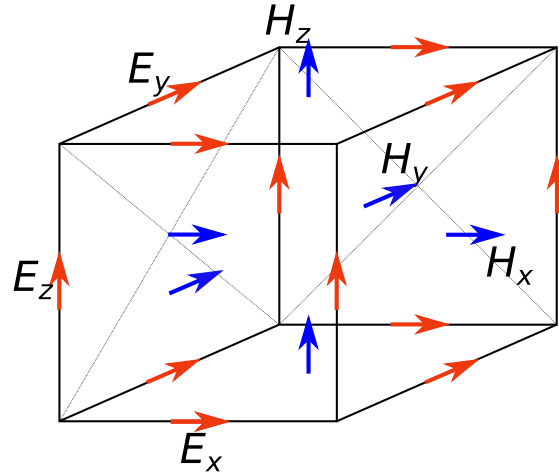


Figure 2.5: Illustration of a Cartesian Yee grid. The electric and magnetic field vector components are staggered at different spatial locations: the E -field components form the edges of the cube, and the H -field components form the normals to the faces of the cube.

The second computational tool for modeling PCSELs is the finite difference time domain (FDTD) method [77–80], which is widely used due to the simplicity of its algorithm and implementation. The computational algorithm is based on the discretization of space and time into a Yee grid (cell) [81], which staggers the electric and magnetic fields

in time and in space as depicted in Fig. 2.5. Each field component is sampled at different spatial locations offset by half a pixel, allowing the time and space derivatives of Maxwell's equations to be formulated as center-difference approximations. The Yee grid has proven to be very robust and remains at the core of many current FDTD softwares.

In this thesis, an open-source software package called MEEP is used [80]. For grid truncation it offers periodic boundary conditions or perfectly matched layers. A sub-pixel smoothing for the dielectric function is included to improve the accuracy and/or reduce the computational time. MEEP is advantageous in broad band simulations when a large range of frequencies are of interest. In this case a single broad band pulse can be used and all the spectral information (including both the central frequency and Q factor) can be extracted with a single simulation. However, it is not guaranteed that the result includes all optical eigenmodes. By accidentally positioning the source or the observation point in an intensity minimum of a mode it may be hidden in the results. A lot of time steps are also needed to resolve little separated peaks in the Fourier spectrum.

The major drawback of the FDTD method, however, is that its memory requirement and computational time scale with the structure dimension. This is especially critical for PCSEL structures which require 3D dimensional simulation because both the surface-normal emission and the in-plane loss in the PC plane need to be taken into account. Due to the Nyquist limit, a resolution of at least 10 pixels is required to spatially sample a single wavelength. For a regular PCSEL with surface normal emission, the lattice constant a is equal to a single wavelength. The modeled laser structure typically has several hundreds of periodicity in the PC (xy) plane and necessitate over $20a$ to map the extended optical field in the vertical (z) direction. Moreover, a higher resolution is required when the lattice point has a complicated geometry, e.g., a triangular shape. Since the computational time increases roughly with the fourth power of the resolution, it is fundamentally challenging to use FDTD simulations to model large-area PCSELs.

2.4.3 Coupled-wave theory: Two-dimensional eight-wave model

The light propagation and diffractions in real space described in Section 2.3 can be understood in an analytical by using a coupled-wave theory (CWT) approach [65]. CWT is widely used in many practical applications, especially in the one dimensional (1D) distributed feedback lasers [3, 5–8]. It provides a powerful approach to understand the physics of the periodic structures. In this section, to introduce the basics of this approach, we first give a short review of earlier 2D eight-wave coupled-wave theory

developed by K. Sakai et al., [62, 63], and then we point out the limitations of this theory.

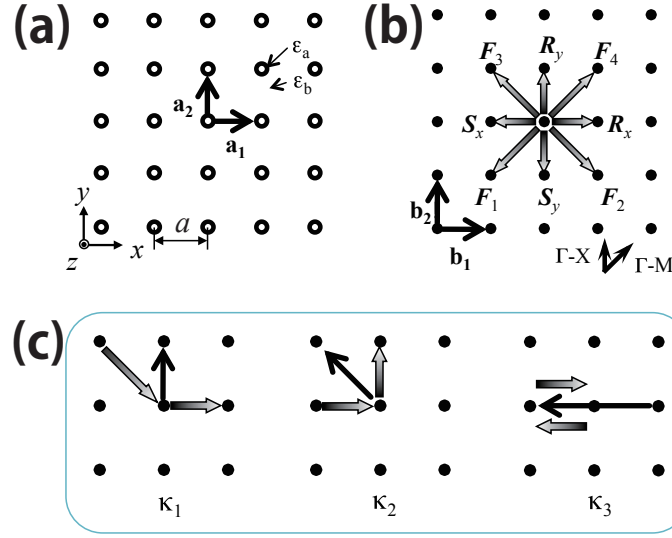


Figure 2.6: (a) Schematic of a square-lattice PC. (b) Reciprocal lattice with eight wavevectors considered in the earlier works [62, 63]. (c) Diffraction diagram for each coupling constant. Gray arrows indicate the wave vectors and black arrows indicate the corresponding reciprocal vectors.

The investigated PC structure consists of a square-lattice of circular holes in the $x - y$ plane with lattice constant a , as shown in Fig. 2.6(a). The dielectric constants of the circular holes and the background material are ϵ_a and ϵ_b , respectively. The structure is assumed to be uniform in the z direction. The reciprocal lattice of a square-lattice PC is depicted in Fig. 2.6(b). The reciprocal lattice vectors $\mathbf{G}_{m,n}$ are given by

$$\mathbf{G}_{m,n} = (m\beta_0, n\beta_0), \quad (2.17)$$

where $\beta_0 = 2\pi/a$, and m and n are arbitrary integers.

For a transverse-electric (TE) mode in square lattice, the magnetic field only has z -oriented component H_z and satisfy the following scalar wave equation

$$\frac{\partial}{\partial x} \left\{ \frac{1}{k^2} \frac{\partial H_z}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ \frac{1}{k^2} \frac{\partial H_z}{\partial y} \right\} + H_z = 0 \quad (2.18)$$

where k^2 is given by

$$k^2 = \frac{\omega^2}{c^2} \epsilon(\mathbf{r}) + i \frac{2\pi \epsilon_0^{1/2}}{\lambda} \alpha \quad (2.19)$$

where ω is the angular frequency. λ (c) is the wavelength (the speed of light) in the free space. ϵ_0 is the averaged dielectric constant and α is the averaged gain constant.

In a 2D periodic structure, the magnetic field H_z can be expanded according to

$$H_z = \sum_{m,n} H_{m,n}(z) e^{-im\beta_0 x - in\beta_0 y}, \quad (2.20)$$

Similarly, the dielectric function $\varepsilon(\mathbf{r})$ can be expressed as

$$\varepsilon(\mathbf{r}) = \varepsilon_0^2 + \sum_{m,n \neq 0} \xi_{m,n}(z) e^{-im\beta_0 x - in\beta_0 y}. \quad (2.21)$$

Then, we have

$$\frac{1}{k^2} \simeq \frac{1}{\beta^4} \beta^2 - i2\alpha\beta + 2\beta \sum_{m,n \neq 0} \kappa_{m,n} e^{-im\beta_0 x - in\beta_0 y}, \quad (2.22)$$

where the coupling coefficient is defined by

$$\kappa_{m,n} = -\frac{\pi}{\lambda \varepsilon_0^{1/2}} \xi_{m,n} - i\frac{\alpha}{2}. \quad (2.23)$$

Although in Eq. 2.20 an infinite set of Bloch waves exist, only eight waves are assumed to contribute significantly to the coupling between light waves [62, 63], i.e. four basic waves with $|\mathbf{G}_{m,n}| = \beta_0$ and four high-order waves with $|\mathbf{G}_{m,n}| = \sqrt{2}\beta_0$, as shown in Fig. 2.6. Then, the expression of magnetic field H_z reduces to

$$\begin{aligned} H_z(\mathbf{r}) = & R_x e^{-i\beta_0 x} + S_x e^{i\beta_0 x} + R_y e^{-i\beta_0 y} + S_y e^{i\beta_0 y} \\ & + F_1 e^{i\beta_0 x + i\beta_0 y} + F_2 e^{-i\beta_0 x + i\beta_0 y} + F_3 e^{i\beta_0 x - i\beta_0 y} + F_4 e^{-i\beta_0 x - i\beta_0 y} \end{aligned} \quad (2.24)$$

Substituting Eq. (2.22)-(2.24) and including diffraction in the direction vertical to the PC plane represented by the coupling coefficient κ_0 , we obtain four coupled-wave equations in the form

$$(\delta + i\alpha)R_x = \left(-\frac{4\kappa_1^2}{\beta_0} + i\kappa_0\right) R_x + (-\kappa_3 - i\kappa_0) S_x - \frac{2\kappa_1^2}{\beta_0} R_y - \frac{2\kappa_1^2}{\beta_0} S_y + i\frac{\partial}{\partial x} R_x, \quad (2.25a)$$

$$(\delta + i\alpha)R_x = (-\kappa_3 - i\kappa_0) R_x + \left(-\frac{4\kappa_1^2}{\beta_0} + i\kappa_0\right) S_x - \frac{2\kappa_1^2}{\beta_0} R_y - \frac{2\kappa_1^2}{\beta_0} S_y - i\frac{\partial}{\partial x} S_x, \quad (2.25b)$$

$$(\delta + i\alpha)R_x = -\frac{2\kappa_1^2}{\beta_0}R_x - \frac{2\kappa_1^2}{\beta_0}S_x + \left(-\frac{4\kappa_1^2}{\beta_0} + i\kappa_0\right)R_y + (-\kappa_3 - i\kappa_0)S_y + i\frac{\partial}{\partial y}R_y, \quad (2.25c)$$

$$(\delta + i\alpha)R_x = -\frac{2\kappa_1^2}{\beta_0}R_x - \frac{2\kappa_1^2}{\beta_0}S_x + (-\kappa_3 - i\kappa_0)R_y + \left(-\frac{4\kappa_1^2}{\beta_0} + i\kappa_0\right)S_y - i\frac{\partial}{\partial y}S_y, \quad (2.25d)$$

Here, the coupling coefficients are defined as follows,

$$\kappa_1 = \kappa_{m,n}|_{m,n} \in \{(1, 0), (-1, 0), (0, 1), (0, -1)\} \quad (2.26a)$$

$$\kappa_3 = \kappa_{m,n}|_{m,n} \in \{(2, 0), (-2, 0), (0, 2), (0, -2)\} \quad (2.26b)$$

$$\kappa_0 = A_0\kappa_1^2 \quad (2.26c)$$

where the constant A_0 is defined empirically as $A_0 = 2\kappa_1^2 L^2/500$ where L is the side length of the laser cavity. The parameter α represents the threshold gain, and δ represents the deviation of the resonant frequency ω from the Bragg frequency ω_0

$$\delta = \beta - \beta_0 = n_{av}(\omega - \omega_0)/c, \quad (2.27)$$

where n_{av} is the averaged refractive index and equal to $\varepsilon_0^{1/2}$.

The above coupled-wave Eqs. (2.25a)-(2.25d) give a description of the complicated coupling mechanism between light waves in 2D PC laser cavity. Their physical interpretations are of great interest. For example, Eq. (2.25a) expresses how the basic wave R_x couples with other three basic waves S_x , R_y and S_y . R_x couples with the counter-propagating basic wave S_x with the strength represented by κ_3 , as shown in Fig. 2.6(c). In the case of TE mode, the basic wave R_x propagating in the x direction can not couple directly with R_y or S_y propagating in the $\pm y$ directions, because their polarization direction is orthogonal. Yet, they can still indirectly couple via the oblique coupling with high-order waves (Fig. 2.6(c)). This oblique coupling provides a 2D optical feedback which contributes to the 2D coherent oscillation. The coupling strength between basic waves and high-order waves is represented by κ_1 . In addition to the in-plane coupling, the basic wave R_x also couples with light waves propagating in the vertical direction with the strength determined by κ_0 . Via this coupling some part of energy inside the laser cavity is radiated into the vertical direction and construct the output power of the

laser cavity. The other three coupled-wave equations can be understood in the same manner.

The coupling coefficients included in Eqs. (2.25a)-(2.25d) depend only on the PC structure and the waveguide structure, and can be analytically calculated by using Eqs. (2.23) and (2.26a)-(2.26c)(2.10). Once the values of these parameter are known, the coupled-wave Eqs. (2.25a)-(2.25d) can be solved numerically as an eigenvalue problem. The eigenvalues α and δ provide the threshold gain and frequency of the resonant modes, respectively. Additionally, the corresponding eigenvectors characterize the resonant modes. Therefore, quantitative understanding of the lasing properties of the laser cavity becomes possible.

2.5 Threshold condition and mode stability

The laser threshold condition corresponds to the situation when the modal gain equals the sum of the intrinsic and total cavity loss. It is well known that, for a simple Fabry-Perot laser, the laser threshold condition is determined by,

$$\Gamma g_{\text{th}} = \alpha_i + \alpha_m \quad (2.28)$$

$$\alpha_m = \frac{1}{2L} \ln \frac{1}{R_1 R_2} \quad (2.29)$$

where Γ is the optical confinement factor, and α_i is the intrinsic loss due to mostly free carrier absorption of the waveguide and scattering loss caused by the waveguide wall roughness. The mirror loss α_m accounts for the transmission losses (output) at the two end mirrors (facets) with reflectivity R_1 and R_2 . L represents the distance between the two mirrors. With an increase in the injection current density J , the gain increases due to the increase of the carrier concentration n . When the threshold condition is reached, the carrier concentration n is pinned at the threshold value n_{th} because the gain is pinned at the threshold value: $g_{\text{th}} = (\alpha_i + \alpha_m)/\Gamma$ [104]. If we adopt a typical linear gain model for the peak gain coefficient versus the carrier density such as,

$$g(n) = g'(n - n_{\text{tr}}), \quad (2.30)$$

where g' is the differential gain, dg/dn , and n_{tr} is a transparency concentration when the gain is zero. Then, the threshold current density becomes

$$n_{\text{th}} = n_{\text{tr}} + (\alpha_i + \alpha_m)/(\Gamma g'). \quad (2.31)$$

For a PCSEL cavity, the total cavity loss α_{total} includes both the in-plane loss ($\alpha_{\parallel}$) and the surface emission loss (α_v),

$$\alpha_{\text{total}} = \alpha_{\parallel} + \alpha_v \quad (2.32)$$

which is depicted schematically in Fig. 2.7. Unfortunately, both $\alpha_{\parallel}$ and α_v cannot be derived explicitly because of the complex coupling mechanism in PCSEL cavity. Quantitative description of these loss terms will necessitate a 3D modeling method.

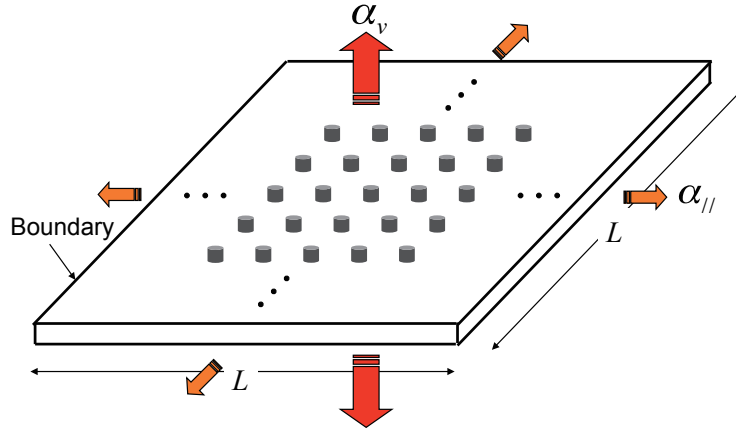


Figure 2.7: (a) Schematic of cavity loss in a PCSEL. The surface emission loss (α_v) and the in-plane loss ($\alpha_{\parallel}$) are represented by the red and orange arrows, respectively.

Because of the wavelength-selective feedback provided by the Bragg reflections at the second-order Γ point of the photonic-band structure (Fig. 2.4(a)), the resonance condition will only be fulfilled for the resonant wavelength that is close to the lattice constant, i.e., $\lambda \simeq a$. This is exactly the mode selection mechanism described in Section 2.3. However, it is important to note that there are for band-edge modes that may satisfy this phase resonance condition. In other word, the Bragg reflection at the at the second-order Γ point solely cannot ensure a single-mode operation. To enable single-mode condition, one more mode selection mechanism is necessary. This provided by the difference in the modal gain which refers to the optical gain minus the laser cavity loss α_{total} experienced by the resonant mode. The mode with the highest modal gain will be favored for lasing. This implies that the laser will lase at the band-edge mode with the lowest α_{total} . The other resonant modes do not receive enough optical gain to overcome the cavity losses and are called the side modes. Typically, the α_{total} of each band-edge modes is different due to their different field pattern, and will be discussed in detail in the next chapter. The difference between the cavity losses of the first lasing mode and the side mode with the second-lowest α_{total} determines how much the side mode suppression ratio, and

hence, the mode stability. Therefore, we conclude that the cavity loss α_{total} plays a key role in determining the lasing and the single-mode stability.

2.6 Discussion

Computer simulations based on the 2D plane-wave expansion method (PWEM) [31, 75, 76] or the finite-difference time-domain (FDTD) method [77–79], can provide valuable information about the lasing properties of the PC laser cavity. However, there are some inherent limitations to these computational approaches. The 2D PWEM is only applicable to infinite structures, and the FDTD method requires substantial computational resources in order to model finite structures with realistically large areas. Moreover, neither simulation approach provides deep analytical insight into improving the design of devices. A group of alternative analytical methods [33, 61] have been developed, based on the concept of one-dimensional (1D) coupled-wave theory (CWT) [65]. However, these methods in their initial formulations consider only four basic waves in the coupled-wave model and disregard 2D optical coupling effects, which are important in 2D square-lattice PCs. Sakai et al. later derived a 2D CWT using an eight-wave model [62, 63] that incorporates both conventional 1D coupling and the more pertinent 2D coupling, allowing 2D coherent lasing action to be explained [34].

Because the previous CWT [62, 63] is essentially a 2D model, it is accurate for 2D systems, while having inherent limitations when trying to model a full three-dimensional (3D) system. The first limitation is attributed to the number of waves considered in the coupled-wave model. As described above, eight Bloch waves are taken into consideration in the previous CWT. As a result, only coupling coefficients of lower orders are considered to contribute significantly to the couplings between these Bloch waves. Since we consider the resonant case at the second-order Γ -point, coupling coefficient $\kappa_{m,n}$ corresponds to the reciprocal lattice vector $\mathbf{G}_{m,n}$ in reciprocal lattice space. Fig. 2.8(a) shows the coupling diagram of all the couplings considered in the previous CWT. The following groups of coupling coefficient $\kappa_{m,n}$ were included

- κ_3 : 1D feedback coupling,
- κ_1 : 2D optical coupling,
- κ_0 : out-of-plane coupling between radiative and basic waves.

The first group κ_3 consists of $\kappa_{2,0}$, $\kappa_{-2,0}$, $\kappa_{0,2}$, and $\kappa_{0,-2}$, the second group κ_1 consists of $\kappa_{1,0}$, $\kappa_{-1,0}$, $\kappa_{0,1}$, and $\kappa_{0,-1}$, and the third group κ_0 was defined as a fitting parameter

proportional to the square of κ_1 . Thus, eventually, all the coupling effects considered in the previous system are expressed by $\kappa_{1,0}$, $\kappa_{-1,0}$, $\kappa_{0,1}$, $\kappa_{0,-1}$, $\kappa_{2,0}$, $\kappa_{-2,0}$, $\kappa_{0,2}$, and $\kappa_{0,-2}$, as depicted in Fig. 2.8(a). Since $\kappa_{m,n}$ is proportional to the Fourier coefficients of the dielectric function $\xi_{m,n}$ (Eq. (2.23)), all the included coupling effects are represented by the limited number of Fourier coefficients : $\xi_{1,0}$, $\xi_{-1,0}$, $\xi_{0,1}$, $\xi_{0,-1}$, $\xi_{2,0}$, $\xi_{-2,0}$, $\xi_{0,2}$, and $\xi_{0,-2}$. This might be a good approximation when the higher-order Fourier components of the dielectric function $\varepsilon(\mathbf{r})$ of the PC are small enough so that they can be neglected, e.g. in the case of a circular air-hole shape (see Fig. Fig. 2.8(b)). However, when the air-hole shape of PC becomes asymmetric, the higher-order Fourier components of $\varepsilon(\mathbf{r})$ could be large, as shown in Fig. 2.8(c) for a right-angled isosceles triangle (RIT) air-hole shape. The components considered in the previous CWT are limited inside the area indicated by the yellow lines. Apparently, beyond the indicated area there exist large components that can not be neglected, e.g. $\varepsilon_{1,1}$ and $\varepsilon_{-1,-1}$, etc. These components are significant to represent the asymmetric nature of the RIT air-hole shape, therefore it is important to include these higher-order coupling coefficients to in order to reflect the effects of the asymmetry.

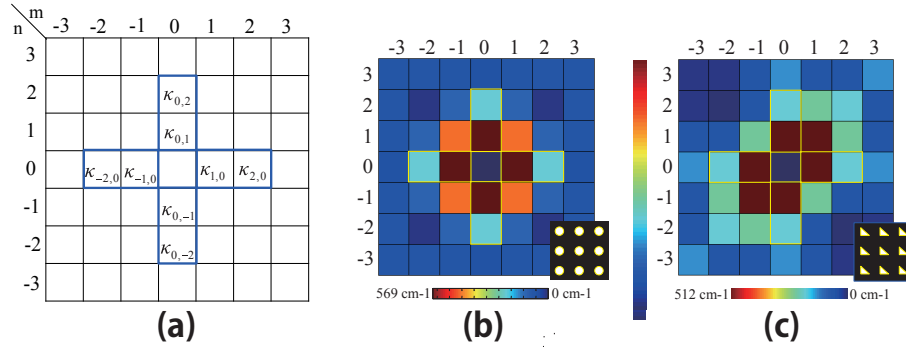


Figure 2.8: (a) Coupling coefficients considered in the previous CWT. Intensity distribution of coupling coefficients (Fourier coefficients) of (b) circular and (c) right-angled isosceles triangle shaped air holes. The components indicated by the yellow line are those included in the previous CWT.

Second, the coupling coefficients are not rigorously defined in the earlier 2D CWT theory. In the previous theory, the coupling coefficient $\kappa_{m,n}$ with a uniform gain constant is defined as [62, 63]

$$\kappa_{m,n} = -\frac{\pi}{\lambda \varepsilon_0^{1/2}} \tilde{\xi}_{m,n}. \quad (2.33)$$

Here, the $\tilde{\xi}_{m,n}$ represents the Fourier coefficient of the effective dielectric constant difference within PC region, which is determined by calculating the electric field profile of the fundamental waveguide mode $\Theta_0(z)$ of the device structure using Transfer matrix

method (TMM) [74]. Then, Eq. (2.33) can be written as

$$\kappa_{m,n} = -\frac{\pi}{\lambda \varepsilon_0^{1/2}} \tilde{\xi}_{m,n} = -\frac{\pi}{\lambda \varepsilon_0^{1/2}} \xi_{m,n} \Gamma_g. \quad (2.34)$$

where $\xi_{m,n}$ is the Fourier coefficient of the realistic dielectric constant difference (e.g., GaAs and air). $\Gamma_g = \int_{PC} |\Theta_0(z)|^2 dz$ is the optical confinement factor of the PC layer and $\Theta_0(z)$ is normalized as where $\Theta_0(z)$ is normalized as $\int_{-\infty}^{\infty} |\Theta_0(z)|^2 dz = 1$. In the resonant case of the second-order Γ point, the in-plane wavenumber of basic waves β_0 is chosen to closely match the wavenumber of the fundamental waveguide mode β ,

$$\beta_0 = \frac{2\pi}{a} = \beta. \quad (2.35)$$

Therefore, the electric field profile of the basic waves in the vertical direction can be approximated by $\Theta_0(z)$. In general, coupling coefficient between two modes depends upon not only the Fourier coefficient associated with the wave vector of the individual modes but also the integrated overlapping field of the individual modes [73]. From Eq. (2.34), we can see that the term representing the integrated overlapping field of the individual modes corresponds to $\int_{PC} |\Theta_0(z)|^2 dz$. Here, it is important to note that the field profile of all the individual modes has been implicitly assumed to be identical to $\Theta_0(z)$. In the case of 1D coupling coefficient κ_3 , both of the field profiles for the two waves involved (i.e., basic waves) is $\Theta_0(z)$, thus the definition given by Eq. (2.34) correctly expresses the integrated overlapping field of the individual modes. However, in the other two cases (κ_1 or κ_0) for which the high-order or radiative waves are involved, Eq. (2.34) is inaccurate. Because the in-plane wavenumber of high-order waves equal to $\sqrt{2}\beta_0$ and that of the radiative waves equals to zero, the large deviation from β_0 indicates that approximating the field profiles of high-order waves and radiative waves using the same $\Theta_0(z)$ would result in a large error, which will be described in greater detail in the next chapter. This suggests that we need to treat the field profile of each Bloch wave very carefully and make the κ 's definition more generally applicable to various coupling situations.

Third, the vertical coupling coefficient κ_0 (Eq. (2.26c)), a very important parameter to describe the surface emission, is still defined empirically via a numerical fit to the experimental data. An explicit expression yet has to be derived, in order to quantitatively evaluate the amount of the radiation power into the vertical direction. Here, we note that, in the case of TE mode, the radiative waves coupled to the vertically direction do not have the H_z component. This suggests that the H_z -based scalar wave equation (Eq. 2.18), which is the starting point of the previous CWT formulation, has fundamental limitation in modeling the surface normal emission. To overcome this limitation, a

vectorial wave equation will be considered in the next chapter.

2.7 Summary

This chapter described the fundamentals of PCSEL devices and their theoretical backgrounds. First was the introduction of the device structures fabricated by using the wafer-bonding techniques. Next the basic lasing principles at the band-edge modes of the second-order Γ point were briefly described. The Bragg diffraction in both in both the x and y directions enables a large-area 2D cavity mode. At the same time, the PC itself diffracts the in-plane resonant light waves into vertical direction, leading to the surface emission behavior. Then, several theoretical tools for modeling PCSELs were introduced. 2D plane-wave expansion method (PWEM), while is a powerful tool for calculating the photonic band structure and field patterns of the eigenmodes, is only applicable to 2D structures and therefore cannot model the surface emission (laser output) which is the principal property of our interest. The 3D finite-difference time-domain (FDTD) method is able to treat the surface emission components but requires substantial computational resources when applied to model a realistically large-area laser cavity. As an alternative analytical methods, a 2D coupled-wave theory (CWT) was developed in the earlier works. Differing from the PWEM and 3D FDTD methods, which are inherently computer simulations, the analytical CWT method provides deep physical insights into the detailed behavior of light waves in PCs because wave couplings and diffraction effects can be formulated explicitly by defining the coupling coefficients. Moreover, various lasing properties of the resonant modes (resonant frequency, threshold gain, field distribution, etc.) can be calculated efficiently. However, after a brief overview of the previous CWT works by focusing on the derivation process of the coupled-wave equations, we revealed that the previous CWT is essentially a 2D model because the device structure was assumed to be uniform in the vertical direction. This assumption is critical because the surface emission components cannot be explicitly described without considering a nonuniform waveguide structure in the vertical direction. Moreover, only eight wavevectors was considered in the previous coupled-wave model, which unavoidably result in inaccuracy when modeling PC geometries with complex air-hole shapes. In the consequent chapter, we shall develop a 3D CWT model to overcome the above-mentioned drawbacks of the previous theory.

Chapter 3

Three-dimensional modeling of wave interactions in PCSELs

3.1 Introduction

As discussed in the end of Chapter 2, the previous CWT [62, 63] has inherent limitations when trying to model a full three-dimensional (3D) system. The fundamental reason lies in the fact that the previous is essentially a 2D model. Therefore, the surface emission in the vertical direction (i.e., the laser output), the principal feature of interest, cannot be modeled. Additionally, difference in the vertical field profiles of the individual Bloch wavevector components was not considered and instead an identical field profile was assumed for all the wavevectors. This assumption is critical because the coupling coefficients cannot be accurately defined without considering the overlapped fields of the individual wavevector components. Furthermore, the eight wavevectors were not enough to reflect the air-hole geometry because the higher-order Fourier components were neglected.

In this Chapter, we develop a 3D coupled-wave model for square-lattice PCSELs with transverse-electric (TE) polarization in order to overcome the limitations discussed above. We present a generalized coupled-wave formulation for a 3D structure by extending the original coupled-wave approach developed by Streifer *et al.* for 1D distributed feedback (DFB) lasers [66]. The separation of variables technique and Green function approximation [67] are employed in order to derive an explicit expression for the coupling coefficients in a 3D system. Our coupled-wave model not only incorporates a large number of high-order wavevectors, but also takes their individual vertical field profiles into account. This model accurately describes all the important coupling effects in 3D systems, and can also be generally applied to the analysis of PC structures with air holes

of arbitrary shape. Next, we further extend the coupled-wave model of band-edge modes to that for the non- Γ -point modes by introducing a small wavevector perturbation into the coupled-wave model. We present numerical examples in which the in-plane and vertical field profiles, as well as the mode frequency and radiation constant of PC structures with different air-hole shapes are calculated. These results are compared with 3D-FDTD simulations in order to confirm the validity of the proposed CWT model. This Chapter is organized as follows. Section 3.2 presents the 3D coupled-wave model for Γ -point band-edge modes and the relevant analysis results. Section 3.3 presents model for non- Γ -point band-edge modes and band structure analysis. A summary of our findings is given in the final Section.

3.2 3D coupled-wave model for Γ -point band-edge modes

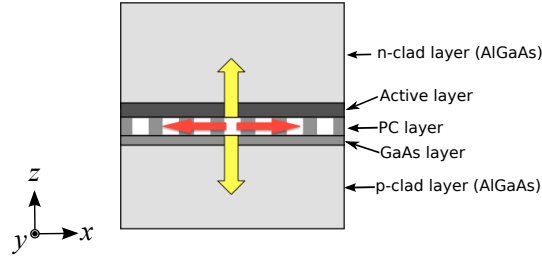


Figure 3.1: Schematic cross-sectional view of a PC-SEL device. This multi-layer waveguide structure represents an approximation of a realistic laser device, which was described in detail in Ref. [46]. We simplify the vertical geometry by not depicting the upper n-substrate and lower p-contact layers and the surrounding air because the penetration of the fundamental waveguide mode field into these layers is negligibly small. For simplicity, we assume that both the upper and lower device surfaces are antireflection coated. The orange and the yellow arrows represent the in-plane guided waves and the light waves diffracted into the vertical direction.

Table 3.1: Waveguide structural parameters.

Layer	Thickness (μm)	Dielectric constant
n-clad(AlGaAs)	1.5	11.0224
Active	0.0885	12.8603
PC	0.1180	ϵ_{av}
GaAs	0.0590	12.7449
p-clad(AlGaAs)	1.5	11.0224

A schematic cross-section of the PC-SEL device considered here is shown in Fig. 3.1, which can be approximated by a multilayer waveguide. The PC layer is embedded in the waveguide structure, which is assumed to support only a single waveguide mode. Details of the device was described in [46] (we simplify the vertical geometry by not depicting the upper n-substrate and lower p-contact layers and the surrounding air because

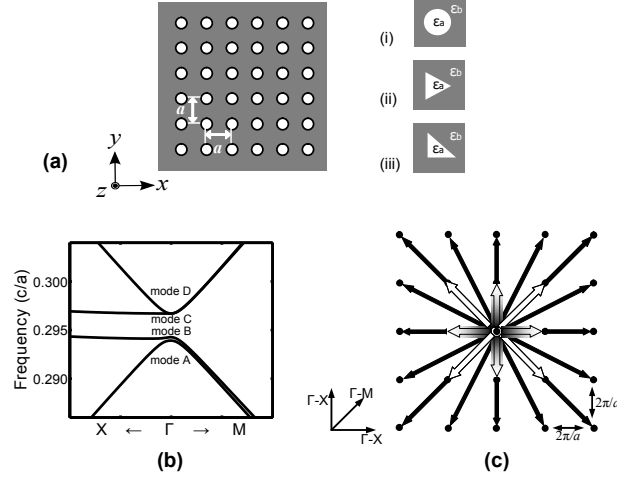


Figure 3.2: (a) Schematic diagram of a square-lattice PC and examples of air-hole designs: (i) circular, (ii) equilateral triangular, (iii) right-angled isosceles triangular. (b) A typical photonic-band structure calculated by 2D-PWEM [46]. (c) Bloch wave state represented by wavevectors (arrows) in reciprocal space. A large number of high-order wavevectors need to be included, in addition to the eight wavevectors (light arrows) considered in the previous study.

the penetration of the fundamental waveguide mode field into these layers is negligibly small). For simplicity, we assume that both the upper and lower device surfaces are antireflection coated. The structural parameters of each layer are summarized in Table 3.1. The average dielectric constant of the PC layer is given by $\epsilon_{av} = f \cdot \epsilon_a + (1 - f) \cdot \epsilon_b$, where ϵ_a is the dielectric constant of air, ϵ_b is the dielectric constant of the background dielectric material (GaAs), f is the filling factor (FF) given by $f = S_{air-hole}/a^2$ (i.e., the fraction of the area of a unit cell occupied by air holes), and a is the lattice constant. The PC layer consists of a square lattice with air holes perpendicular to the xy plane, as shown in the left side of Fig. 3.2(a). In this paper, the shape of the air-holes is not restricted to circular but can be arbitrary. The right side of Fig. 3.2(a) depicts examples of air-hole shapes that are considered later in this paper: (i) circles, (ii) equilateral triangles, and (iii) right-angled isosceles triangles. The lattice constant a is designed to match the wavelength of light in the waveguide such that the photonic lattices serve to provide a 2D distributed feedback effect induced by Bragg diffraction. It should be noted that, in contrast to the vertical-cavity surface-emitting lasers (VCSELs) [9], PCSELs are band-edge lasers where a single stable longitudinal and transverse mode gives rise to coherent large-area lasing [29]. Fig. 3.2(b) shows a typical photonic-band structure in the vicinity of the second-order Γ -point for a square lattice PC with TE polarization (for further details, see Ref. [46]). There exist four band-edge modes, which we refer to as modes A, B, C and D, in order of increasing frequency.

The second-order Γ -point is particularly interesting since it provides the in-plane distributed feedback effect to form the lasing cavity and light is simultaneously diffracted

in the direction normal to the PC surface (yellow arrows in Fig. 3.1) due to first-order Bragg diffraction of the in-plane guided waves (orange arrows in Fig. 3.1). The radiated light waves constitute the laser output (i.e. surface emission) and dominate the threshold gain of the laser cavity with a large area (the side length of our band-edge laser device is usually larger than $100\ \mu\text{m}$ or 300 periods such that PCs can be practically regarded to be infinity and the in-plane loss can be neglected [78]). Therefore, it is important to quantify this radiation effect in the analysis of PCSELs. However, the previous study [63] did not explicitly formulate this effect as the limited 2D model cannot describe waves that are diffracted into an extra dimension (i.e. the vertical direction). As a result, one of the objectives of this paper is to develop a rigorous formulation of the full 3D structure to model this radiation effect.

Light propagating inside a PC must obey Bloch's theorem, which states that the amplitude of the light must conform to the imposed periodicity [71]. The Bloch wave state ψ at the Γ -point can be expressed as a Fourier series of plane waves:

$$\psi(\mathbf{r}) = \sum_{m,n} a_{m,n}(z) e^{-i(m\beta_0 x + n\beta_0 y)}, \quad (3.1)$$

where $a_{m,n}$ represents the field amplitude of a wave with wavevector $(m\beta_0, n\beta_0)$, m and n are arbitrary integers, and $\beta_0 = 2\pi/a$. It is implied by Eq. (3.1) that the Bloch wave state is composed of multiple wavevectors, including the wavevectors indicated by arrows in the reciprocal space diagram in Fig. 3.2(c), as well as wavevectors outside the plotted range. In the vicinity of the second-order Γ -point, the resonant states are primarily made up of fields of four wavevectors with in-plane wavenumber: $(\pm\beta_0, 0)$ and $(0, \pm\beta_0)$ (the shortest light arrows in Fig. 3.2(c)). In the case of TE polarization, the wavevectors $(\pm\beta_0, 0)$ and $(0, \pm\beta_0)$ cannot couple directly, thus high-order wavevectors need to be introduced to explain the 2D coupling phenomenon [62]. However, the 2D coupling reported in the previous study took into account only the contribution of low-order Fourier components of the PC refractive index profile, as only four high-order wavevectors: $(\pm 1, \pm 1)\beta_0$ (see the four oblique light arrows in Fig. 3.2(c)) were included. Yet, when we consider an arbitrary air-hole geometry, asymmetric air-hole shapes in particular, contributions of higher-order Fourier components cannot be neglected. Furthermore, the vertical field profile for each in-plane wavevector shown in Fig. 3.2(c) was assumed to be identical in the previous 2D theory, this therefore is another major limitation in describing full 3D laser device. To overcome these limitations mentioned above, we develop a generalized CWT formulation in a full 3D model as follows.

Here, we focus our discussion on the TE polarization because PCSELs. We choose to start our formulation from Maxwell's equations using the electric-field components, because scalar wave equations for the magnetic field (H_z) [62] cannot include waves

diffracted in the vertical direction (see the yellow arrows in Fig. 3.1). In a 3D waveguide structure as shown in Fig. 3.1, the electric field can be expressed as $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{i\omega t}$. By eliminating the magnetic field from Maxwell's equations, we obtain

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) = k_0^2 \tilde{n}^2(\mathbf{r}) \mathbf{E}(\mathbf{r}), \quad (3.2)$$

where $k_0 (= \omega/c)$ is the free-space wavenumber, ω is the angular frequency, c is the velocity of light in free space and $\tilde{n}$ is the refractive index (a complex number) that satisfies [66]

$$k_0^2 \tilde{n}^2(\mathbf{r}) = k_0^2 n^2(\mathbf{r}) + 2ik_0 n(\mathbf{r}) \tilde{\alpha}(\mathbf{r}) - \tilde{\alpha}^2(\mathbf{r}), \quad (3.3)$$

where $n(\mathbf{r})$ is the real part of $\tilde{n}(\mathbf{r})$ and $\tilde{\alpha}(z)$ represents the gain ($\tilde{\alpha} > 0$) or loss ($\tilde{\alpha} < 0$) in each region. In the following derivation, we neglect the third term $\tilde{\alpha}^2(z)$ because $|\tilde{\alpha}| \ll k_0 n_0$ [66]. The TE polarization fields $\mathbf{E}(\mathbf{r}) = (E_x(\mathbf{r}), E_y(\mathbf{r}), 0)$ can be expanded according to Bloch theorem

$$E_i(z) = \sum E_{i,mn}(z) e^{-im\beta_0 x - in\beta_0 y}, i = x, y. \quad (3.4)$$

Besides, we expand the refractive index profile as

$$n^2(\mathbf{r}) = n_0^2(z) + \sum_{m \neq 0, n \neq 0} \xi_{m,n}(z) e^{-im\beta_0 x - in\beta_0 y}. \quad (3.5)$$

Here, m, n are arbitrary integers; $n_0^2(z) = \varepsilon_0(z)$, $\varepsilon_0(z)$ is the average dielectric constant of the material at position z , and $\xi_{m,n}(z)$ is the high-order Fourier coefficient term. We note that $\xi_{m,n}(z)$ is zero outside the PC region. Inside the PC region, $n_0^2(z) = \varepsilon_{av}$ and $\xi_{m,n}(z)$ can be expressed as $\xi_{m,n}(z) = \frac{1}{a^2} \iint_{-a/2}^{a/2} n^2(x, y) e^{im\beta_0 x + in\beta_0 y} dx dy$. In order to simplify the formulation, we have assumed that air holes within the PC region have perfectly vertical sidewalls (a formulation for air holes with tilted sidewalls will be given elsewhere [85]) such that n_0^2 and $\xi_{m,n}$ are independent of z within this region.

By combining Eqs. (3.2) -(3.5), and collecting all terms that are multiplied by the factor $e^{-im\beta_0 x - in\beta_0 y}$, we obtain

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 + 2i\tilde{\alpha}k_0 n_0(z) - n^2 \beta_0^2 \right] E_{x,m,n} + mn\beta_0^2 E_{y,m,n} \\ = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{x,m',n'}, \end{aligned} \quad (3.6a)$$

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 + 2i\tilde{\alpha}k_0 n_0(z) - m^2 \beta_0^2 \right] E_{y,m,n} + mn\beta_0^2 E_{x,m,n} \\ = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{y,m',n'}, \end{aligned} \quad (3.6b)$$

$$\frac{\partial}{\partial z} [mE_{x,mn} + nE_{y,mn}] = 0. \quad (3.6c)$$

In this work, the derivative terms of E_x and E_y with respect to x and y have been eliminated because we assume an infinite periodic PC structure (the corresponding formulation for a finite periodic PC structure will be given elsewhere).

The wavevectors can be classified into three groups according to their in-plane wavenumber, $\sqrt{m^2 + n^2}\beta_0$.

- Basic waves: $\sqrt{m^2 + n^2} = 1$,
- High-order waves: $\sqrt{m^2 + n^2} > 1$,
- Radiative waves: $m = 0, n = 0$.

It is possible to solve Eqs. (3.6a)-(3.6c) using the method of separation of variables by assuming a separable form of solutions for the fields. In the resonant case at the second-order Γ -point [62], the basic waves can be expressed as

$$E_{x,1,0} = 0, \quad E_{y,1,0} = R_x \Theta_0(z), \quad (3.7a)$$

$$E_{x,-1,0} = 0, \quad E_{y,-1,0} = S_x \Theta_0(z), \quad (3.7b)$$

$$E_{x,0,1} = R_y \Theta_0(z), \quad E_{y,0,1} = 0, \quad (3.7c)$$

$$E_{x,0,-1} = S_y \Theta_0(z), \quad E_{y,0,-1} = 0. \quad (3.7d)$$

Here, R_x and S_x represent the amplitudes of basic waves propagating in the $+x$ and $-x$ directions, respectively, and likewise R_y and S_y represent the amplitudes of waves propagating in the $+y$ and $-y$ directions, respectively. These four basic waves are assumed to have identical field profiles in the z -direction, denoted by $\Theta_0(z)$, which is the same as the field profile of the fundamental waveguide mode for a waveguide with no periodic structure [66, 67]. We express the wave equation for the fundamental waveguide

mode in terms of $\Theta_0(z)$ as

$$\frac{\partial^2 \Theta_0}{\partial z^2} + [k_0^2 n_0^2(z) - \beta^2] \Theta_0 = 0, \quad (3.8)$$

where β is the propagation constant. The solutions for β and $\Theta_0(z)$ in Eq. (3.8) can be obtained by employing the transfer matrix method (TMM) [74].

In order to obtain the equations satisfied by the basic waves, Eqs. (3.7a)-(3.7d) are substituted into Eqs. (3.6a)-(3.6c) for $(m, n) = \{(1, 0), (-1, 0), (0, 1), (0, -1)\}$. Without any loss of generality, we focus here on the case where $(m, n) = (1, 0)$. We then only need to consider Eqs. (3.7a) and (3.6b). Substitution of Eq. (3.7a) into Eq. (3.6b) gives

$$\begin{aligned} & \left[\frac{\partial^2 \Theta_0}{\partial z^2} + (k_0^2 n_0^2 + 2i\tilde{\alpha} k_0 n_0(z) - \beta_0^2) \Theta_0 \right] R_x \\ &= -k_0^2 \sum_{\substack{m' \neq 1, \\ n' \neq 0}} \xi_{1-m', -n'} E_{y, m', n'}. \end{aligned} \quad (3.9)$$

Next, Eq. (3.8) is substituted into Eq. (3.9) to yield

$$\begin{aligned} & (\beta^2 - \beta_0^2) R_x \Theta_0 + 2i\tilde{\alpha} k_0 n_0(z) R_x \Theta_0 \\ &= -k_0^2 \sum_{\substack{m' \neq 1, \\ n' \neq 0}} \xi_{1-m', -n'} E_{y, m', n'}. \end{aligned} \quad (3.10)$$

Specifically, we express the radiative waves, i.e., the field amplitudes of the waves with $(m, n) = (0, 0)$ as

$$E_{x,0,0} = \Delta E_x(z), E_{y,0,0} = \Delta E_y(z). \quad (3.11)$$

Finally, we can obtain the coupled-wave equation for $(m, n) = (1, 0)$ by multiplying Eq. (3.10) by $\Theta_0^*(z)$ on both sides and integrating over $(-\infty, \infty)$ along the z direction. Three more coupled-wave equations for $(m, n) = \{(-1, 0), (0, 1), (0, -1)\}$ can be derived in analogous fashion. We write the four coupled-wave equations in the following form:

$$\begin{aligned} (\delta + i\alpha) R_x &= \kappa_{2,0} S_x - \frac{k_0^2}{2\beta_0} \xi_{1,0} \int_{PC} \Delta E_y(z) \Theta_0^*(z) dz \\ &- \frac{k_0^2}{2\beta_0} \sum_{\substack{m' \neq 1, \\ \sqrt{m'^2 + n'^2} > 1}} \xi_{1-m', -n'} \int_{PC} E_{y, m', n'}(z) \Theta_0^*(z) dz, \end{aligned} \quad (3.12a)$$

$$\begin{aligned}
(\delta + i\alpha)S_x &= \kappa_{-2,0}R_x - \frac{k_0^2}{2\beta_0}\xi_{-1,0}\int_{PC}\Delta E_y(z)\Theta_0^*(z)dz \\
&\quad - \frac{k_0^2}{2\beta_0}\sum_{\substack{-n \\ \sqrt{m^2+n^2}>1}}\xi_{-1-m,-n}\int_{PC}E_{y,m,n}(z)\Theta_0^*(z)dz,
\end{aligned} \tag{3.12b}$$

$$\begin{aligned}
(\delta + i\alpha)R_y &= \kappa_{0,2}S_y - \frac{k_0^2}{2\beta_0}\xi_{0,1}\int_{PC}\Delta E_x(z)\Theta_0^*(z)dz \\
&\quad - \frac{k_0^2}{2\beta_0}\sum_{\substack{-m \\ \sqrt{m^2+n^2}>1}}\xi_{1-n,-m}\int_{PC}E_{x,m,n}(z)\Theta_0^*(z)dz,
\end{aligned} \tag{3.12c}$$

$$\begin{aligned}
(\delta + i\alpha)S_y &= \kappa_{0,-2}R_y - \frac{k_0^2}{2\beta_0}\xi_{0,-1}\int_{PC}\Delta E_x(z)\Theta_0^*(z)dz \\
&\quad - \frac{k_0^2}{2\beta_0}\sum_{\substack{-m \\ \sqrt{m^2+n^2}>1}}\xi_{-1-n,-m}\int_{PC}E_{x,m,n}(z)\Theta_0^*(z)dz,
\end{aligned} \tag{3.12d}$$

Here, $\delta = \beta - \beta_0 = n_{eff}(\omega - \omega_0)/c$ is the deviation from the Bragg condition, ω_0 is the Bragg frequency, n_{eff} is the effective refractive index of the PC layer, and α is the mode gain/loss given by

$$\alpha = \frac{k_0}{\beta_0}\int_{-\infty}^{\infty}n_0(z)\tilde{\alpha}(z)|\Theta_0(z)|^2dz, \tag{3.13}$$

where $\Theta(z)$ is normalized as $\int_{-\infty}^{\infty}|\Theta_0(z)|^2dz = 1$.

The parameters $\kappa_{\pm 2,0}, \kappa_{0,\pm 2}$ are the conventional 1D (forward-backward) coupling coefficients given by

$$\kappa_{\pm 2,0} = -\frac{k_0^2}{2\beta_0}\xi_{\pm 2,0}\int_{PC}|\Theta_0(z)|^2dz, \tag{3.14a}$$

$$\kappa_{0,\pm 2} = -\frac{k_0^2}{2\beta_0}\xi_{0,\pm 2}\int_{PC}|\Theta_0(z)|^2dz. \tag{3.14b}$$

The integrals in Eqs. (3.14a)-(3.14b), as well as those in Eqs. (3.12a)-(3.12d), extend only over the PC region because $\xi_{mn} = 0$ outside that range.

As the fields of the radiative waves ($\Delta E_x(z), \Delta E_y(z)$) and the high-order waves ($E_{x,m,n}(z), E_{y,m,n}(z)$) are unknown, we cannot yet evaluate the right-hand sides of Eqs. (3.12a)-(3.12d). In order to determine these fields, Eqs. (3.6a)-(3.6c) must be solved for these waves. Details concerning the solutions of $\Delta E_x(z), \Delta E_y(z), E_{x,m,n}(z)$, and $E_{y,m,n}(z)$ are shown in the Appendix. Finally, we find that the coupled-wave equations can be treated as an eigenvalue problem in the form

$$(\delta + i\alpha)\mathbf{V} = \mathbf{C}\mathbf{V}, \tag{3.15}$$

where

$$\mathbf{V} = \begin{pmatrix} R_x, & S_x, & R_y, & S_y \end{pmatrix}^t, \quad (3.16)$$

$$\mathbf{C} = \mathbf{C}_{1D} + \mathbf{C}_{rad} + \mathbf{C}_{2D}. \quad (3.17)$$

Here, the three matrices, $\mathbf{C}_{1D}$, $\mathbf{C}_{rad}$ and $\mathbf{C}_{2D}$ correspond to the first, second, and third terms on the right-hand sides of the couple-wave Eqs. (3.12a)-(3.12d), respectively. All their matrix elements are dependent on the PC geometry and the multilayer waveguide structure, as will be defined analytically in the next section.

It is informative to examine the physical interpretation of the three matrices: $\mathbf{C}_{1D}$, $\mathbf{C}_{rad}$, $\mathbf{C}_{2D}$. $\mathbf{C}_{1D}$ represents the conventional 1D coupling effects, i.e., the feedback coupling between two counter-propagating basic waves. $\mathbf{C}_{rad}$ represents coupling between the radiative waves and the basic waves, i.e., the out-of-plane coupling coefficient arising from first-order diffractions. Unlike the previous 2D theory [63], this term is explicitly derived in a 3D model, allowing an accurate prediction of the device output (surface emission). $\mathbf{C}_{2D}$ represents the 2D optical coupling coefficient via high-order waves. As the infinite summations were taken into account, the 2D coupling described by our coupled-wave equations is far richer in nature than previous 2D theory, thus making it possible to capture all the important 2D optical coupling effects in 3D systems. The generalized formalism above is capable of treating air holes of any arbitrary shape by inclusion of the appropriate high-order Fourier components.

3.2.1 Analytical solutions of partial waves

The partial waves, i.e., radiative and high-order waves included on the right-hand side of the coupled-wave eqs. (3.12a)-(3.12b), can be solved analytically, by assuming that:

- (1) Only basic waves are important in generating radiative waves and high-order waves;
- (2) $\tilde{\alpha}$ is small and thus may be neglected [66].

First, we consider the radiative waves $\Delta E_x(z)$ and $\Delta E_y(z)$ for $(m, n) = (0, 0)$. In this case, Eqs. (3.6a)-(3.6b) are reduced to the following two expressions:

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) \right] \Delta E_x(z) &= -k_0^2 \sum_{m', n' \neq 0} \xi_{-m', -n'} E_{x, m', n'} \\ &\simeq -k_0^2 (\xi_{0, -1} R_y + \xi_{0, 1} S_y) \Theta_0(z), \end{aligned} \quad (3.18a)$$

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) \right] \Delta E_y(z) &= -k_0^2 \sum_{m', n' \neq 0} \xi_{-m', -n'} E_{y, m', n'} \\ &\simeq -k_0^2 (\xi_{-1, 0} R_x + \xi_{1, 0} S_x) \Theta_0(z). \end{aligned} \quad (3.18b)$$

These equations can be solved by employing the Green's function approximation [67], where the Green's function $G(z, z')$ satisfies

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2\right]G(z, z') = -\delta(z, z'), \quad (3.19)$$

which gives $G(z, z') \simeq -\frac{i}{2\beta_z} e^{-i\beta_z|z-z'|}$ with $\beta_z = k_0 n_0(z)$ represents the wavenumber of radiative waves in the z direction (for simplicity, here we use an approximate form of the Green's function that neglects reflections occurring at the lower-index-contrast waveguide layer interfaces. A more accurate expression is derived in Ref. [85] to improve accuracy). In terms of $G(z, z')$, the radiative waves can then be expressed as

$$\Delta E_x(z) = k_0^2(\xi_{0,-1}R_y + \xi_{0,1}S_y) \int_{PC} G(z, z')\Theta_0(z')dz', \quad (3.20a)$$

$$\Delta E_y(z) = k_0^2(\xi_{-1,0}R_x + \xi_{1,0}S_x) \int_{PC} G(z, z')\Theta_0(z')dz'. \quad (3.20b)$$

As a consequence, the second terms of the right-hand sides of the coupled-wave equations (3.12a)-(3.12d) can be replaced by terms only associated with the basic waves.

Next, we obtain solutions for high-order waves, $E_{x,m,n}(z)$ and $E_{y,m,n}(z)$, where $\sqrt{m^2 + n^2} > 1$. It is difficult to solve Eqs. (3.6a)-(3.6c) directly, thus we introduce a proper linear combination of $E_{x,m,n}(z)$ and $E_{y,m,n}(z)$ and obtain a set of equations of the form

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2\right](mE_{x,m,n} + nE_{y,m,n}) = \\ -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m'} \frac{1}{n-n'} (mE_{x,m',n'} + nE_{y,m',n'}), \end{aligned} \quad (3.21a)$$

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 - (m^2 + n^2)\beta_0^2\right](nE_{x,m,n} - mE_{y,m,n}) = \\ -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m'} \frac{1}{n-n'} (nE_{x,m',n'} - mE_{y,m',n'}), \end{aligned} \quad (3.21b)$$

$$\frac{\partial}{\partial z}[mE_{x,m,n} + nE_{y,m,n}] = 0. \quad (3.21c)$$

The substitution of Eq. (3.21c) into Eq. (3.21a) yields

$$n_0^2(mE_{x,m,n} + nE_{y,m,n}) = - \sum_{m' \neq m, n' \neq n} \xi_{m-m'} \frac{1}{n-n'} (mE_{x,m',n'} + nE_{y,m',n'}). \quad (3.22)$$

It is worthwhile noting that Eq. (3.22) is equivalent to the transversality constraint; i.e., $\nabla \cdot (\mathbf{D}(\mathbf{r})) = \nabla \cdot (\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r})) = 0$ must be satisfied. Next, we solve Eqs. (3.21b) and (3.22) to obtain solutions for the high-order waves $E_{x,m,n}(z)$ and $E_{y,m,n}(z)$. The linear combination $(nE_{x,m,n} - mE_{y,m,n})$ can be solved from Eq. (3.21b) by using a similar

Green's function approach. The Green's function $G_{m,n}(z, z')$ satisfies

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 - (m^2 + n^2)\beta_0^2\right]G_{m,n}(z, z') = -\delta(z, z'), \quad (3.23)$$

where $G_{m,n}(z, z') \simeq \frac{1}{2\beta_{z,m,n}}e^{-\beta_{z,m,n}|z-z'|}$, with $\beta_{z,m,n} = \sqrt{(m^2 + n^2)\beta_0^2 - k_0^2 n_0^2(z)}$. Then, we obtain

$$\begin{aligned} (nE_{x,m,n} - mE_{y,m,n}) &= k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m'} \cdot \\ &\int_{PC} (nE_{x,m',n'}(z') - mE_{y,m',n'}(z'))G_{m,n}(z, z')dz'. \end{aligned} \quad (3.24)$$

Under the assumption that only the basic waves are important in generating high-order waves, Eqs. (3.22) and (3.24) can be rewritten as

$$\begin{aligned} mE_{x,m,n} + nE_{y,m,n} &\simeq -\frac{1}{n_0^2}(n\xi_{m-1,n}R_x + n\xi_{m+1,n}S_x + m\xi_{m,n-1}R_y + m\xi_{m,n+1}S_y)\Theta_0(z) \\ &\triangleq E^+(z), \end{aligned} \quad (3.25a)$$

$$\begin{aligned} nE_{x,m,n} - mE_{y,m,n} &\simeq k_0^2(-m\xi_{m-1,n}R_x - m\xi_{m+1,n}S_x + n\xi_{m,n-1}R_y + n\xi_{m,n+1}S_y) \cdot \\ &\int_{PC} G_{m,n}(z, z')\Theta_0(z')dz' \\ &\triangleq E^-(z). \end{aligned} \quad (3.25b)$$

We then obtain

$$\begin{pmatrix} E_{x,m,n}(z) \\ E_{y,m,n}(z) \end{pmatrix} = \frac{1}{m^2 + n^2} \begin{pmatrix} n & m \\ -m & n \end{pmatrix} \begin{pmatrix} E^-(z) \\ E^+(z) \end{pmatrix}. \quad (3.26)$$

By multiplying both sides of Eq. (3.26) by $\Theta_0^*(z)$ and integrating over the PC region, we obtain

$$\begin{aligned} \begin{pmatrix} \int_{PC} E_{x,m,n}(z)\Theta_0^*(z)dz \\ \int_{PC} E_{y,m,n}(z)\Theta_0^*(z)dz \end{pmatrix} &= \frac{1}{m^2 + n^2} \begin{pmatrix} n & m \\ -m & n \end{pmatrix} \cdot \\ &\begin{pmatrix} -m\mu_{m,n}^{(1,0)} & -m\mu_{m,n}^{(-1,0)} & n\mu_{m,n}^{(0,1)} & n\mu_{m,n}^{(0,-1)} \\ n\nu_{m,n}^{(1,0)} & n\nu_{m,n}^{(-1,0)} & m\nu_{m,n}^{(0,1)} & m\nu_{m,n}^{(0,-1)} \end{pmatrix} \mathbf{V}, \\ &\triangleq \begin{pmatrix} \varsigma_{x,m,n}^{(1,0)} & \varsigma_{x,m,n}^{(-1,0)} & \varsigma_{x,m,n}^{(0,1)} & \varsigma_{x,m,n}^{(0,-1)} \\ \varsigma_{y,m,n}^{(1,0)} & \varsigma_{y,m,n}^{(-1,0)} & \varsigma_{y,m,n}^{(0,1)} & \varsigma_{y,m,n}^{(0,-1)} \end{pmatrix} \mathbf{V}, \end{aligned} \quad (3.27)$$

where $\mathbf{V} = \begin{pmatrix} R_x, & S_x, & R_y, & S_y \end{pmatrix}^t$,

$$\mu_{m,n}^{(r,s)} = k_0^2 \iint_{PC} \xi_{m-r, n-s}(z') G_{m,n}(z, z') \Theta_0(z') \Theta_0^*(z) dz' dz, \quad (3.28)$$

$$\nu_{m,n}^{(r,s)} = - \int_{PC} \frac{1}{n_0^2(z)} \xi_{m-r, n-s}(z) |\Theta_0(z)|^2 dz. \quad (3.29)$$

As a consequence, the third terms of the right-hand sides of the coupled-wave equations (3.12a)-(3.12d) can also be replaced by terms only associated with the basic waves. Finally, the coupled-wave equations (3.12a)-(3.12d) leads to an eigensystem that can be written in matrix form as

$$(\delta + i\alpha)\mathbf{V} = \mathbf{C}\mathbf{V}. \quad (3.30)$$

Here, $\mathbf{C} = \mathbf{C}_{1D} + \mathbf{C}_{rad} + \mathbf{C}_{2D}$,

$$\mathbf{C}_{1D} = \begin{pmatrix} 0 & \kappa_{2,0} & 0 & 0 \\ \kappa_{-2,0} & 0 & 0 & 0 \\ 0 & 0 & 0 & \kappa_{0,2} \\ 0 & 0 & \kappa_{0,-2} & 0 \end{pmatrix}, \quad (3.31)$$

$$\mathbf{C}_{rad} = \begin{pmatrix} \zeta_{1,0}^{(1,0)} & \zeta_{1,0}^{(-1,0)} & 0 & 0 \\ \zeta_{-1,0}^{(1,0)} & \zeta_{-1,0}^{(-1,0)} & 0 & 0 \\ 0 & 0 & \zeta_{0,1}^{(0,1)} & \zeta_{0,1}^{(0,-1)} \\ 0 & 0 & \zeta_{0,-1}^{(0,1)} & \zeta_{0,-1}^{(0,-1)} \end{pmatrix}, \quad (3.32)$$

$$\mathbf{C}_{2D} = \begin{pmatrix} \chi_{y,1,0}^{(1,0)} & \chi_{y,1,0}^{(-1,0)} & \chi_{y,1,0}^{(0,1)} & \chi_{y,1,0}^{(0,-1)} \\ \chi_{y,-1,0}^{(1,0)} & \chi_{y,-1,0}^{(-1,0)} & \chi_{y,-1,0}^{(0,1)} & \chi_{y,-1,0}^{(0,-1)} \\ \chi_{x,0,1}^{(1,0)} & \chi_{x,0,1}^{(-1,0)} & \chi_{x,0,1}^{(0,1)} & \chi_{x,0,1}^{(0,-1)} \\ \chi_{x,0,-1}^{(1,0)} & \chi_{x,0,-1}^{(-1,0)} & \chi_{x,0,-1}^{(0,1)} & \chi_{x,0,-1}^{(0,-1)} \end{pmatrix}, \quad (3.33)$$

and

$$\zeta_{p,q}^{(r,s)} = -\frac{k_0^4}{2\beta_0} \iint_{PC} \xi_{p,q} \xi_{-r,-s} G(z, z') \Theta_0(z') \Theta_0^*(z) dz' dz, \quad (3.34)$$

$$\chi_{i,p,q}^{(r,s)} = -\frac{k_0^2}{2\beta_0} \sum_{\sqrt{m^2+n^2}>1} \xi_{p-m,q-n} \zeta_{i,m,n}^{(r,s)}, i = x, y. \quad (3.35)$$

Note that matrices $\mathbf{C}_{1D}$, $\mathbf{C}_{rad}$, and $\mathbf{C}_{2D}$ correspond to the conventional 1D feedback coupling, radiative coupling, and 2D couplings via high-order waves, respectively. It should also be noted that $\mathbf{C}_{1D}$ and $\mathbf{C}_{2D}$ are Hermitian matrices, whereas $\mathbf{C}_{rad}$ is not an Hermitian one.

3.2.2 In-plane and vertical field profiles

As described above, we have developed a 3D CWT formulation by incorporating high-order effects. The formulation allows us to obtain various quantities of interest, including: in-plane electromagnetic-field pattern, vertical field profile, radiation constant, and mode frequency of the resonant modes. In all the following calculations, the waveguide structural parameters listed in Table 3.1, the dielectric constants $\varepsilon_a = 1.0$, $\varepsilon_b = 12.7449$, and the lattice constant $a = 295$ nm are used. Unless otherwise stated, we include a large number of high-order waves by truncating the summation terms in matrix $\mathbf{C}_{2D}$ at $|m, n| \leq 10$ (the effects of the wave truncation order will be discussed later).

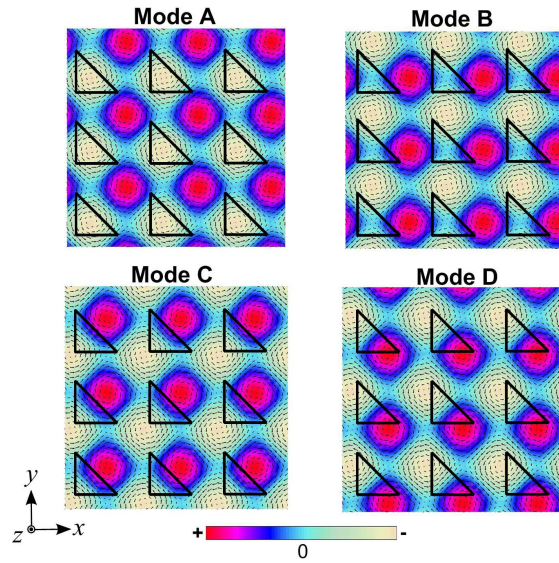


Figure 3.3: (Color online) In-plane E-field vector distribution (arrows) and H-field patterns (in color) of four band-edge modes (A-D) at the 3D structure. The thick black triangles indicate the shapes and locations of air holes. The E-fields (E_x, E_y) are calculated by using Eq. (3.4). In the calculation, we use the waveguide parameters shown in Table 3.1, $\varepsilon_a = 1.0$, $\varepsilon_b = 12.7449$, FF=0.16, and $a = 295$ nm. A large number of high-order waves are included by truncating the summation terms in matrix $\mathbf{C}_{2D}$ (see Appendix) at $|m, n| \leq 10$.

Fig. 3.3 shows in-plane E-field vector distribution (arrows) and H-field patterns (in color) of four band-edge modes (A-D) at the 3D structure. The fields at the center of the PC layer (see Fig. 3.1) are plotted for square-lattice PC with right-angled isosceles triangular (RIT) air-hole shapes. It can be seen from the figure that, these band-edge

modes are characterized by different field patterns distributed in two dimensions. Modes C and D correspond to the symmetric mode (leaky mode) of 1D-DFB lasers, and thus have significant loss. In contrast, modes A and B correspond to the anti-symmetric mode (non-leaky mode) of 1D-DFB lasers, and lase more easily than modes C and D [47, 48]. Therefore, we restrict the following discussion to modes A and B only.

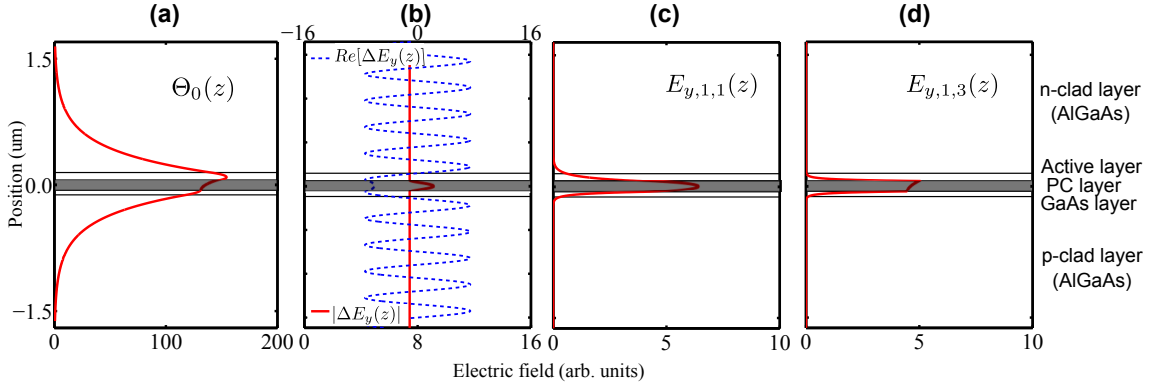


Figure 3.4: (Color online) Vertical field profiles for wavevectors with different in-plane wavenumbers: (a) basic waves, (b) radiative waves, high-order waves with (c) $(m, n) = (1, 1)$ and (d) $(m, n) = (1, 3)$. The shaded regions indicate the PC layer. The vertical field profile of basic waves is the same as that of the fundamental waveguide mode $\Theta_0(z)$ described by Eq. (??). The vertical field profiles of radiative and high-order waves are plotted for the mode A (similar features are observed for other modes) and are calculated based on Eqs. (??) and (6.25), respectively (field outside the PC layer is calculated by imposing continuity conditions on E-field at the layer interfaces). Parameters used in the calculation is the same as those shown in Fig. 3.3.

In addition to the in-plane (xy plane) field patterns, our 3D formulation also allows us to calculate the field profile in the vertical (z) direction for each wavevector. As mentioned above, wavevectors involved in the couplings are classified into three groups: basic waves, radiative waves and high-order waves. Fig. 3.4 shows the vertical electric-field profiles for these wavevectors that are calculated by employing Eqs. (3.8), (3.20b) and (3.26), respectively. Here, we show the results for right-angled isosceles triangular air-hole shapes with $FF=0.16$ (similar results are obtained for other shapes). The basic waves (see Fig. 3.4(a)) have the same field profile as the fundamental waveguide mode $\Theta_0(z)$ described by Eq. (3.8), the amplitude of which has a peak at the active layer and decays slowly towards the upper and lower cladding layers. The radiative waves (see Fig. 3.4(b)) possess an oscillating field (see the dashed blue line that represents the real part of the electric field) along the z direction and emanate in the direction normal to the PC plane to constitute the laser output (surface emission). The field amplitude (red line) is constant and *non-zero* at both sides of the PC layer, quantifying the energy leaking out of the PC laser cavity. The field profile of the high-order waves

is more complicated. As an example, here we show the profiles of high-order waves with $(m, n) = (1, 1)$ and $(m, n) = (1, 3)$ in Fig. 3.4(c) and (d), respectively. It is apparent that the high-order waves are more strongly confined within the PC layer compared to the basic waves, and that they decay evanescently outside the PC layer. In addition, it can easily be found that the field profile is largely dependent on the order of the waves (m, n) : the higher the wavevector order, the more strongly the field is confined in the PC layer. In short, the field profiles for the individual wavevectors in a 3D structure are extremely complicated, which represents the fundamental difference between 3D and 2D systems. Therefore, each field profile must be treated very carefully in order to accurately quantify the coupling effects in a 3D system. In the previously reported CWT analyses [62, 63], an approximation based on the effective refractive index [31] was used in the 2D calculations to compensate for the effects of the 3D nature. This approximation implies that all the individual wavevectors have the same field profile in the vertical direction as the fundamental waveguide mode. Failing to reflect these complicated field profile changes can lead to significant inaccuracy.

3.2.3 Analysis results and comparison with 3D FDTD simulation

By solving the coupled-wave Eq. (3.15) as an eigenvalue problem, we can directly evaluate two most important properties of the band-edge modes, i.e., the radiation constant α_r ($\alpha_r = 2\alpha$: the modal power loss due to the surface emission) and the mode frequency ω . In order to understand the effects of asymmetric air-hole shapes, we present numerical results for the three shapes shown in Fig. 3.2(a): circular (CC), equilateral triangular (ET), and right-angled isosceles triangular (RIT) shapes.

When solving Eq. (3.15), we need to truncate the summation terms at an appropriate order of m and n . Here, we define a quantity D such that $|m, n| \leq D$. For a given wave truncation order D , the total number of the included waves is $(2D + 1)^2$. The effects of truncating the summations can be observed by plotting the radiation constant and the mode frequency as a function of the wave truncation order D , as shown in Fig. 3.5. For illustration, we only show results for the asymmetric RIT air-hole shape (FF=0.16), the modeling of which requires the inclusion of many more high-order waves than the CC and ET shapes. It is apparent from Fig. 3.5 that the radiation constant is more sensitive to D than the mode frequency, which indicates that a large number of wavevectors must be included in order to calculate the radiation constant accurately. Both the radiation constant and mode frequency converge well when D is larger than 10, hence we use $D = 10$ in all of the following calculations.

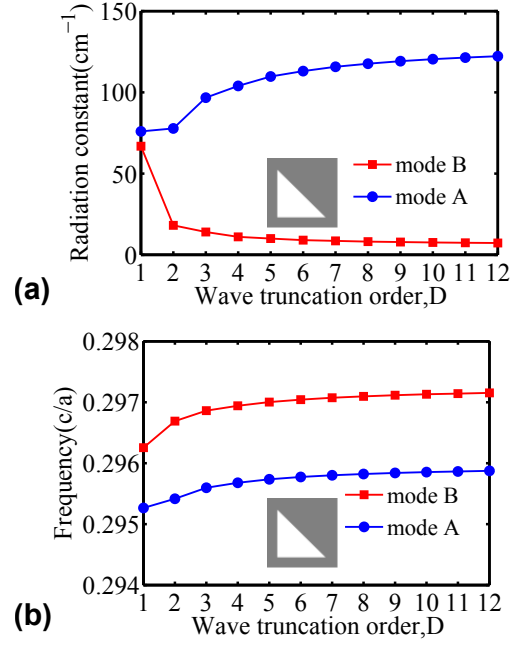


Figure 3.5: (Color online) Radiation constant and mode frequency as a function of the wave truncation order D . The total number of the included waves is $(2D + 1)^2$. These plots are calculated by using the same parameters shown in Fig. 3.3.

In order to confirm the accuracy of the above CWT analysis results, we also performed 3D-FDTD simulations [79, 80] for the structure shown in Fig. 3.1. We used a computational cell of $40 \times 40 \times 640$ pixels ($x \times y \times z$), corresponding to $1 \times 1 \times 16$ lattice periods, with absorbing boundary layers in the z direction and periodic boundary conditions in x and y . The Q factor obtained by the 3D-FDTD method was used to compute the radiation constant via the following relationship [69]:

$$\alpha_r \simeq \frac{\beta_0}{Q} = \frac{2\pi/a}{Q}. \quad (3.36)$$

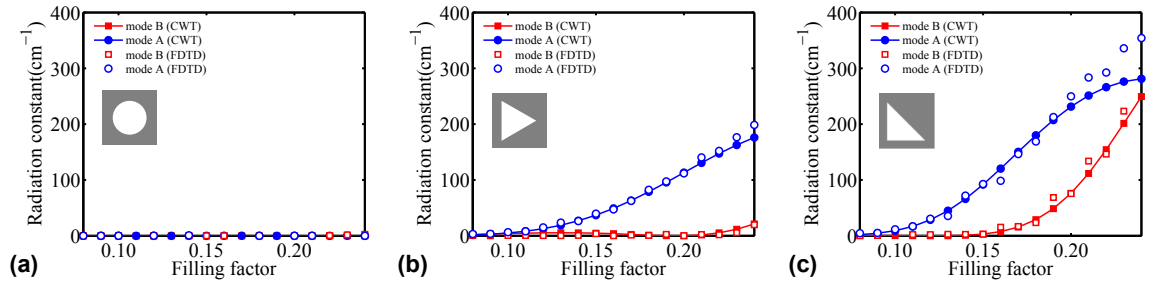


Figure 3.6: Radiation constant as a function of FF for (a) CC, (b) ET, and (c) RIT air-hole shapes. The CWT data are calculated by using $D=10$, $\varepsilon_a = 1.0$, $\varepsilon_b = 12.7449$, $a = 295$ nm and the waveguide parameters shown in Table 3.1. The 3D-FDTD data are calculated for the same structure. Some 3D-FDTD points are missing in the case of the CC shape because Q is infinitely large.

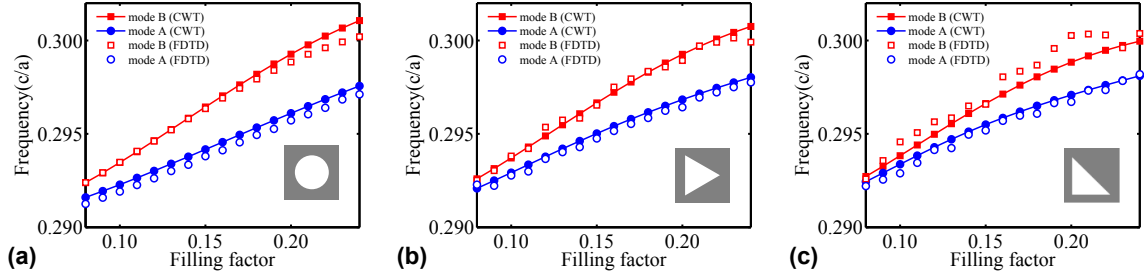


Figure 3.7: (Color online) Mode frequency as a function of FF for (a) CC, (b) ET, and (c) RIT air-hole shapes. Parameters used for the calculations are the same as those shown in Fig. 3.6.

Figures 3.6 and 3.7 show the radiation constant and mode frequency as a function of FF, obtained by both the CWT and 3D-FDTD methods. It is clear that the CWT results are in good agreement with the 3D-FDTD simulations. Deviation between the two methods, increasing for large FF, can be attributed to numerical effects (i.e., low resolution of 3D-FDTD) as well as the approximations used in our theory: separation of variables (see Eqs. (5.1-5.4)) and Green's functions neglecting the reflections occurring at the low-index-contrast waveguide layer interfaces. It is possible to improve the accuracy by employing an iterative technique described in Ref. [68] and a generalized Green's function incorporating the reflection effects [69, 85]. Nevertheless, the current treatment still allows us to obtain qualitatively reliable results even at large filling factors. The calculation time required for the two methods is markedly different. For a specific FF, the 3D-FDTD simulation takes ~ 4 hours using a supercomputer system (64 cores and 9.0 GB memory), whereas the CWT analysis takes less than 1 second with a personal computer (1 core@2.20GHz and negligible memory usage). Although a large number of wavevectors were included in the CWT analysis, the calculation time is nevertheless short due to the semi-analytical nature of the algorithm.

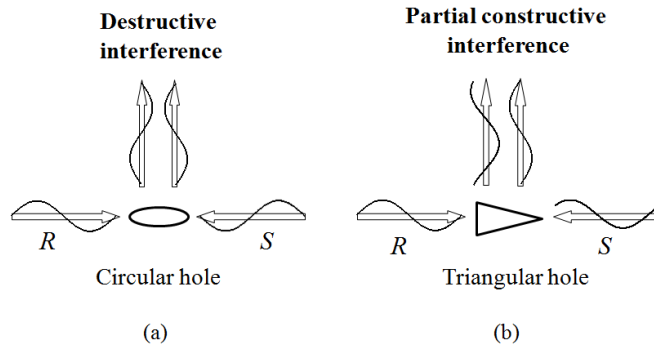


Figure 3.8: Schematic illustration of the interference occurring in the vertical direction for (a) circular holes and (b) triangular holes. The arrows represent the propagation directions of the basic waves and radiative waves, and the sine curves represent the phases of the fields for these waves. The destructive interference is suppressed when air-hole shape becomes asymmetric.

It is noteworthy that the radiation constant for the symmetric CC air-hole shape is zero (corresponding to an infinite Q factor in the 3D-FDTD method) at every value of FF, whereas it increases with FF when the air-hole shapes are asymmetric (ET or RIT). This difference can be physically interpreted by considering the interference occurring in the vertical direction, as illustrated in Fig. 3.8. The radiation field depends on the phase difference of the waves diffracted vertically, which arise from counter-propagating basic waves in the PC plane. In the case of the symmetric CC air-hole shape, the two basic waves propagating in the x or y direction are intrinsically out of phase [47] and their diffracted waves thus have a phase difference of π . Therefore, destructive interference occurs and the two diffracted waves cancel each other out. In contrast, when the air-hole shape is asymmetric, such as for the ET and RIT shapes, the counter-propagating basic waves are no longer out of phase and the phase difference of the diffracted waves will deviate from π . The destructive interference is consequently suppressed, giving rise to partial constructive interference. Therefore, a higher output power can be expected when asymmetric air-hole shapes are used.

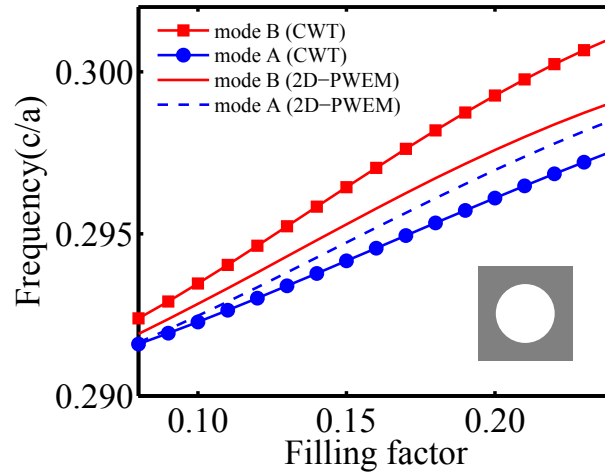


Figure 3.9: (Color online) Mode frequency for CC air holes as a function of FF, calculated using the CWT and 2D-PWEM approaches. This figure replots the CWT data shown in Fig. 3.7(a). The 2D-PWEM data are obtained by using 441 plane waves with modified dielectric constants (calculated by using the structural parameters shown in Table 3.1 based on the effective refractive index approximation described in Ref. [46]).

We note that the mode frequency plotted in Fig. 3.7 was calculated for a 3D structure, which should be different from that calculated for a 2D structure. In order to elucidate the difference between 3D and 2D calculations, we evaluated the mode frequency for the CC air-hole shape using the 2D-PWEM approach [31], which is plotted versus FF in Fig. 3.9 together with the CWT results of Fig. 3.7(a). A total of 441 plane waves were used in the 2D-PWEM calculation and the effective refractive index approximation [46] was employed. Comparing the results for the two methods, it is apparent that the

mode gap between modes A and B ($\omega_B - \omega_A$) calculated using the present CWT model is significantly larger than that calculated using the 2D-PWEM approach. We suggest that a physical explanation can be found by considering the fact that in a 3D structure, the high-order waves (generated by basic waves) are more strongly confined in the PC layer, as depicted in Fig. 3.4(c-d). As a consequence, the 2D optical coupling strength is greater in a 3D structure than in a 2D structure, leading to a larger mode gap in a 3D structure.

3.3 Extension to non- Γ -point modes

In the previous section, for simplicity, we have restricted our analysis to band-edge modes (i.e., Γ -point modes). However, lasing action of non- Γ -point modes has also been observed in the experiments. Therefore, it is important to theoretically study and understand the physical principles and properties of this kind of lasing modes. In this section, we present a coupled-wave analysis on non- Γ -point modes by extending our previous CWT formulation.

3.3.1 Extended coupled-wave formulation

The non- Γ -point modes are deviated from the Γ point band edges as shown in Fig. 3.10(a). The schematic diagram of coupled-wave model for these modes is shown in Fig. 3.10(b), which is similar to the case of Γ -point modes except that the four basic waves (gray arrows) have a small wavenumber deviation $\Delta\mathbf{k}$ (red arrows) from the Γ point. Note here that, the wavenumber deviation $\Delta\mathbf{k}$ can be in an arbitrary direction. In addition to the four basic waves, the high-order waves also have a wavenumber deviation $\Delta\mathbf{k}$ and contribute to the 2D coupling.

The Bloch vector $\Delta\mathbf{k}$ at a non- Γ point implies that the wavevectors of the four basic waves have different amplitudes, and they no longer lie along primitive vectors. Therefore, the phase matching conditions of the four basic waves are slightly different in principle, and hence, their vertical profiles are not identical. However, since Δ_x/β_0 and Δ_y/β_0 are considerably small, we assume that the basic waves have an identical vertical profile $\Theta_0(z)$. For $(m, n) = \{(1, 0), (-1, 0), (0, 1), (0, -1)\}$, we have

$$E_{x,mn} = \rho_{mn} A_{mn} \Theta_0(z), E_{y,mn} = \eta_{mn} A_{mn} \Theta_0(z) \quad (3.37)$$

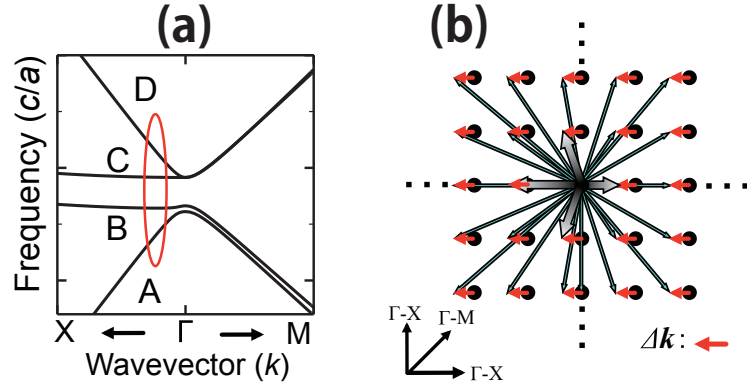


Figure 3.10: (a) Non- Γ -point modes in the square-lattice band structure (red circle). (b) Schematic diagram of coupled-wave model at non- Γ -point modes. Gray arrows represent basic waves, and red arrows represent a small wavenumber deviation $\Delta \mathbf{k}$ from the Γ point.

with

$$\rho_{mn} = \frac{n_{y,mn}}{\sqrt{m_{x,mn}^2 + n_{y,mn}^2}}, \quad \eta_{mn} = -\frac{m_{x,mn}}{\sqrt{m_{x,mn}^2 + n_{y,mn}^2}} \quad (3.38)$$

where $A_{mn} = \{R_x, S_x, R_y, S_y\}$ for the given (m, n) , respectively, and it does not depend on x, y because an infinite periodical PC structure is assumed here for simplicity. In fact, ρ_{mn}, η_{mn} denote the perturbation of the basic waves' polarizations; then, from Eqs. (3.6a)-(3.6c) we obtain

$$\left[\frac{\partial^2}{\partial z^2} + n_0^2 k_0^2 - (m_x^2 + n_y^2) \beta_0^2 \right] \sqrt{m_x^2 + n_y^2} \Theta_0(z) A_{mn} = -k_0^2 \sum_{m', n'} \xi_{m-m'} \frac{n_y E_{x, m'n'} - m_x E_{y, m'n'}}{n-n'} \quad (3.39)$$

Under resonant conditions, the basic wave profile $\Theta_0(z)$ can be determined by the waveguide mode profile. It is noteworthy that since the phase matching conditions for the four basic waves are different, the corresponding waveguide mode frequencies are also different. The wavenumber is denoted by as $k_{0;mn}$ for the case of A_{mn} , and $\Theta_0(z)$ satisfies as

$$\frac{\partial^2 \Theta_0}{\partial z^2} + [n_0^2 k_{0;mn}^2 - (m_x^2 + n_y^2) \beta_0^2] \Theta_0(z) = 0 \quad (3.40)$$

The above equation can be solved numerically by the transfer matrix method (TMM)[74, 84]. Combining Eq. (3.39) with Eq. (3.40), then multiplying the complex conjugate

field $\Theta_0^*(z)$ on both sides, and integrating over $(-\infty, \infty)$, we obtain

$$\begin{aligned} (k_0 - k_{0;mn})A_{mn} = & \sum_{\substack{|r^2+s^2|=1; \\ r \neq m, s \neq n}} \kappa_{mn}^{(rs)} A_{rs} \\ & - \frac{k_0^2}{h_{mn}} \sum_{|m'^2+n'^2| \neq 1} \xi_{m-m'} n_y \int_{PC} E_{x,m'n'} \Theta_0^*(z) dz \\ & + \frac{k_0^2}{h_{mn}} \sum_{|m'^2+n'^2| \neq 1} \xi_{m-m'} m_x \int_{PC} E_{y,m'n'} \Theta_0^*(z) dz \end{aligned} \quad (3.41)$$

where

$$\kappa_{mn}^{(rs)} = - \int_{PC} \frac{k_0^2}{h_{mn}} \xi_{m-r} (n_{y,mn} \rho_{rs} - m_{x,mn} \eta_{rs}) |\Theta_0(z)|^2 dz,$$

and

$$h_{mn} = 2k_{0;mn} \sqrt{m_x^2 + n_y^2} \int_{-\infty}^{\infty} \varepsilon_0(z) \Theta_0(z) \Theta_0^*(z) dz.$$

Here, the normalization condition $\int_{-\infty}^{\infty} \Theta_0(z) \Theta_0^*(z) dz = 1$ is used. However, the radiative wave and high-order profiles $E_{y,m'n'}(z)$ remain unknown; they will be determined in the Appendix, and they only depend on the PC geometry and the multilayer waveguide structure. Since all the terms in Eq. (3.41) are solved analytically, similar treatment of other basic waves gives the eigenvalue problem equations for the basic wave vector $\mathbf{V} = (R_x, S_x, R_y, S_y)^t$ with the coupling matrix $\mathbf{C}$:

$$k_0 \mathbf{V} = \mathbf{C} \mathbf{V} \quad (3.42)$$

The complex frequencies ω can be obtained from the eigenvalues by solving Eq. (3.42) with $\omega = k_0 c$. In this case, the Q factors of the band-edge modes can be determined from the real and imaginary parts of ω , as $Re(\omega)/|2Im(\omega)|$, and directly compared with the FDTD simulation results without using any ambiguous definition of the effective refractive index. Hence, the radiation constant is given by Eq. (3.36).

3.3.2 Band structure analysis and comparison with 3D FDTD simulation

Fig. 3.11 shows the calculated results using the extended CWT model of the band structure for a square-lattice PCSEL. The air-hole filling factor $f = 0.12$. The real part of the eigenvalues corresponds to the mode frequency, and the imaginary part corresponds to radiation constant (i.e. vertical radiation loss). For the infinite periodic

structure with circular air holes, radiation constant of both modes A and B becomes zero at the band edges (Γ point) because destructive interference due to the perfect symmetry. On the other hand, band-edge modes C and D have a large radiation constant due to their symmetric nature. Therefore, modes A and B are usually favored for lasing. When

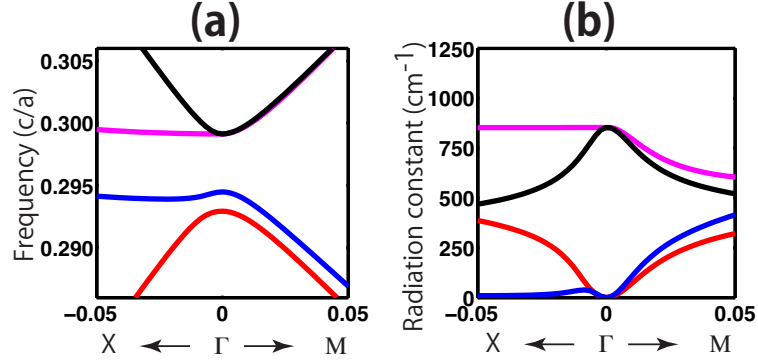


Figure 3.11: (a) Calculated band structure of a square-lattice PC laser structure calculated by CWT. (a) Frequency (real part), (b) Radiation constant (imaginary part). The plot was calculated for circular air holes with air-hole filling fraction $f = 0.12$.

the wavenumber is slightly deviated from Γ point, radiation constants of both modes A and B increase, and hence, ensure the lasing stability of Γ point modes. However, it is worthwhile to note that there also exist no- Γ -point modes with a very lower group velocity (almost zero at $|\Delta k| = 0.018 - 0.022$) at band B along $\Gamma = X$ direction. We refer to these modes as flat-band modes. In close view of Fig. 3.11(b), we find that these flat-band modes have a noticeably low radiation constant (loss), which indicates that these modes may compete with band-edge modes for lasing.

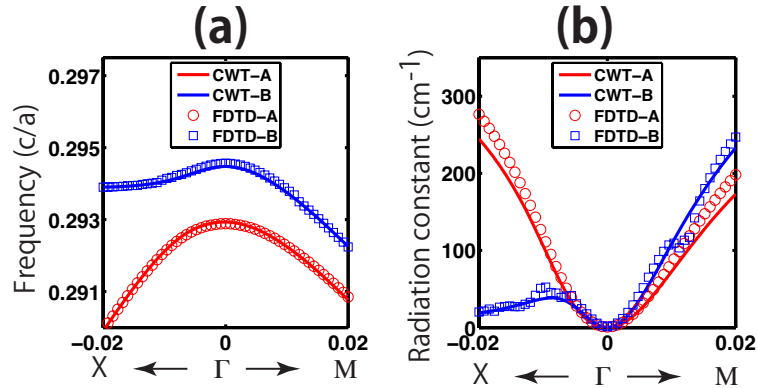


Figure 3.12: (a) Comparison of photonic band structures calculated by CWT and 3D-FDTD method. (a) Frequency, (b) Radiation constant. The plot was calculated for circular air holes with air-hole filling fraction $f = 0.12$.

In order to confirm the accuracy of the CWT analysis results, we also performed 3D-FDTD simulations for the same structure (FF=12%) [80]. Here, we focus on the modes

located on bands A and B because they are more favored for lasing. The comparison of CWT results with 3D-FDTD simulations are shown in Fig. 3.12. The CWT results are in good agreement with 3D-FDTD simulations, thereby confirming the validity of the extended non- Γ -point CWT model.

3.4 Summary

This chapter presented a fully 3D CWT model for square-lattice PCSELs with TE polarization. We have derived a generalized formulation for both the Γ -point band-edge modes and non- Γ -point modes by including a large number of high-order wavevectors and carefully treating the vertical field profile of each wavevector in a full 3D model. Our general coupled-wave formulation can be applied to air holes of arbitrary shape. The accuracy of our 3D CWT model has been confirmed by comparison with 3D-FDTD simulations, which require significantly greater computation time.

In the first main section, we focus our analysis on the band-edge modes. We have shown that not only the inclusion of a sufficiently large number of in-plane high-order wavevectors but also a 3D treatment incorporating the vertical field profile is important for an accurate study of the band-edge modes. The surface emission, our principal feature of interest, and 2D coupling effects can be explicitly modeled based on our model, neither of which can be accurately described by the previous 2D model. We have also discussed the essential differences between 3D and 2D systems. We find that the vertical field profile of the wavevectors is extremely complicated in a 3D system and the effective refractive index approximation employed in the 2D calculation cannot compensate for the complexity caused by the 3D nature. By evaluating the radiation constant and mode frequency of the band-edge modes for several different air-hole shapes, we have found that asymmetric air holes are beneficial for improving the output power of 2D PCSELs because destructive interference in the vertical direction can be suppressed, which is in agreement with our experimental findings.

In the second main section of this chapter, we further extend our analysis to the on- Γ -point mode analysis. The essence of this extension is to introduce a small wavenumber deviation to the individual wavevectors. The perturbed wavevectors would slightly vary the polarization directions of basic waves and accordingly modify the overlapped fields between the individual partial waves. The extended model allows us to calculate the complex band structure (including both real and imaginary parts of the mode frequency), which provides an important insights to the radiation nature of each band. The accuracy of the calculated was compared with 3D-FDTD and good agreement was found. In particular, we find that the radiation constant (loss) of the flat-band modes located

in the $\Gamma - X$ direction of band B is found to be noticeably small and may influence the mode stability of PCSELs. This well explains our experimental observations where lasing action sometimes occurs at these undesirable modes.

To the best of our knowledge, the coupled-wave theory presented in this chapter is the first to provide a full 3D model for describing the surface emission and 2D coupling effects in PCSELs. For the first step of constructing our theoretical framework, we have restricted our analysis to infinite periodic square-lattice PC structures with perfectly vertical sidewalls. However, the framework presented dhere can be extended to the analysis of finite-size structures, triangular-lattice PCs, and more complicated PC geometries with tilted sidewalls without modifying the basic methodology. These extension will be presented in subsequent chapters.

Chapter 4

Finite-size coupled-wave analysis

4.1 Introduction

As presented in the previous chapter, we developed a 3D CWT model that affords an exact analytical treatment of the full 3D structure of typical laser devices and achieves a very accurate and efficient analysis of the surface emission properties. This theory incorporates the key issues in modeling surface-emitting-type PC lasers, i.e. the surface emission in the surface normal direction and the in-plane higher-order coupling effects [84], neither of which was appropriately described in the previous works [33, 61–63].

Nevertheless, in the previous chapter, for simplicity we restricted our analyses to *infinite* periodic structures [84]. To predict and improve the performance of the practical PCSEL device, however, it is essential to consider a *finite-size* structure. For example, following the arguments of the analysis results in the previous chapter, two antisymmetric band-edge modes of PCs with circular air holes should be excited simultaneously without emitting a laser beam because both of their radiation constants (i.e. parameters quantifying the surface radiation loss) are shown to be zero. This is in contrast to the experimental results where a laser with a doughnut-shaped beam pattern operating stably at one of the two antisymmetric modes was demonstrated [35, 46, 51]. The physical mechanism of this lasing behavior cannot be explained without considering the *finite-size* effects of the laser device, as we will show later on. This is our motivation for the present work, where we develop a 3D CWT model capable of treating the *finite-size* laser device by extending our previous framework [84]. Our objective in this chapter is not to exhaustively quantify the dependence on the large number of parameters that determine device behavior. Rather, we focus on clarifying the underlying physical mechanism of the effects caused by finiteness of the device.

The remainder of this chapter is organized as follows. Section 4.2 describes derivations of the coupled-wave equations for finite systems. Section 4.3 presents analysis results and discusses the finite-size effects including mode selectivity and mode stability. Comparison with experiments will also be presented. Section 4.4 concludes with our findings.

4.2 Coupled-wave equations for finite-size structures

In this section, we will present the derivations of the coupled-wave equations for finite systems. We shall not give a complete description of the formulation, but highlight only the major differences from our previous study. For a more detailed derivation and discussion, please refer to the previous Chapter. 3.

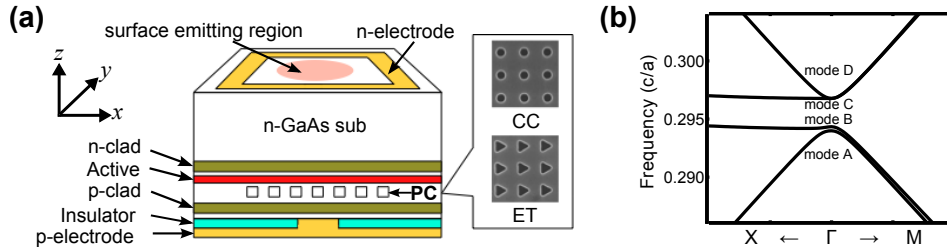


Figure 4.1: (a) Schematic structure of square-lattice PCSEL device with circular (CC) and equilateral triangular (ET) air holes (inset: scanning electron microscope images). (b) A typical photonic-band structure calculated by 2D-PWEM. There exist four band-edge modes in the vicinity of the second-order Γ point, which we refer to as modes A, B, C and D, in order of increasing frequency.

The schematic structure of PCSELs is shown in Fig. 4.1(a), in which the electric field can be expressed as $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{i\omega t}$. By eliminating the magnetic field from Maxwell's equations, we obtain

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) = k_0^2 \tilde{n}^2(\mathbf{r}) \mathbf{E}(\mathbf{r}), \quad (4.1)$$

where $k_0 (= \omega/c)$ is the free-space wavenumber, ω is the angular frequency, c is the velocity of light in free space and $\tilde{n}$ is the refractive index (a complex number) satisfying $k_0^2 \tilde{n}^2(\mathbf{r}) \simeq k_0^2 n^2(\mathbf{r}) + 2ik_0 n_0(z) \tilde{\alpha}(z)$ [66, 84], where $n^2(\mathbf{r})$ is a periodic function of x and y , $n_0(z)$ represents the average refractive index of the material at position z , and $\tilde{\alpha}(z)$ represents the gain ($\tilde{\alpha} > 0$) or loss ($\tilde{\alpha} < 0$) in each region. Here, we still focus our analysis on the transverse electric (TE) polarization because the lasing mode has been identified experimentally as being a TE mode [46]. For TE polarization, $\mathbf{E}(\mathbf{r}) = (E_x(\mathbf{r}), E_y(\mathbf{r}), 0)$ can be expanded according to Bloch's theorem

$$E_j(\mathbf{r}) = \sum_{m,n} E_{j,m,n}(x, y, z) e^{-im\beta_0 x - in\beta_0 y}, \quad j = x, y, \quad (4.2)$$

and the periodic function $n^2(\mathbf{r})$ can be expanded as

$$n^2(\mathbf{r}) = n_0^2(z) + \sum_{m \neq 0, n \neq 0} \xi_{m,n}(z) e^{-im\beta_0 x - in\beta_0 y}. \quad (4.3)$$

Here, $\beta_0 = 2\pi/a$, a is the lattice constant, m, n are arbitrary integers, and $\xi_{m,n}(z)$ is the high-order Fourier coefficient term. We note that $\xi_{m,n}(z)$ is zero outside the PC region. For simplicity, we assume that air holes within the PC region have perfectly vertical sidewalls (tilted case is discussed in Ref. [85]) such that $n_0^2(z)$ represents the average dielectric constant of PC and that $\xi_{m,n}$ is independent of z within the PC region. By substituting Eqs. (4.2) and (4.3) into Eq. (4.1) and collecting all terms that are multiplied by the factor $e^{-im\beta_0 x - in\beta_0 y}$, we obtain

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) + 2ik_0 n_0(z) \tilde{\alpha}(z) - n^2 \beta_0^2 \right] E_{x,m,n} &= 2in\beta_0 \frac{\partial E_{x,m,n}}{\partial y} + \frac{\partial^2 E_{x,m,n}}{\partial y^2} + mn\beta_0^2 E_{y,m,n} \\ &\quad - \frac{\partial^2 E_{y,m,n}}{\partial x \partial y} + i\beta_0 \left(m \frac{\partial E_{y,m,n}}{\partial y} + n \frac{\partial E_{y,m,n}}{\partial x} \right) = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{x,m',n'}, \end{aligned} \quad (4.4)$$

$$\begin{aligned} \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) + 2ik_0 n_0(z) \tilde{\alpha}(z) - m^2 \beta_0^2 \right] E_{y,m,n} &= 2im\beta_0 \frac{\partial E_{y,m,n}}{\partial x} + \frac{\partial^2 E_{y,m,n}}{\partial x^2} + mn\beta_0^2 E_{x,m,n} \\ &\quad - \frac{\partial^2 E_{x,m,n}}{\partial x \partial y} + i\beta_0 \left(m \frac{\partial E_{x,m,n}}{\partial y} + n \frac{\partial E_{x,m,n}}{\partial x} \right) = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{y,m',n'}, \end{aligned} \quad (4.5)$$

$$\frac{\partial}{\partial z} \left[\left(\frac{\partial E_{x,m,n}}{\partial x} + \frac{\partial E_{y,m,n}}{\partial y} \right) - i\beta_0 (m E_{x,mn} + n E_{y,mn}) \right] = 0. \quad (4.6)$$

Here, as we are considering a finite system, we have retained the spatial derivative terms of E_x and E_y with respect to x and y . As defined previously [84], the wavevectors can be classified into three groups according to their in-plane wavenumber, $\sqrt{m^2 + n^2} \beta_0$: basic waves ($\sqrt{m^2 + n^2} = 1$), high-order waves ($\sqrt{m^2 + n^2} > 1$), and radiative waves ($m = n = 0$). By assuming a separable form of solutions for the fields, we can solve Eqs. (4.4)-(4.6) analytically. In the resonant case at the second-order Γ point shown in Fig. 4.1(b), the four basic waves can be expressed as

$$E_{x,1,0} = 0, \quad E_{y,1,0} = R_x(x, y) \Theta_0(z), \quad (4.7)$$

$$E_{x,-1,0} = 0, \quad E_{y,-1,0} = S_x(x, y) \Theta_0(z), \quad (4.8)$$

$$E_{x,0,1} = R_y(x, y) \Theta_0(z), \quad E_{y,0,1} = 0, \quad (4.9)$$

$$E_{x,0,-1} = S_y(x, y) \Theta_0(z), \quad E_{y,0,-1} = 0. \quad (4.10)$$

Here, $R_x(x, y)$ and $S_x(x, y)$ represent the amplitudes of basic waves propagating in the $+x$ and $-x$ directions, respectively, and likewise, $R_y(x, y)$ and $S_y(x, y)$ represent the amplitudes of waves propagating in the $+y$ and $-y$ directions, respectively. These four basic waves are assumed to have identical field profiles in the z -direction, denoted

by $\Theta_0(z)$, which is the same as the field profile of the fundamental guided mode for a multilayer structure without PCs [66]. We express the wave equation for the fundamental guided mode in terms of $\Theta_0(z)$ as

$$\frac{\partial^2 \Theta_0}{\partial z^2} + [k_0^2 n_0^2(z) - \beta^2] \Theta_0 = 0, \quad (4.11)$$

where β is the propagation constant, which satisfies $\beta \simeq \beta_0$ in the vicinity of the second-order Γ point. In this chapter, we calculate β and $\Theta_0(z)$ in Eq. (4.11) by employing the transfer matrix method [74] and normalize $\Theta_0(z)$ as $\int_{-\infty}^{\infty} |\Theta_0(z)|^2 dz = 1$.

In order to obtain the coupled-wave equations, Eqs. (4.7)-(4.10) are substituted into Eqs. (4.4)-(4.6) for $(m, n) = \{(1, 0), (-1, 0), (0, 1), (0, -1)\}$. Here, without loss of generality, we focus on the case for which $(m, n) = (1, 0)$. We then only need to consider Eqs. (4.7) and (4.5). Substitution of Eq. (4.7) into Eq. (4.5) gives

$$\begin{aligned} & \left[\frac{\partial^2 \Theta_0}{\partial z^2} + (k_0^2 n_0^2(z) + 2ik_0 n_0(z) \tilde{\alpha}(z) - \beta_0^2) \Theta_0 \right] R_x - 2i\beta_0 \frac{\partial R_x}{\partial x} \Theta_0 \\ & = -k_0^2 \sum_{m' \neq 1, n' \neq 0} \xi_{1-m', -n'} E_{y, m', n'}. \end{aligned} \quad (4.12)$$

Here, the basic wave R_x is assumed to vary slowly compared to $\exp(-i\beta_0 x)$ so that its second spatial derivative terms in Eq. (4.5) can be neglected. Then Eq. (4.11) is substituted into Eq. (4.12) to yield

$$(\beta^2 - \beta_0^2) R_x \Theta_0 + 2ik_0 n_0(z) \tilde{\alpha}(z) R_x \Theta_0 - 2i\beta_0 \frac{\partial R_x}{\partial x} \Theta_0 = -k_0^2 \sum_{m' \neq 1, n' \neq 0} \xi_{1-m', -n'} E_{y, m', n'}. \quad (4.13)$$

The term $E_{y, m', n'}$ on the right-hand side of Eq. (4.13) represents all the waves that may couple to R_x , including basic, high-order, and radiative waves as described above. Specifically, we express the radiative waves [for which $(m', n') = (0, 0)$] as

$$E_{x, 0, 0} = \Delta E_x(z), \quad E_{y, 0, 0} = \Delta E_y(z). \quad (4.14)$$

Finally, we can obtain the coupled-wave equation for $(m, n) = (1, 0)$ by multiplying Eq. (4.13) by $\Theta_0^*(z)$ on both sides and integrating over $(-\infty, \infty)$ along the z direction. Three more coupled-wave equations for $(m, n) = \{(-1, 0), (0, 1), (0, -1)\}$ can be derived

in analogous fashion. We write the four coupled-wave equations in the following form:

$$-i\frac{\partial R_x}{\partial x} + (\delta + i\alpha)R_x = \kappa_{2,0}S_x - \frac{k_0^2}{2\beta_0}\xi_{1,0}\int_{PC}\Delta E_y(z)\Theta_0^*(z)dz - \frac{k_0^2}{2\beta_0}\sum_{\sqrt{m^2+n^2}>1}\xi_{1-m,-n}\int_{PC}E_{y,m,n}(z)\Theta_0^*(z)dz, \quad (4.15)$$

$$i\frac{\partial S_x}{\partial x} + (\delta + i\alpha)S_x = \kappa_{-2,0}R_x - \frac{k_0^2}{2\beta_0}\xi_{-1,0}\int_{PC}\Delta E_y(z)\Theta_0^*(z)dz - \frac{k_0^2}{2\beta_0}\sum_{\sqrt{m^2+n^2}>1}\xi_{-1-m,-n}\int_{PC}E_{y,m,n}(z)\Theta_0^*(z)dz, \quad (4.16)$$

$$-i\frac{\partial R_y}{\partial y} + (\delta + i\alpha)R_y = \kappa_{0,2}S_y - \frac{k_0^2}{2\beta_0}\xi_{0,1}\int_{PC}\Delta E_x(z)\Theta_0^*(z)dz - \frac{k_0^2}{2\beta_0}\sum_{\sqrt{m^2+n^2}>1}\xi_{-m,1-n}\int_{PC}E_{x,m,n}(z)\Theta_0^*(z)dz, \quad (4.17)$$

$$i\frac{\partial S_y}{\partial y} + (\delta + i\alpha)S_y = \kappa_{0,-2}R_y - \frac{k_0^2}{2\beta_0}\xi_{0,-1}\int_{PC}\Delta E_x(z)\Theta_0^*(z)dz - \frac{k_0^2}{2\beta_0}\sum_{\sqrt{m^2+n^2}>1}\xi_{-m,-1-n}\int_{PC}E_{x,m,n}(z)\Theta_0^*(z)dz \quad (4.18)$$

Here, $\delta = (\beta^2 - \beta_0^2)/2\beta_0 \simeq \beta - \beta_0 = n_{eff}(\omega - \omega_0)/c$ is the deviation from the Bragg condition, ω_0 is the Bragg frequency, n_{eff} is the effective refractive index for the fundamental guided mode, and α is the mode loss given by $\alpha = \frac{k_0}{\beta_0}\int_{-\infty}^{\infty}n_0(z)\tilde{\alpha}(z)|\Theta_0(z)|^2dz$. $\kappa_{\pm 2,0}$ and $\kappa_{0,\pm 2}$ are the backward coupling coefficients defined as

$$\kappa_{\pm 2,0} = -\frac{k_0^2}{2\beta_0}\xi_{\pm 2,0}\int_{PC}|\Theta_0(z)|^2dz, \quad (4.19)$$

$$\kappa_{0,\pm 2} = -\frac{k_0^2}{2\beta_0}\xi_{0,\pm 2}\int_{PC}|\Theta_0(z)|^2dz, \quad (4.20)$$

respectively, which are equivalent to the conventional one dimensional (1D) coupling coefficients [65]. The second and third terms on the right-hand sides of Eqs. (4.15)-(4.18) represent the out-of-plane and 2D optical couplings, respectively. It should be noted that integrals in Eqs. (4.1)-(4.4), as well as those in Eqs. (4.19)-(4.20), extend only over the PC region because the Fourier coefficient $\xi_{mn} = 0$ outside that range.

The solutions of the radiative waves ($\Delta E_x(z)$, $\Delta E_y(z)$) and the high-order waves ($E_{x,m,n}(z)$, $E_{y,m,n}(z)$) can be expressed analytically by terms only associated with basic waves, as derived in Chapter 3. Then, the coupled-wave Eqs. (4.15)-(4.18) can be rewritten in

matrix form as

$$(\delta + i\alpha) \begin{pmatrix} R_x \\ S_x \\ R_y \\ S_y \end{pmatrix} = \mathbf{C} \begin{pmatrix} R_x \\ S_x \\ R_y \\ S_y \end{pmatrix} + i \begin{pmatrix} \partial R_x / \partial x \\ -\partial S_x / \partial x \\ \partial R_y / \partial y \\ -\partial S_y / \partial y \end{pmatrix}. \quad (4.21)$$

Here, $\mathbf{C}$ is a 4×4 matrix (see Appendix A). By considering a finite laser cavity area with $0 \leq x, y \leq L$ (L : laser cavity length in both x and y directions) and defining appropriate boundary conditions, Eq. (4.21) can be discretized using the staggered-grid finite-difference method [82]. This creates an eigenvalue problem with eigenvectors $(R_x^{j,k}, S_x^{j,k}, R_y^{j,k}, S_y^{j,k}, R_x^{j+1,k}, S_x^{j+1,k}, R_y^{j+1,k}, S_y^{j+1,k}, \dots)^t$ and normalized eigenvalues $(\delta + i\alpha)L$.

4.3 Analysis results

In this section, we will show numerical results of the calculated lasing properties. By solving the coupled-wave Eq. (4.21), we can obtain various properties of interest, including mode frequency, threshold gain, field intensity envelope profile within the device, far-field patterns (including the polarization profile) of the band-edge modes. The effects of finite size on these properties will be discussed.

The structural parameters of the laser structure [see Fig. 4.1(a)] to be studied are shown in Tab. 4.1. The PC layer is embedded inside the multilayer structure, which is assumed to support only a single guided mode. The average refractive index of the PC layer is given by $n_{av} = \sqrt{fn_a^2 + (1-f)n_b^2}$, where n_a is the refractive index of air, n_b is the refractive index of the background dielectric material (GaAs), and f is the air-hole filling factor (i.e., the fraction of the area of a unit cell occupied by air holes). In this work, we focus our analyses on two typical air-hole shape designs [see the inset of Fig. 4.1(a)]: circular (CC) and equilateral triangular (ET), both of which have been studied experimentally in our previous works [35, 51]. We consider a boundary condition that is defined as

$$R_x(0, y) = S_x(L, y) = R_y(x, 0) = S_y(x, L) = 0, \quad (4.22)$$

which includes fixing the field amplitude to zero at only one of two sides, generalizing a similar concept for 1D distributed feedback (DFB) laser structure originally proposed by Kogelnik and C. V. Shank [65]. Unless otherwise noted in the following examples, the lattice constant $a = 295$ nm and the air-hole filling factor $f = 0.16$, the device length

$L=70\text{ }\mu\text{m}$ (all these values were inferred from experimental data). Here, it is important to note that $L=70\text{ }\mu\text{m}$ approximately corresponds to a $240a \times 240a$ lasing area, which is almost impossible to use 3D FDTD method to compute.

Table 4.1: Structural parameters of the 2D PCSEL device.

Layer	Thickness (nm)	Refractive index
n -clad (AlGaAs)	1500	3.307
Spacer (GaAs)	30	3.524
Active (3QW, InGaAs/GaAs)	64	3.553
Spacer (GaAs)	40	3.524
Cladding (AlGaAs)	40	3.279
GaAs	22	3.524
PC	118	n_{av}
GaAs	20	3.524
p -clad (AlGaAs)	1500	3.307

4.3.1 Threshold gain and field intensity profile

In finite systems, mode frequency and threshold gain correspond to the real part and imaginary part of the normalized eigenvalue of Eq. (??), $(\delta + i\alpha)L$, respectively. As an example, we show in Fig. 4.2(i) a plot of the normalized threshold gain (αL) as a function of deviation from the Bragg condition (δL) for a PCSEL with ET air holes. Though a large number of modes exist due to the numerical calculation, we identify the four band-edge modes (A, B, C and D) using the techniques described in Ref. [63]. First, we evaluate the field intensity envelope of the individual modes throughout the laser cavity, which modulates the fast-varying Bloch waves in the PC lattice and can be determined by [63]

$$P(x, y) = |R_x(x, y)|^2 + |S_x(x, y)|^2 + |R_y(x, y)|^2 + |S_y(x, y)|^2. \quad (4.23)$$

We extract the solutions of interest that have a singled-lobed profile throughout the laser cavity. Then, we further identify the four band-edge modes by plotting their field distribution patterns inside a unit cell located at the center of the cavity and comparing these patterns with those calculated by 2D-PWEM. Figure 4.2(ii) shows the field intensity envelope profiles of the individual band-edge modes, indicating that energy can be well confined inside the laser cavity. Figure 4.2(iii) shows field distributions of each mode inside a unit cell located at the center of the cavity. Modes A and B correspond to the antisymmetric (nonleaky) mode of 1D DFB lasers, whereas modes C and D correspond to the symmetric (leaky) mode of 1D DFB lasers [47].

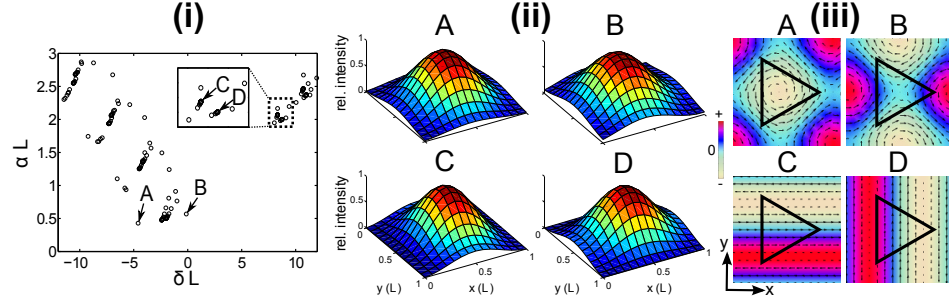


Figure 4.2: (i) Normalized threshold gain (αL) as a function of normalized mode frequency deviation (δL) for a PCSEL with ET air holes. The four band-edge modes A-D are indicated by arrows. (ii) Field intensity envelopes of the individual band-edge modes. (iii) Field distributions inside a unit cell located at the center of the cavity, in which colors and arrows represent H- and E-fields, respectively. Thick black triangles indicate the air holes. In the calculations, we use the structural parameters shown in Tab. 4.1, the air-hole filling factor $f = 0.16$, the lattice constant $a = 295$ nm, and the device length $L = 70$ μm . The laser is divided into 14 sections for which the eigenvalues (αL and δL) converge well.

Table 4.2: Normalized threshold gain (αL) of the four band-edge modes A-D for CC and ET air-hole shapes ($f = 0.16$, $a = 295$ nm, and $L = 70$ μm).

Shape	$\alpha_A L$	$\alpha_B L$	$\alpha_C L$	$\alpha_D L$
CC	0.23	0.52	2.18	2.18
ET	0.43	0.57	2.08	2.01

The normalized threshold gains of modes A-D are shown in Tab. 4.2 in which the values for the CC air-hole case were obtained in the same manner. We note that modes C and D exhibit a much higher threshold gain compared with modes A and B, which is attributed to the symmetric nature of their electric-field distributions with respect to the air holes as shown in Fig. 4.2(iii). As the lasing action occurs at the mode with the lowest threshold gain (loss), Tab. 4.2 indicates that mode A is favored for lasing for both CC and ET air holes when the device length $L = 70$ μm , with a large threshold-gain discrimination of over 20 cm^{-1} against mode B. This is consistent with the experimental observations [46, 51] where stable single-mode operations at mode A were demonstrated.

It is important to note that the single-mode lasing behavior at mode A cannot be explained based on the infinite solutions [84]. For an infinite periodic system with the vertical structure shown in Tab. 4.1, the radiation constants α_{inf} of modes A and B are $\alpha_{inf,A} = \alpha_{inf,B} = 0$ cm^{-1} for CC and $\alpha_{inf,A} = 12.35$ cm^{-1} , $\alpha_{inf,B} = 0.82$ cm^{-1} for ET air holes, respectively. From these results, one might expect that both modes A and B are favored for lasing for the CC air holes because both of their radiation constants (losses) are equal to zero; and for the ET air holes, mode B lases due to its much smaller radiation constant compared with that of mode A. Apparently, these predictions are in

contrast to our finite analysis results and experimental findings. We suggest that the in-plane loss of finite structures might have a great impact on the mode selection of PCSELs, which will be discussed in detail in the following sections.

4.3.2 Far-field pattern and polarization

The far-field pattern and polarization of the output laser beam is one of the most unique features of 2D PCSELs. As demonstrated in Refs. [29, 35], both far-field pattern and polarization can be tailored by appropriately engineering the PC geometry. Theoretically, it is possible to calculate the far-field patterns of 2D PCSELs based on our 3D CWT model since the radiation field emanating from the surface of the finite-size laser structure is formulated explicitly (see Sec. 3.2.1). The time-dependent amplitude of the far field $F_{j=x,y}$ (subscripts denote the x and y components, respectively), a function of the deflection angle (θ_x, θ_y) from the surface normal, can be found by taking the Fourier transform of the radiation field and multiplying by an obliquity factor $(\cos \theta_x + \cos \theta_y - 1)$ [97],

$$F_j(\theta_x, \theta_y, t) \propto (\cos \theta_x + \cos \theta_y - 1) \iint_0^L \Delta E_j(x, y, z = d_{PC}/2) e^{i\omega t} \cdot e^{-ik_0(\tan \theta_x x + \tan \theta_y y)} dx dy, \quad j = x, y, \quad (4.24)$$

where $\Delta E_j(x, y, z = d_{PC}/2)$ is the complex radiation field just above the PC surface (see Eqs. (3.20a)-(3.20b) and note the x and y dependence of ΔE_j), d_{PC} is the depth of the PC layer, and $z = 0$ is defined at the center of the PC layer. Then, the time-averaged far-field intensity (i.e. beam pattern) is given as

$$\langle B(\theta_x, \theta_y) \rangle = \langle B_x(\theta_x, \theta_y) \rangle + \langle B_y(\theta_x, \theta_y) \rangle, \quad (4.25)$$

where

$$\langle B_j(\theta_x, \theta_y) \rangle = \frac{1}{T} \int_0^T |Re[F_j(\theta_x, \theta_y, t)]|^2 dt, \quad j = x, y, \quad T = 2\pi/\omega. \quad (4.26)$$

By calculating the x and y components of the far field using Eq. (4.26), we can directly evaluate the effect of the air holes on the polarization of the output beam.

Figures 4.3(a) and (b) show the calculated far-field patterns of mode A (i.e. the lowest threshold mode) for the two air-hole shapes. A doughnut-shaped profile is obtained for CC, whereas a single-lobed profile is obtained for ET air holes. The insets show the x and y components of the far field, indicating that CC air holes exhibit an azimuthal polarization, and ET ones exhibit an almost linear polarization in the y direction. These

semi-analytical results closely match our experimental observations shown in Figs. 4.3(c) and (d) [35, 51]. The beam divergence angle of all of the far-field patterns is around 1° , reflecting the large area of coherent oscillation. The small side lobes of the calculated far-field patterns are caused by the abrupt termination of the radiation field at the edges of the laser cavity.

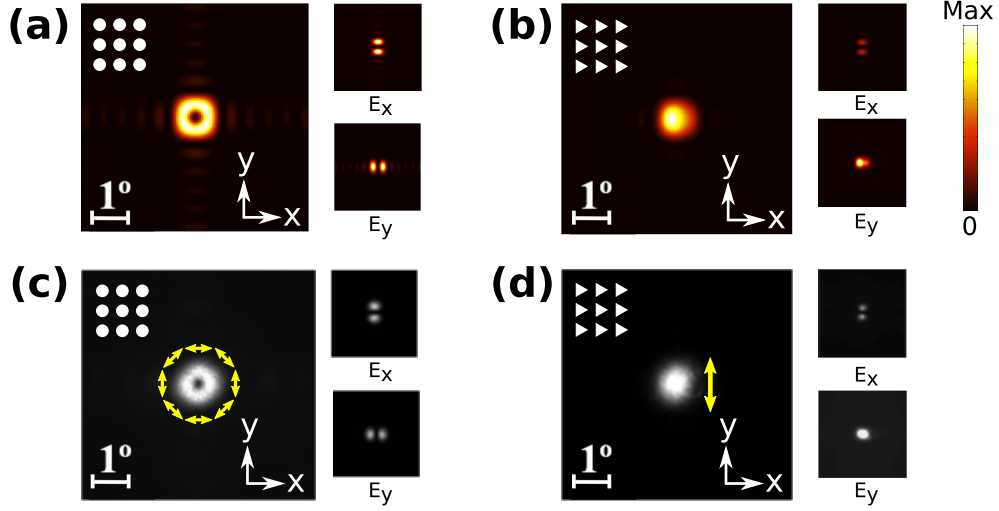


Figure 4.3: Calculated far-field patterns (FFPs) of mode A (i.e. the lowest threshold mode) for (a) CC and (b) ET air holes and experimentally observed FFPs for (c) CC and (d) ET air holes. The insets in (a) and (b) represent the x and y components of the far field. Parameters used for the calculations are the same as those shown in Fig. 4.2. The yellow arrows in (c) and (d) indicate the directions of polarization.

It is interesting to note that the quantity of surface emission for the symmetric CC air-hole shape is zero when an infinite periodic structure is considered [84], whereas it has a finite value for a finite periodic structure. This difference can be understood by considering the effect of finite device length on the electromagnetic field distribution within the device. For an infinite periodic structure, the light from mode A cannot be coupled to the external system because perfect destructive interference occurs everywhere due to the antisymmetric field distribution pattern with respect to the perfectly symmetric air holes. On the other hand, the mode field is spatially restricted for a finite system, leading to a small shift of the electromagnetic field with respect to the air holes. Figure 4.4(a) shows the electromagnetic field distribution patterns at (i) the center of the device and toward (ii-vi) the edges of the device. Although the mode field is kept antisymmetric with respect to the air holes in the center region, the field in the regions away from the center is no longer antisymmetric with respect to the air holes, thereby resulting in an imperfect destructive interference.

To examine the resultant interference effect in further detail, we plot in Fig. 4.4(b) the intensities of basic waves propagating in the $\pm x$ directions (i.e. $|R_x|^2$ and $|S_x|^2$) and

the radiation field intensity along the line $y = L/2$. The radiation field intensity can be represented by $|R_x + S_x|^2$, which reflects the interference effects of the two counter-propagating basic waves R_x and S_x (see Eqs. (3.20a)-(3.20b) by noting that Fourier coefficient terms $\xi_{m,n}$ for CC air holes are real numbers). From Fig. 4.4(b), we can clearly see that the interference is indeed perfectly destructive at the center but becomes imperfect toward the edges of the device. The situation for ET can be understood in the same manner except that even at the central region the perfect destructive interference is suppressed because of the asymmetric air-hole effects [89].

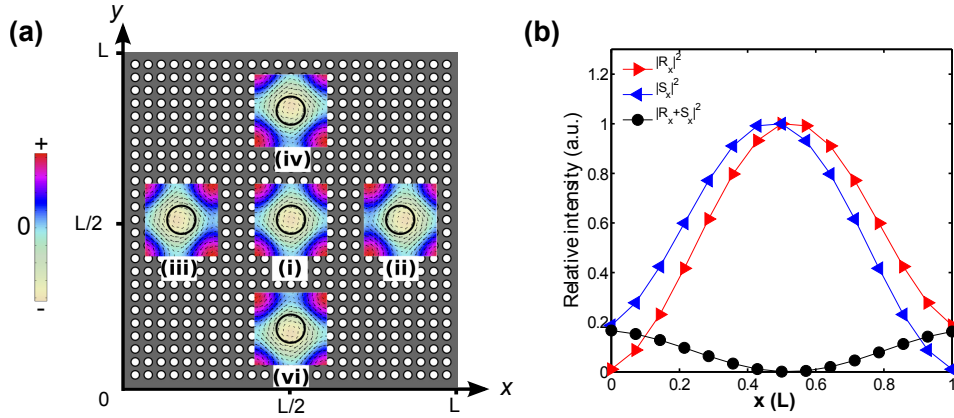


Figure 4.4: (a) Illustrative field distribution patterns (plotted in a single unit cell) of mode A for CC air holes at the center of the cavity (i): $(\frac{L}{2}, \frac{L}{2})$ and toward the edges (ii): $(\frac{6L}{7}, \frac{L}{2})$, (iii): $(\frac{L}{7}, \frac{L}{2})$, (iv): $(\frac{L}{2}, \frac{6L}{7})$, and (vi): $(\frac{L}{2}, \frac{L}{7})$. Colors and arrows represent H- and E-fields, respectively. Thick black circles indicate the locations of air holes with respect to the unit cell. (b) Field intensities of basic waves propagating in the $\pm x$ directions, $|R_x|^2$ and $|S_x|^2$ (red and blue curves), and the radiation field intensity represented by $|R_x + S_x|^2$ (black curve) along the axis $y = L/2$. Note that R_x and S_x are zero at $x = 0$ and $x = L$, respectively, which corresponds to the boundary condition described by Eq. (4.22).

The divergence angle of the far-field pattern is closely related to the finite size of the device. When the device is infinitely large, the surface emission is strictly in the surface normal direction. However, the realistic device has a finite length L , and therefore allows a wavenumber fluctuation of $\delta k \simeq 2\pi/L$ from the Γ point, which was demonstrated by 3D FDTD simulations for finite structures [78, 79]. In fact, this wavenumber fluctuation corresponds to the slightly shifted electromagnetic field distributions discussed above [see Fig. 4.4(a)]. Due to this fluctuation, the emitted beam deviates from the surface normal direction with a deflection angle $\delta\theta$. The relation between $\delta\theta$ and the wavenumber fluctuation can be expressed as

$$k_0 \sin(\delta\theta) = \delta k, \quad (4.27)$$

where $k_0 = 2\pi/\lambda$ (λ : the resonance wavelength in free space). For example, when $\lambda = 960$ nm, $L=70$ μm , $\delta\theta \simeq 0.8^\circ$, which is a good approximation of the results shown in Fig. 4.3.

4.3.3 Device length dependence of threshold gain

The analysis for an infinite system corresponds to the case when $L \rightarrow \infty$. In this case, threshold gain and mode selection properties are determined only by the surface radiation loss (for simplicity, in this work we do not consider absorption loss). However, for a finite structure, influence of the in-plane loss (i.e. the power escaping from the edges of the laser cavity) has to be taken into account. To clarify the effects of the in-plane loss and highlight the difference between finite and infinite analyses, we investigate the threshold dependence on device length.

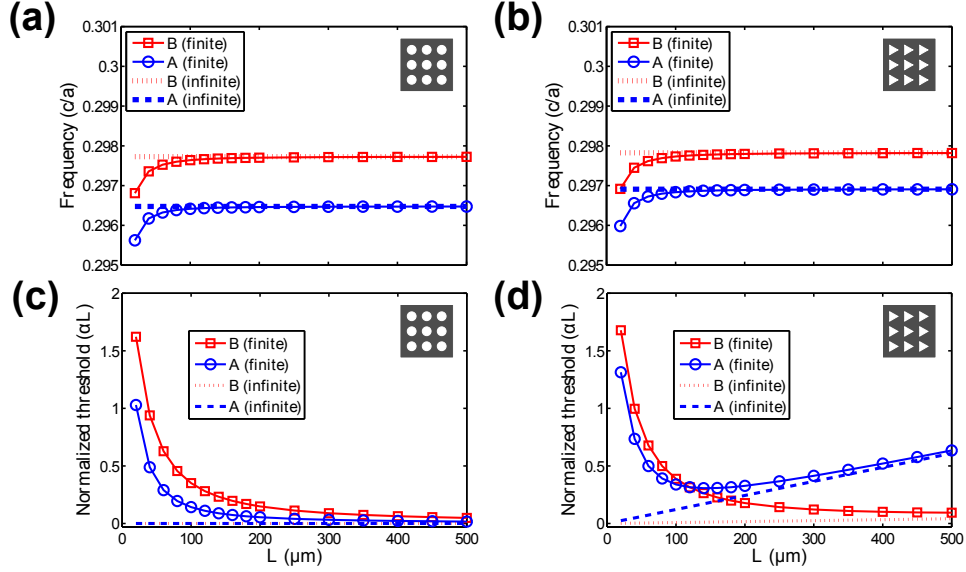


Figure 4.5: Normalized mode frequency (a, b) and threshold gain (c, d) as a function of the device length L for CC and ET air holes ($f = 0.16$ and $a=295$ nm). The solid curves and dashed lines are calculated for finite and infinite structures, respectively.

We plot in Fig. 4.5 the normalized mode frequency and threshold gain as a function of the device length L for CC and ET air holes. Also included as dashed lines are the infinite solutions (δ and α are first calculated for infinite periodic structures and then normalized by using $(\delta + \beta_0)/(n_{eff}\beta_0)$ [84] and αL , respectively). From Figs. 4.5(a) and (b), we note that mode frequency increases with respect to L and converges quickly to the infinite solutions (dashed lines). The threshold gain, in contrast, shows a quite different behavior: as shown in Figs. 4.5(c) and (d), in both cases, the laser threshold gain (solid curves) initially decreases with increasing L and then begins to be asymptotic

to the infinite solutions (dashed lines). This behavior can be intuitively understood as follows. For small values of L , the dominant loss mechanism in the laser is the in-plane loss. In particular, at very short lengths, the optical power exits the gain region at the edges of the laser cavity without being diffracted out of the PC surface, leading to a high threshold gain. However, for larger values of L , the in-plane loss steadily decreases and the surface radiation loss becomes dominant. In fact, infinite solutions can correctly predict the lasing mode (i.e. the lowest threshold mode) of the device only when L is large enough, e.g. $L > 400 \mu\text{m}$ (see Fig. 4.5). For a relatively small L , e.g. $L < 100 \mu\text{m}$, the influence of the in-plane loss on threshold behavior should not be neglected.

To evaluate the influence of the in-plane loss quantitatively, we derive a formula (Appendix B) to describe the power flow in 2D PCSELs by extending the energy conservation theorem developed for 1D DFB lasers [90], which can be expressed as

$$P_{stim} = P_{edge} + P_{rad}. \quad (4.28)$$

Here, P_{stim} , P_{edge} , and P_{rad} represent the stimulated emission power, the power escaping from the edges of the laser cavity (i.e. the in-plane loss), and the surface radiation power, respectively. Therefore, the percentage of the in-plane loss power with respect to the total stimulated power is given by

$$P_{edge}/P_{stim} = 1 - P_{rad}/P_{stim}. \quad (4.29)$$

Table 4.3: Percentage of the in-plane loss with respect to the total stimulated power, P_{edge}/P_{stim} for CC and ET air holes with different device lengths ($f = 0.16$ and $a=295 \text{ nm}$).

Shape/mode		L=70 μm	L=400 μm
CC	mode A	67%	26%
	mode B	69%	26%
ET	mode A	58%	2%
	mode B	71%	19%

Table 4.3 shows the calculated P_{edge}/P_{stim} of modes A and B for CC and ET air holes with different device lengths. We can clearly see that, for both air-hole shapes, when $L = 70 \mu\text{m}$, the in-plane loss is indeed noticeably larger than the surface radiation loss, indicating that in-plane loss plays a very important role in the mode selections of the laser device. While when $L=400 \mu\text{m}$, the in-plane loss drastically decreases and its influence on mode selections might be neglected. Here, it is important to note that, in the case of ET air holes, when the device length L is increased from $70 \mu\text{m}$ to $400 \mu\text{m}$, the lasing mode likely switches from mode A to mode B which has a smaller radiation constant

[see Fig. 4.5(d)]. This kind of mode switching will be experimentally demonstrated in the following section.

4.3.4 Demonstration of mode selectivity controlled by cavity length

Understanding the mechanism of the mode selection behavior is particularly important in designing PCSELs, because the lasing mode may be possibly favored at different band-edge states which exhibit completely different surface emission nature. In this section, we experimentally demonstrate that the lasing band-edge mode can be selectively controlled by changing the laser cavity length L . Here, for the PC air-hole shape design, we adopted a right-angled isosceles triangle (RIT) because this shape provides identical feedback in both the x and y directions and lasing action tends to occur at the band-edge modes [59, 60].

Figure 4.6(a) shows the calculated band structure of a PC with right-angled isosceles triangle (RIT) air-hole shape. The field patterns of band-edge modes A and B are shown in the insets. Figure 4.6(b) presents the calculated threshold gain (αL) as a function of L for band-edge modes A and B . As the lasing action occurs at the mode with the lowest threshold, Figure 4.6(b) indicates that mode A is favored for lasing when the cavity length is less than $100 \mu\text{m}$, and when L is increased further mode B will be favored for lasing.

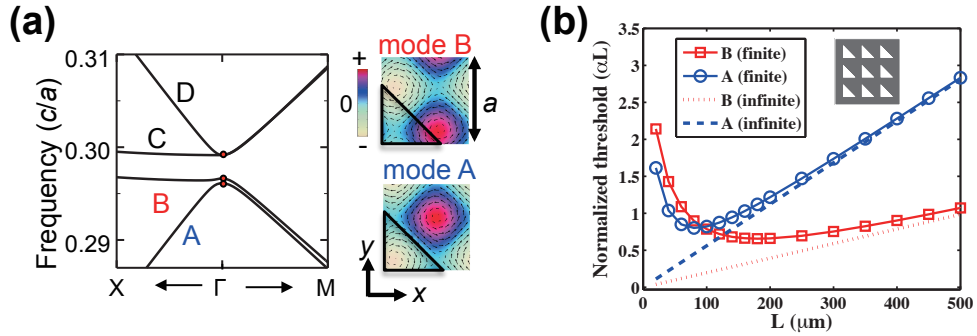


Figure 4.6: (a) Calculated band structure of a PC with right-angled isosceles triangle (RIT) air holes. Field patterns of modes A and B are shown in the insets.(b) Calculated threshold gain as a function of the device length L for the RIT air holes. In the calculation the air-hole fraction $f = 0.20$ and the lattice constant $a=295 \text{ nm}$). The solid curves and dashed lines are calculated for finite and infinite structures, respectively.

Next, to demonstrate the mode selectivity behavior, on the same wafer we fabricated two samples that have different cavity lengths: $L=50 \mu\text{m}$, and $L=200 \mu\text{m}$. The measured band structures of these two samples are shown in Figs. 4.7(a) and 4.8(a), respectively. These band structure were measured well below the laser threshold and showed similar

features. The spontaneous emission spectrum at the Γ point is shown in Figs. 4.7(b) and 4.8(b), respectively. Above the laser threshold, the $L=50\text{ }\mu\text{m}$ sample lased at the band-edge mode A but the $L=200\text{ }\mu\text{m}$ sample lased at the band-edge mode B . This is the direct experimental demonstration of the theoretical prediction presented in Fig. 4.6(b).

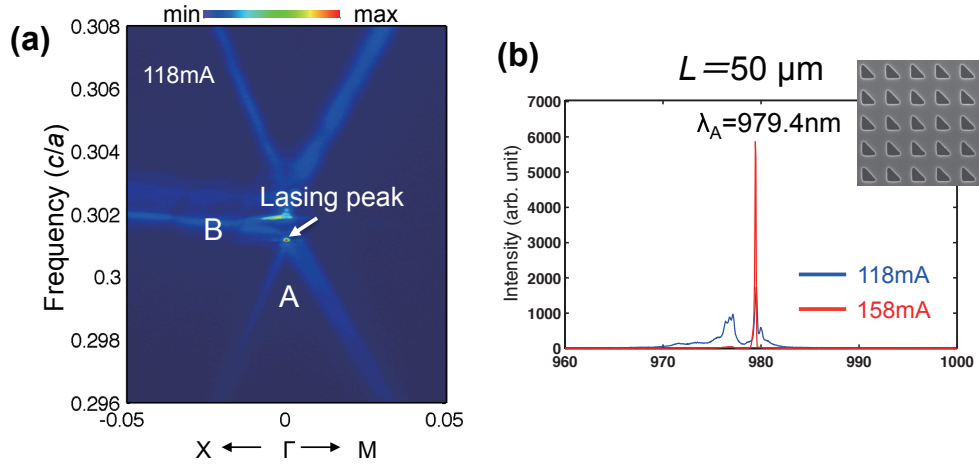


Figure 4.7: Characteristic of a $L = 50\text{ }\mu\text{m}$ device: measured (a) band structure and (b) lasing spectrum.

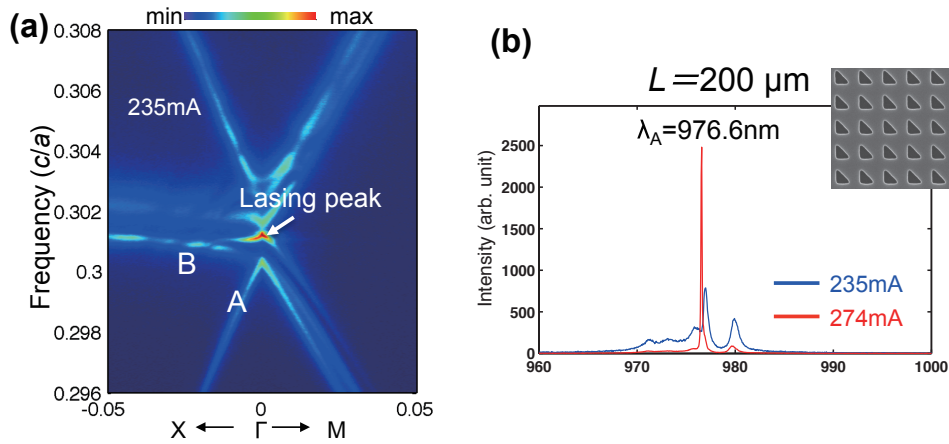


Figure 4.8: Characteristic of a $L = 200\text{ }\mu\text{m}$ device: measured (a) band structure and (b) lasing spectrum.

The experimental FFPs observed from these two samples are presented in Fig. 4.9. The $L=50\text{ }\mu\text{m}$ sample exhibited a single-lobed FFP, whereas the $L = 200\text{ }\mu\text{m}$ exhibited a doughnut-like FFP. These results are in good agreement with the calculated FFPs (lower pannels). Here, it should be mentioned that, in the calculation, the roundness of the experimental RIT shapes were taken into account. A curvature ratio $r/a = 0.08$ (r : radii of circles that represent the roundness of the RIT angles) was used, which was inferred from the SEM images of the fabricated samples.

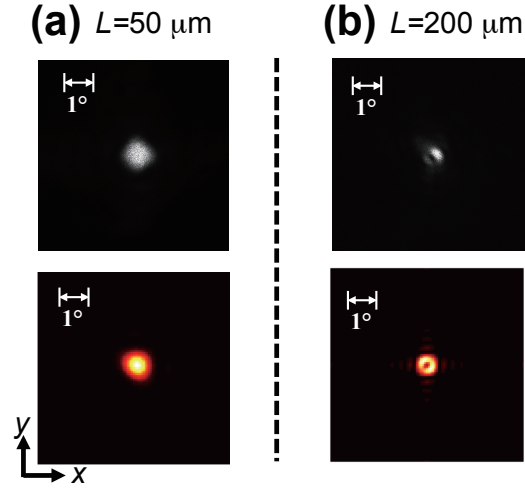


Figure 4.9: Far-field patterns (FFPs) of the (a) $L = 50 \mu\text{m}$ and (b) $L = 200 \mu\text{m}$ samples. The upper and lower panels show the experimental and calculated FFPs, respectively.

4.3.5 Single-mode stability in large-area PCSELs

In general, a large device dimension is beneficial for improving output power. However, in the field of distributed-feedback (DFB) lasers, it is widely recognized that single-mode DFB lasers with a large coupling-coefficient-length product κL become unstable under high current levels, where κ is the coupling coefficient between counterpropagating basic waves and L is the laser cavity length [91]. This is due not only to reduced modal discrimination at a large L [66, 109], but also to the spatial hole burning (SHB) effect that is closely associated with κL [91]. For multidirectional distributed-feedback PCSELs, the situation becomes more complicated; this is because the coupling mechanism in PCSELs is represented by two kinds of coupling coefficients: κ_{1D} and κ_{2D} [84]. The former represents the direct coupling strength of basic waves propagating along one axis and corresponds to κ in DFB lasers. The latter represents the indirect two-dimensional (2D) coupling strength via oblique partial waves and does not exist in DFB lasers [63, 84]. The combined effect of these coupling coefficients determines the unique 2D resonant characteristics of PCSEL cavities [29, 31, 35, 40] and distinguishes PCSELs from conventional DFB lasers. In this letter, as the first step to study the influence of the coupling-coefficient-length product on mode stability in PCSELs, we focus on $\kappa_{1D}L$ and investigate mode stability in large-area PCSELs in which $\kappa_{1D}L$ exceeds 6. We show that, contrary to single-mode operation obtained near threshold, other competing modes are excited at higher currents above threshold. The origin of the observed competing modes will be clarified by our theoretical analysis. The influence of the cavity length and the SHB effect on the mode stability is also discussed.

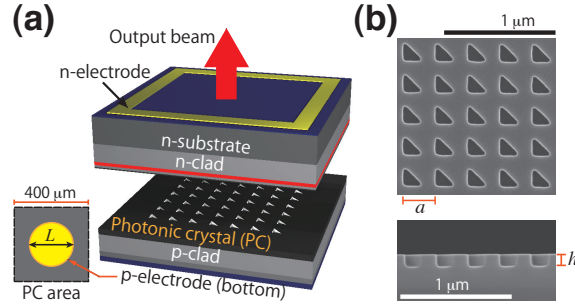


Figure 4.10: (a) Schematic structure of a PCSEL device. Lower left panel illustrates bottom side view of circular p-electrode with diameter L . (b) Scanning electron microscope (SEM) images (top and cross-sectional views) of fabricated PCs. Lattice constant $a = 295$ nm and air-hole depth $h = 108$ nm. Corners of the fabricated right-angled isosceles triangle (RIT)-shaped air holes are rounded and described in the text.

Figure 4.10(a) shows a schematic of the PCSEL, which was fabricated using a wafer bonding technique [34, 46]. The vertical multilayer structure is the same as that previously described [86]. The embedded PC has a square patterned area of $400\ \mu\text{m} \times 400\ \mu\text{m}$. Fig. 4.10(b) presents SEM images of a portion of the fabricated square-lattice PCs. We adopted a right-angled isosceles triangle (RIT)-shaped air-hole design because its asymmetry is beneficial for efficient out-of-plane coupling [84]. The p-electrode at the bottom of the device is circular and its diameter is L (lower left inset). Since the p-electrode is located $\sim 2\ \mu\text{m}$ below the active layer, the active cavity area is approximately equal to the p-electrode area. In this work, on the same wafer we fabricated two samples, which have identical PC geometry (Fig. 4.10(b)) but different active cavity areas: $L = 200\ \mu\text{m}$ and $L = 150\ \mu\text{m}$. Note that even at $L = 150\ \mu\text{m}$ the active cavity area is seven times larger than those previously reported [34, 35, 46].

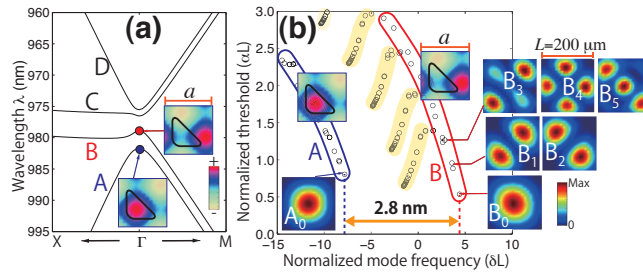


Figure 4.11: (a) Calculated TE-mode band structure. Insets show the H -field patterns (in color) of band-edge modes A and B , where triangles indicate air holes. (b) Mode spectra calculated for a finite-size PCSEL with $L = 200\ \mu\text{m}$. Band-edge modes A and B are grouped with blue and red circles, respectively; each group includes multiple resonant states with different field intensity envelopes (e.g., insets labeled as A_0 , B_0 , and B_1 - B_5). Additional modes between A and B (highlighted in yellow) are artifacts due to the numerical algorithm [63, 86].

Figure 5.4(a) shows the calculated band structure using the three-dimensional coupled-wave theory by assuming a periodic boundary condition [84, 87]. In the calculation, we used the experimental parameters shown in Fig. 4.10(b). The experimental air-hole shape takes the form of a RIT with rounded corners. The curvature of the 45° and 90° corners are found to be accurately described by circles with radii of 18 nm and 27 nm, respectively. The length of the short side of the RIT obtained by drawing a tangential line to the outer edges of each pair of circles is 185 nm. From Fig. 5.4(a), we see four band-edge modes A - D exist in the vicinity of the second-order Γ point, in order of decreasing wavelength. We are especially interested in band-edge modes A and B with lower frequency (insets: H -field patterns within one unit cell), because they are more favorable for lasing due to their less radiative nature.[84] To understand the threshold behavior of modes A and B within the *finite-size* laser cavity, we present in Fig. 5.4(b) the calculated mode spectra [86] (normalized threshold gain αL versus normalized mode frequency δL) for $L = 200 \mu\text{m}$. For simplicity, we have neglected the material absorption loss and assumed square cavity area with a side length of L .

In Fig. 5.4(b) we identified band-edge modes A and B (blue and red circles) by examining their relative spectral positions and field patterns as described previously [63, 86]. Note that, in contrast to the infinitely periodic structure where only one band-edge mode A or B exists, a group of multiple resonant states exist for each mode due to the quantized wave vector within a finite-size laser cavity [65, 67]. The multiple resonant states are characterized by different field intensity envelopes. For example, modes B_0 - B_5 shown in the insets of Fig. 5.4(b) all have the same H -field pattern within a unit cell but different field intensity envelopes. The mode that has only one antinode is called fundamental mode B_0 , and modes that have multiple antinodes are called high-order modes B_1 - B_5 , in order of increasing wavelength. Similar denotation also applies to mode A ; fundamental mode A_0 is shown in the inset. The mode (wavelength) spacing between modes A_0 and B_0 is 2.8 nm, in correspondence with that of the infinitely periodic structure (Fig. 5.4(a)). Since the lasing action is onset at the mode with the lowest threshold gain (α_{th}), Fig. 5.4(b) indicates that mode B_0 ($\alpha_{\text{th}}=26.9 \text{ cm}^{-1}$) will be the first mode to reach the threshold. The second and third lowest-threshold modes are A_0 and B_1 with $\alpha_{\text{th}}=40.3 \text{ cm}^{-1}$ and $\alpha_{\text{th}}=44.7 \text{ cm}^{-1}$, respectively. Note that the additional modes between A and B (highlighted in yellow) are artifacts resulting from our numerical algorithm based on finite-difference method [63, 86] and, hence, are not considered for lasing.

Figure 3(a) shows the measured surface-emission spectra of the $L = 200 \mu\text{m}$ sample under room temperature pulsed condition (1 kHz, 500 ns). The measurement was made in the surface-normal direction (corresponding to the Γ point) using a spectrometer with $\sim 0.045 \text{ nm}$ resolution. The threshold current I_{th} was 230 mA. Below threshold, band-edge modes A - D are apparent, as indicated in the lower panel of Fig. 4.12(a). The

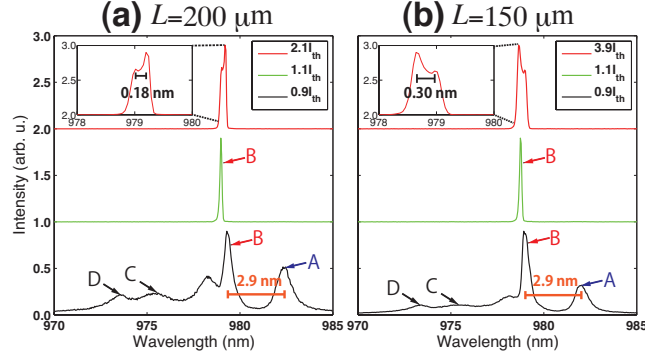


Figure 4.12: Surface-emission spectra measured at three different current levels for samples with (a) $L = 200 \mu\text{m}$ and (b) $L = 150 \mu\text{m}$. Spectrum measured at each current is normalized and shifted in vertical ordinate for clarity. Below threshold, four TE-mode resonant peaks (A - D) appeared with an additional TM-mode peak [46] between B and C (lower panels). Just above threshold, both samples exhibited single-mode operation at mode B (middle panels). Far above threshold, however, multimode lasing was observed (upper panels). The insets show the enlarged spectra of the multimode lasing.

mode spacing between modes A and B was 2.9 nm and closely matches the calculated spacing (2.8 nm) between modes A_0 and B_0 (Fig. 5.4(b)). When above-threshold current $1.1I_{\text{th}}$ was injected, single-mode lasing was observed at mode B , corresponding to lowest-threshold mode B_0 in Fig. 5.4(b). Therefore, resonant peaks A and B in the lower panel of Fig. 4.12(a) correspond to modes A_0 and B_0 , respectively. The single-mode operation was maintained up to a current level as high as $\sim 2.0I_{\text{th}}$. However, at a higher current around $I = 2.1I_{\text{th}}$, a competing mode at the longer wavelength side also began to lase. The mode spacing between this competing mode and the main mode was 0.18 nm. In Fig. 4.12(b) we show similar measurements performed for the $L = 150 \mu\text{m}$ sample. This sample exhibited similar behavior as the $L = 200 \mu\text{m}$ case; single-mode operation initially occurred at band-edge mode B , and a competing mode was excited at the longer wavelength side of the main lasing mode at a higher current level. In the sub-threshold spontaneous emission spectrum, the mode spacing between resonant peaks A and B (2.9 nm) did not change while the cavity length decreased. However, when compared in more detail to the $L = 200 \mu\text{m}$ device, we note that the competing mode of the $L = 150 \mu\text{m}$ device had relatively larger mode spacing (0.30 nm) with the main lasing mode and was onset at a higher current level ($3.9I_{\text{th}}$ with $I_{\text{th}} = 185 \text{ mA}$).

From the calculated mode spectra in Fig. 5.4(b), we note that the third lowest-threshold mode B_1 is located at the longer wavelength side of B_0 (i.e., the observed lasing mode) with fairly narrow wavelength spacing. Therefore, we predict that the competing side mode observed above threshold stems from B_1 (and/or B_2 considering the fabrication imperfection and disorders). To examine our prediction, in Fig. 4.13(a) we calculated the resonant wavelength of modes B_1 and B_0 as a function of L (for simplicity, hereafter

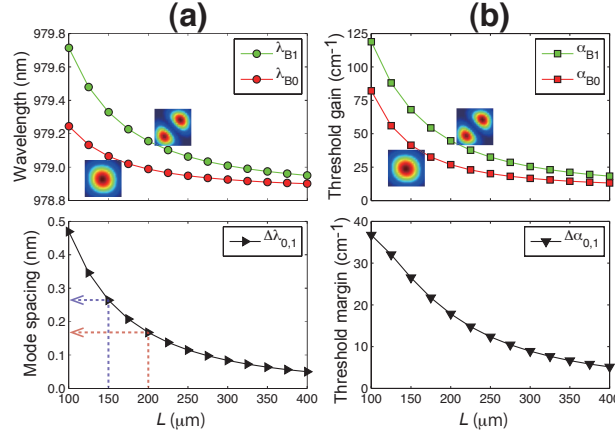


Figure 4.13: Calculated (a) wavelength and (b) threshold gain of modes B_1 and B_0 versus L . Mode spacing ($\Delta\lambda_{0,1}$) and threshold margin ($\Delta\alpha_{0,1}$) of these two modes are shown in the lower panels. Dashed lines in the lower panel of (a) indicate that, $\Delta\lambda_{0,1}=0.17$ nm at $L = 200$ μm and $\Delta\lambda_{0,1}=0.26$ nm at $L = 150$ μm , in good agreement with the mode spacings shown in the upper panels of Fig. 4.12.

our discussion focuses on B_1 because B_2 shows almost the same behavior). The mode spacing between these two modes ($\Delta\lambda_{0,1}$) is shown in the lower panel. We can clearly see that the resonant wavelength of each mode and $\Delta\lambda_{0,1}$ decrease with increasing L . In particular, at $L = 200$ μm and $L = 150$ μm , $\Delta\lambda_{0,1}$ equals 0.17 nm and 0.26 nm (dashed lines), respectively. This closely matches the measured mode spacings (upper panels in Fig. 4.12). This result therefore suggests that the multimode lasing observed in our experiments originates from high-order mode B_1 (and/or B_2). Figure 4.13(b) presents the calculated threshold gain (α) dependence on L . The threshold gains of modes B_0 and B_1 and their threshold margin (difference) $\Delta\alpha_{0,1}$ steadily decrease when L is increased. $\Delta\alpha_{0,1}$ equals 26.5 cm^{-1} at $L = 150$ μm and decreases to 17.8 cm^{-1} at $L = 200$ μm . Since $\Delta\alpha_{0,1}$ determines the suppression of the competing mode B_1 and hence, single-mode operation, the smaller $\Delta\alpha_{0,1}$ at $L = 200$ μm explains why the $L = 200$ μm laser more easily encounters multimode lasing than the $L = 150$ μm case (Fig. 4.12).

It is important to note that, although the calculated threshold gain of mode A_0 is lower than that of mode B_1 (Fig. 5.4(b)), we did not observe any mode competition originating from A_0 above the threshold. We attribute this to the spatial hole burning (SHB) effect [91], which can be understood as follows. When the laser initially operates at fundamental mode B_0 , most of the photons are confined near the cavity center (Fig. 5.4(b)). Consequently, the carrier density near the center is depleted due to the stimulated recombination and the local optical gain at the center is reduced. This modified spatial gain overlaps more effectively with high-order mode B_1 than fundamental mode

A_0 (Fig. 5.4(b)), reducing the effective threshold gain of B_1 and threshold margin $\Delta\alpha_{0,1}$ [110].

Rigorous analysis of the above-described SHB effect involves complex laser dynamics [94] and will be presented elsewhere. However, a simple but useful evaluation can be made by considering an F factor that quantifies the flatness of the mode intensity distribution at threshold [91, 94]. To evaluate the mode intensity flatness in PCSELs, we extend the definition of F factor for DFB lasers [91] as follows:

$$F = \iint_{\text{cavity}} (P(x, y) - 1)^2 / L^2 dx dy, \quad (4.30)$$

where mode intensity distribution $P(x, y)$ is normalized as $\iint_{\text{cavity}} P(x, y) / L^2 dx dy = 1$ and the laser cavity covers an area of $0 \leq x, y \leq L$. Figure 4.14 presents the calculated F as a function of L and $\kappa_{1D}L$. A minimum value (~ 0.02) of F was obtained around $L = 40 \mu\text{m}$ ($\kappa_{1D}L = 1.6$). However, F increased remarkably with increasing L : $F = 0.6$ at $L = 150 \mu\text{m}$ ($\kappa_{1D}L = 6.1$) and $F = 0.8$ at $L = 200 \mu\text{m}$ ($\kappa_{1D}L = 8.1$). At these large F values, highly inhomogeneous $P(x, y)$ was observed (insets). Note that the calculated F values at $L = 150 \mu\text{m}$ and $L = 200 \mu\text{m}$ are comparable to those (~ 0.8) reported for strongly-coupled quarter-wave-shifted DFB lasers ($\kappa L = 3.6$), in which SHB induced multimode lasing [91].

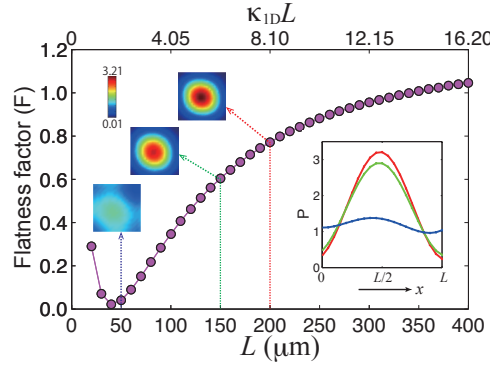


Figure 4.14: (a) Calculated flatness (F) factor of mode B_0 versus L (lower axis) and $\kappa_{1D}L$ (upper axis). $\kappa_{1D} = 405 \text{ cm}^{-1}$. Small F features flat intensity distribution $P(x, y)$. Upper-left insets show normalized $P(x, y)$ at different L s: $50 \mu\text{m}$, $150 \mu\text{m}$, and $200 \mu\text{m}$ (dashed arrows). Cross-sectional plots of P (which includes the peak intensity) at these L s are shown in the bottom-right inset. The slightly asymmetric distribution of P is due to asymmetry of the RIT air holes.

We therefore conclude that SHB's influence on mode stability in our lasers is critical. To achieve stable single-mode operation at a higher current level, PCSELs must be designed to have both a large threshold margin $\Delta\alpha_{0,1}$ and a small F factor. Vertically

asymmetric air-hole geometry with a smaller filling fraction, which provides weaker in-plane confinement but features larger out-of-plane coupling, might be a good candidate [85]. Furthermore, a double-hole unit cell is favorable for reducing κ_{1D} and obtaining uniform mode intensity distribution [52]. We believe that designing such unit cells with a reduced κ_{1D} but a moderate κ_{2D} would be a promising approach. Lastly, extending structures such as chirped gratings [109, 111], multiple-phase-shift gratings [92], and nonuniform pumping [110] that were proposed for suppressing SHB in DFB lasers may be feasible. To explain the above experimental results, we will develop an above-threshold theory in Chapter 6.

4.4 Summary

In this chapter, we developed a CWT model for finite-size square-lattice PCSELs with TE polarization by extending the 3D CWT framework presented in the previous chapter. Using this model, we calculated various properties of 2D PCSELs, including threshold gain, mode frequency, field intensity envelope within the device, and the profile of the output beam (far-field pattern and polarization), threshold dependence on cavity length. The theoretical predictions of the lowest threshold mode and the output beam profile, as well as the mode selectivity dependence on cavity length, showed good agreement with our experimental findings, thereby affirming the validity of our analyses. In the final section, we further investigate the mode stability in large-area PCSEL cavities towards designing single-mode high-power PCSELs.

Our finite-size analysis results demonstrate that finite device length indeed strongly influences surface emission and mode selection properties of the PCSEL device. Phenomena that cannot be explained by the infinite CWT analysis are clarified by considering the finite-size effects of the device. We showed that the finite device length may lead to a small shift of the electromagnetic field with respect to the air holes. This slightly shifted field suppresses the otherwise perfect destructive interference and thus enhances surface emission from the regions away from the center of the cavity, which accounts for the finite surface radiation loss emitted from the non-radiative (antisymmetric) mode of the CC air holes. By investigating the cavity length dependence of threshold gain, we find that, the mode selectivity is very sensitive to the cavity length L . At a very large L regime (e.g. $L > 200 \mu\text{m}$), the finite-size analysis results become asymptotic to the infinite solutions, and therefore the mode with the smallest radiation constant will be selected for lasing. In contrast, at a relatively small L (e.g. $L < 100 \mu\text{m}$), the predicted lasing mode obtained using the finite-size analysis may be quite different from the infinite solutions. This mode selection mechanism is attributed to the in-plane loss,

which can be noticeably large at short device lengths. The mode selectivity behavior controlled by L was clearly demonstrated by our experiments.

The mode stability in PCSELs with a large-area ($L > 150 \mu\text{m}$ or $\kappa_{1D}L > 6$) was studied, and mode competition was observed at high current levels above threshold. Competing modes are found to be in close correspondence with the high-order band-edge modes manifested by our theoretical analysis. We also found that the threshold margin ($\Delta\alpha$) between the main lasing mode and the competing high-order modes, which determines the single-mode stability, steadily decreases with increasing cavity length; these findings well explained our experimental observations. Multimode lasing observed above threshold suggested the influence of spatial hole burning (SHB), which results from highly inhomogeneous mode intensity distribution. To achieve stable single-mode operation far above threshold, PC structures with both a large $\Delta\alpha$ and a reduced SHB must be considered. This issue and design strategy will be discussed in detail in Chapter 6 by incorporating the SHB effects into the 3D CWT.

Chapter 5

Extended analysis of a generalized photonic-crystal geometry

5.1 Introduction

In the previous chapters, we have demonstrated the accuracy and efficiency of our developed 3D CWT model by comparing its analysis results with FDTD and experimental results. Nevertheless, from the viewpoint of PC geometry that can be treated, there are still several limitations in our current theory. First, we have focused our analyses on the square-lattice PCs [84, 86]. Second, while our theory is able to treat air-holes of any arbitrary shape in the PC plane, the sidewalls of the air holes have been assumed to be uniform within the PC layer. In order to further exploit the design freedom of PCSELs, it is important to investigate different crystal geometries. For example, in the earlier PCSEL works, the triangular lattice has been widely studied [27, 28, 30, 31]. This lattice structure has six-fold rotational symmetry and is expected to have stronger two-dimensional couplings [63, 70]. More recently, with the advances of PCSEL fabrication technology, metal organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) have been adopted to fabricate PCSELs [50, 54]. In these fabrication processes, the developed PC air holes are usually nonuniform in the vertical direction. It is important to develop a theoretical model to treat these more complicated PC geometries. In this chapter, we first extend the 3D CWT frameworks [84, 86] to develop a coupled-wave model for triangular-lattice PCSELs. Various modal properties of interest, including the band structure, radiation constant, threshold gain, field intensity envelope profile, and far-field pattern (FFP). The calculated results of the band structure and FFP of the predicted lasing mode are compared with experimental data to validate our theory. Next, we further extend the CWT model to investigate effects

of the vertical sidewalls on the laser properties of PCSELs including radiation constant and FFP, etc.

5.2 Extension to triangular lattice

In this section, three-dimensional coupled-wave theory is extended to model triangular-lattice photonic-crystal surface-emitting lasers with transverse-electric polarization. A generalized coupled-wave equation is derived to describe the sixfold symmetry of the eigenmodes in a triangular lattice. The extended theory includes the effects of both surface radiation and in-plane losses in a finite-size laser structure. Modal properties of interest including the band structure, radiation constant, threshold gain, field intensity profile, and far-field pattern (FFP) are calculated. The calculated band structure and FFP, as well as the predicted lasing mode, are compared with experimental results. The effect of air-hole size on mode selection is also studied and confirmed by experiment.

5.2.1 Generalized formulas

5.2.1.1 Derivation of 3D couple-wave equations for triangular lattice

A schematic of the PCSEL device investigated in this chapter is shown in Fig. 5.1(a). The PC layer is embedded inside a multilayer structure that is assumed to support only a single fundamental guided mode. Details of the device are described in [46, 86]. The average refractive index of the PC layer is given by $n_{av} = \sqrt{fn_a^2 + (1-f)n_b^2}$, where n_a is the refractive index of air, n_b is the refractive index of the background dielectric material (GaAs), and f is the air-hole filling factor (i.e., the fraction of the area of a unit cell occupied by air holes). For circular-shape air holes, $f = (2\pi/\sqrt{3})r^2/a^2$, where r is the hole radius and a is the lattice constant. A typical band structure calculated by the 2D plane-wave expansion method [31] is shown in Fig. 5.1(b). We are particularly interested in the band-edge modes in the vicinity of the second-order Γ point (red circle), where the group velocity of light becomes zero. At these band edges, the PC lattice serves both to provide the 2D distributed feedback and to couple the in-plane guided waves into the surface normal to construct the output.

Figure 5.2(a) shows a schematic of a triangular-lattice PC. The primitive translation vectors of the triangular lattice, $\mathbf{a}_1$ and $\mathbf{a}_2$, can be expressed as

$$\mathbf{a}_1 = (\sqrt{3}a/2, -a/2), \quad \mathbf{a}_2 = (\sqrt{3}a/2, a/2). \quad (5.1)$$

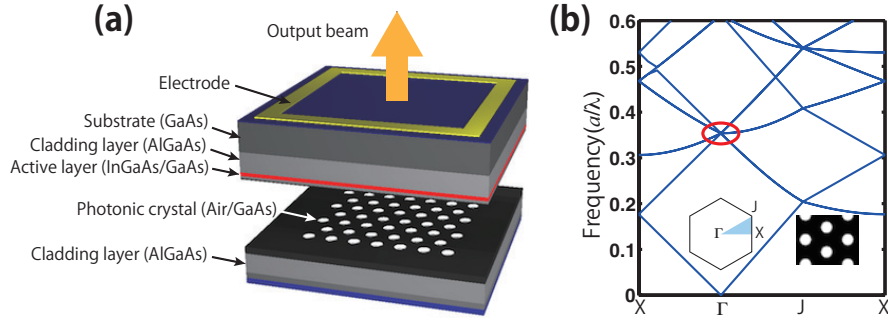


Figure 5.1: (a) Schematic structure of a photonic-crystal surface-emitting laser device with a triangular lattice. (b) Band structure of triangular-lattice PCs calculated by the 2D plane-wave expansion method for transverse-electric (TE) mode [31]. The red circle indicates the second-order Γ point. The inset shows the high-symmetry points at the corners of the irreducible Brillouin zone (shaded light blue).

Then, the corresponding reciprocal lattice vector shown in Fig. 5.2(b) is given by

$$\mathbf{G}_{mn} = m\mathbf{b}_1 + n\mathbf{b}_2 = \frac{m+n}{2}\beta_0\hat{x} + \frac{\sqrt{3}(n-m)}{2}\beta_0\hat{y} \equiv m_{0x}(m,n)\beta_0\hat{x} + n_{0y}(m,n)\beta_0\hat{y}, \quad (5.2)$$

where the primitive reciprocal lattice vectors are $\mathbf{b}_1 = (\beta_0/2, -\sqrt{3}\beta_0/2)$ and $\mathbf{b}_2 = (\beta_0/2, \sqrt{3}\beta_0/2)$, $\beta_0 = 4\pi/\sqrt{3}a$, and m and n are integers.

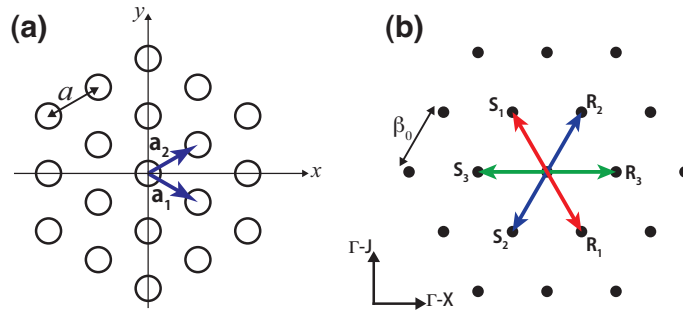


Figure 5.2: (a) Schematic of a triangular-lattice PC in real space. The blue arrows denote the primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and a is the lattice constant. (b) Reciprocal lattice space of a triangular-lattice PC. The colored arrows indicate the six basic waves: R_1 , S_1 , R_2 , S_2 , R_3 , and S_3 at the second-order Γ point, whose wavenumber is equal to $\beta_0 = 4\pi/\sqrt{3}a$.

Light propagating inside a PC must obey Bloch's theorem, and the Bloch wave state $u(\mathbf{r})$ can be expressed as

$$u(\mathbf{r}) = \sum_{\mathbf{G}_{mn}} a_{mn}(z) e^{-i(\Delta\mathbf{k} + \mathbf{G}_{mn}) \cdot \mathbf{r}}, \quad (5.3)$$

where a_{mn} represents the field amplitude of a wave of the order of (m, n) and $\Delta \mathbf{k} = \Delta_x \beta_0 \hat{x} + \Delta_y \beta_0 \hat{y}$ represents the wavenumber deviation from the Γ point [87]. Specifically, in the vicinity of the second-order Γ point ($\Delta \mathbf{k} \simeq 0$), only the field amplitudes of the waves with $|\mathbf{G}_{mn}| = \beta_0$ are dominant [31, 84, 87]. We refer to these waves as basic waves: R_1, S_1, R_2, S_2, R_3 , and S_3 , as illustrated in Fig. 5.2(b).

By following Refs. [84, 86, 87], we seek solutions to

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) = k_0^2 \tilde{n}^2(\mathbf{r}) \mathbf{E}(\mathbf{r}), \quad (5.4)$$

where the time dependence of the electric field $\mathbf{E}(\mathbf{r})$ is $e^{i\omega t}$, $k_0 (= \omega/c)$ is the free-space wavenumber, ω is the angular frequency, c is the velocity of light in free space, and $\tilde{n}$ is the refractive index (a complex number) satisfying $k_0^2 \tilde{n}^2(\mathbf{r}) \simeq k_0^2 n^2(\mathbf{r}) + 2ik_0 n_0(z) \tilde{\alpha}(z)$ [86]; $n_0(z)$ represents the average refractive index of the material at position z , and $\tilde{\alpha}(z)$ represents the gain ($\tilde{\alpha} > 0$) or loss ($\tilde{\alpha} < 0$) in each region. For TE polarization, the electric field can be assumed as $(E_x, E_y, 0)$ and expanded as

$$E_j(z) = \sum_{m,n} E_{j,m,n}(z) e^{-im_{x,mn}\beta_0 x - in_{y,mn}\beta_0 y}, \quad j = x, y, \quad (5.5)$$

where $m_{x,mn} \equiv m_{0x}(m, n) + \Delta_x$ and $n_{y,mn} = n_{0y}(m, n) + \Delta_y$. Similarly, the periodic function of $n^2(\mathbf{r})$ can be expanded as

$$n^2(\mathbf{r}) = n_0^2(z) + \sum_{m \neq 0, n \neq 0} \xi_{m,n}(z) e^{-im_{0x}\beta_0 x - in_{0y}\beta_0 y}, \quad (5.6)$$

where $\xi_{m,n}(z) = 0$ outside the PC layer, and air holes within the PC region are assumed to have perfectly vertical sidewalls [85]; thus, $n_0^2(z)$ and $\xi_{m,n}$ are constant within every region.

By substituting Eqs. (5.6) and (5.5) into Eq. (5.4) and collecting all terms that are multiplied by the factor $e^{-im_{x,mn}\beta_0 x - in_{y,mn}\beta_0 y}$, we obtain

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) + 2ik_0 n_0(z) \tilde{\alpha}(z) - n_y^2 \beta_0^2 \right] E_{x,m,n} + m_x n_y \beta_0^2 E_{y,m,n} - 2in_y \beta_0 \frac{\partial E_{x,m,n}}{\partial y} + i\beta_0 \left(m_x \frac{\partial E_{y,m,n}}{\partial y} + n_y \frac{\partial E_{y,m,n}}{\partial x} \right) = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{x,m',n'}, \quad (5.7)$$

$$\left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2(z) + 2ik_0 n_0(z) \tilde{\alpha}(z) - m_x^2 \beta_0^2 \right] E_{y,m,n} + m_x n_y \beta_0^2 E_{x,m,n} - 2im_x \beta_0 \frac{\partial E_{y,m,n}}{\partial x} + i\beta_0 \left(m_x \frac{\partial E_{x,m,n}}{\partial y} + n_y \frac{\partial E_{x,m,n}}{\partial x} \right) = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} E_{y,m',n'}, \quad (5.8)$$

$$\frac{\partial}{\partial z} \left[\frac{\partial E_{x,m,n}}{\partial x} + \frac{\partial E_{y,m,n}}{\partial y} - i\beta_0 (m_x E_{x,m,n} + n_y E_{y,m,n}) \right] = 0. \quad (5.9)$$

Here, we have neglected the second-order spatial derivatives [86].

By introducing a proper linear combination of $E_{x,m,n}(z)$ and $E_{y,m,n}(z)$, i.e., $(n_y E_{x,m,n} - m_x E_{y,m,n})$ as described in [84, 87], we obtain

$$\begin{aligned} & \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 + 2ik_0 n_0(z) \tilde{\alpha}(z) - (m_x^2 + n_y^2) \beta_0^2 \right] (n_y E_{x,m,n} - m_x E_{y,m,n}) \\ & + i\beta_0 \left[m_x n_y \frac{\partial E_{y,m,n}}{\partial y} - (m_x^2 + 2n_y^2) \frac{\partial E_{x,m,n}}{\partial y} \right] + i\beta_0 \left[-m_x n_y \frac{\partial E_{x,m,n}}{\partial x} + (n_y^2 + 2m_x^2) \frac{\partial E_{y,m,n}}{\partial x} \right] \\ & = -k_0^2 \sum_{m' \neq m, n' \neq n} \xi_{m-m', n-n'} (n_y E_{x,m',n'} - m_x E_{y,m',n'}). \end{aligned} \quad (5.10)$$

We are interested in the modes in the vicinity of the second-order Γ point, for which $\Delta_x, \Delta_y \ll 1$. We assume that all of the six basic waves have an identical vertical field profile $\Theta_0(z)$ [87], which satisfies

$$\frac{\partial^2 \Theta_0}{\partial z^2} + [k_0^2 n_0^2 - \beta^2] \Theta_0(z) = 0, \quad (5.11)$$

where the propagation constant β ($\beta \simeq \beta_0$) and the vertical field profile $\Theta_0(z)$ can be calculated by employing the transfer matrix method (TMM) [84], and Θ_0 is normalized as $\int_{-\infty}^{\infty} \Theta_0(z) \Theta_0^*(z) dz = 1$. We further assume that basic waves are transverse waves. Thus, for basic waves, we can express the $E_{x,m,n}$ and $E_{y,m,n}$ as

$$E_{x,m,n} = \rho_{mn} A_{m,n}(x, y) \Theta_0(z), \quad E_{y,m,n} = \eta_{mn} A_{m,n}(x, y) \Theta_0(z), \quad (5.12)$$

with

$$\rho_{mn} = \frac{n_{y,mn}}{\sqrt{m_{x,mn}^2 + n_{y,mn}^2}}, \quad \eta_{mn} = -\frac{m_{x,mn}}{\sqrt{m_{x,mn}^2 + n_{y,mn}^2}}, \quad (5.13)$$

where $(m, n) \in \{(1, 0), (-1, 0), (0, 1), (0, -1), (1, 1), (-1, -1)\}$ which correspond, in order, to $\{R_1, S_1, R_2, S_2, R_3, S_3\}$ for $A_{m,n}(x, y)$, as shown in Fig. 5.2(b); ρ_{mn} and η_{mn} denote the perturbation of the basic waves' polarizations [87]. By substituting Eqs. (5.12) and (5.13) in Eq. (5.10), we obtain

$$\begin{aligned} & \left[\frac{\partial^2}{\partial z^2} + k_0^2 n_0^2 + 2ik_0 n_0(z) \tilde{\alpha}(z) - (m_x^2 + n_y^2) \beta_0^2 \right] A_{m,n} \Theta_0(z) - 2i\beta_0 \left(m_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} \right) A_{m,n} \Theta_0(z) \\ & = -k_0^2 \sum_{m', n'} \xi_{m-m', n-n'} (\rho_{mn} E_{x,m',n'} + \eta_{mn} E_{y,m',n'}). \end{aligned} \quad (5.14)$$

By substituting Eq. (5.11) in Eq. (5.14), multiplying $\Theta_0^*(z)$ on both sides, and integrating over $(-\infty, \infty)$, we obtain a coupled-wave equation of the following form:

$$\begin{aligned} & \left[\delta + i\alpha + (1 - \sqrt{m_x^2 + n_y^2})\beta_0 \right] A_{m,n} - i \left(m_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} \right) A_{m,n} \\ &= \sum_{|r^2+s^2|=1; r \neq m, s \neq n} \kappa_{mn}^{(rs)} A_{r,s} \\ & - \frac{k_0^2}{2\beta_0} \sum_{|m'^2+n'^2| \neq 1} \xi_{m-m', n-n'} \int_{PC} (\rho_{mn} E_{x,m',n'} + \eta_{mn} E_{y,m',n'}) \Theta_0^*(z) dz, \end{aligned} \quad (5.15)$$

where

$$\kappa_{mn}^{(rs)} = -\frac{k_0^2}{2\beta_0} \int_{PC} \xi_{m-r, n-s} (\rho_{mn} \rho_{rs} + \eta_{mn} \eta_{rs}) |\Theta_0(z)|^2 dz \quad (5.16)$$

represents direct couplings between basic waves, $\delta = \beta - \beta_0 = n_{eff}\omega/c - \beta_0$ is the deviation from the Bragg condition, n_{eff} is the effective refractive index for the fundamental guided mode, α is the modal loss defined by $\alpha = \frac{k_0}{\beta_0} \int_{-\infty}^{\infty} n_0(z) \tilde{\alpha}(z) |\Theta_0(z)|^2 dz$. Note that the integrals in Eqs. (5.15) and (5.16) extend only over the PC region because $\xi_{m,n} = 0$ outside that range. The field profiles [i.e., $E_{x,m',n'}(z)$ and $E_{y,m',n'}(z)$] of radiative ($m' = n' = 0$) and high-order ($|m'^2 + n'^2| > 1$) waves can be expressed in terms of basic waves as described in Appendix B.

The 3D coupled-wave Eq. (5.15) derived above includes both the in-plane high-order coupling and vertical diffraction effects, neither of which was included or appropriately described in the previous 2D CWT models for triangular-lattice PCSELs [33, 63, 64]. It is important to note that, Eq. (5.15) is a very general formula capable of treating any type of centered-rectangular lattice [44] by replacing the basic waves terms. Furthermore, the derivative terms of the basic waves, which are crucial factors for treating the finite-size laser structures but not considered in the previous 3D CWT model for centered-rectangular lattices [87], are now included.

5.2.1.2 Staggered-grid finite-difference method on hexagonal grids

The coupled-wave equation for finite systems can be solved by using a staggered-grid finite-difference method. We rewrite the coupled-wave Eq. (5.15) for the band-edge

modes (for which $\Delta_x = \Delta_y = 0$) in the following form:

$$(\delta + i\alpha) \begin{bmatrix} R_1 \\ S_1 \\ R_2 \\ S_2 \\ R_3 \\ S_3 \end{bmatrix} = [\mathbf{C}] \begin{bmatrix} R_1 \\ S_1 \\ R_2 \\ S_2 \\ R_3 \\ S_3 \end{bmatrix} + i \begin{bmatrix} \frac{1}{2} \frac{\partial R_1}{\partial x} - \frac{\sqrt{3}}{2} \frac{\partial R_1}{\partial y} \\ -\frac{1}{2} \frac{\partial S_1}{\partial x} + \frac{\sqrt{3}}{2} \frac{\partial S_1}{\partial y} \\ \frac{1}{2} \frac{\partial R_2}{\partial x} + \frac{\sqrt{3}}{2} \frac{\partial R_2}{\partial y} \\ -\frac{1}{2} \frac{\partial S_2}{\partial x} - \frac{\sqrt{3}}{2} \frac{\partial S_2}{\partial y} \\ \frac{\partial R_3}{\partial x} \\ -\frac{\partial S_3}{\partial x} \end{bmatrix}, \quad (5.17)$$

where $\mathbf{C}$ is a 6×6 matrix composed of coupling coefficients defined by Eqs. (B7)–(B11) in Appendix B.

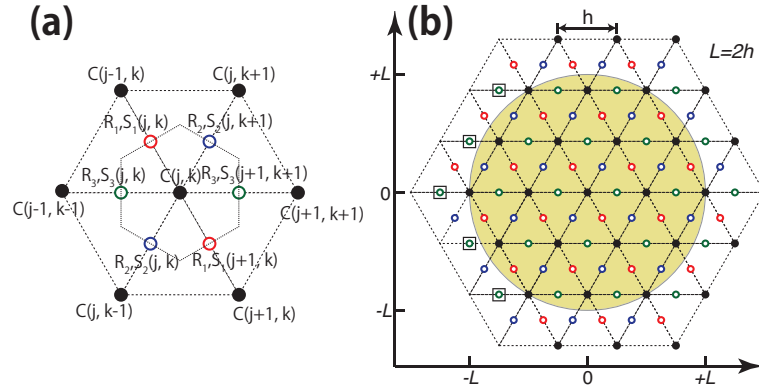


Figure 5.3: (a) Location of field components (basic waves) and coupling coefficients in the vicinity of the (j, k) th hexagonal cell of the grid. Positions of the unknown field components (colored hollow dots) are staggered from the positions of the known coupling coefficients (solid dots). The colored hollow dots correspond to the points that are updated using the finite-difference scheme, while the solid points are points that are not solved. (b) Schematic of a circular computational domain (yellow shaded region) discretized on the hexagonal grids with $L = 2h$ (L is the radius of the circular shape and h is the distance between two adjacent grid points). The green hollow dots inside the black squares indicate the boundary of R_3 ; these are set to be zero in the calculations.

To model a triangular-lattice PC having a sixfold symmetry, we discretize the computational domain on a hexagonal grid (see, e.g., Sec. 3.7.2 of Ref. [83]). The location of the six basic-wave components and the coupling coefficients in the vicinity of the (j, k) th

hexagonal cell of the grid is illustrated in Fig. 5.3(a). Then, Eq. (5.17) becomes

$$\frac{1}{2}(\delta + i\alpha) \begin{bmatrix} R_1^{j+1,k} + R_1^{j,k} \\ S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} + R_2^{j,k} \\ S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} + R_3^{j,k} \\ S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix} = \frac{1}{2}[\mathbf{C}] \begin{bmatrix} R_1^{j+1,k} + R_1^{j,k} \\ S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} + R_2^{j,k} \\ S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} + R_3^{j,k} \\ S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix} + i\frac{1}{h} \begin{bmatrix} R_1^{j+1,k} - R_1^{j,k} \\ -S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} - R_2^{j,k} \\ -S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} - R_3^{j,k} \\ -S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix}, \quad (5.18)$$

where h is the distance between two adjacent grid points and the coupling coefficients C_{mn} ($1 \leq m, n \leq 6$) are assumed to be constant throughout the laser cavity. Figure 5.3(b) shows a schematic of the circular-shape computational domain (yellow shaded region) considered in this work. The computational domain physically corresponds to the gain region determined by the electrode geometry. Because the shape of the electrode at the bottom of the fabricated device is circular (see Ref. [44] for details), we consider a circular computational domain. We define the radius of the circular-shape gain region as $L = Nh$ (N : integer). Schematic depicted in Fig. 5.3(b) corresponds to the case when $N = 2$. By multiplying $2L$ on both sides of Eq. (6.24), we obtain

$$L(\delta + i\alpha) \begin{bmatrix} R_1^{j+1,k} + R_1^{j,k} \\ S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} + R_2^{j,k} \\ S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} + R_3^{j,k} \\ S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix} = L[\mathbf{C}] \begin{bmatrix} R_1^{j+1,k} + R_1^{j,k} \\ S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} + R_2^{j,k} \\ S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} + R_3^{j,k} \\ S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix} + i2N \begin{bmatrix} R_1^{j+1,k} - R_1^{j,k} \\ -S_1^{j+1,k} + S_1^{j,k} \\ R_2^{j,k+1} - R_2^{j,k} \\ -S_2^{j,k+1} + S_2^{j,k} \\ R_3^{j+1,k+1} - R_3^{j,k} \\ -S_3^{j+1,k+1} + S_3^{j,k} \end{bmatrix}, \quad (5.19)$$

which can be treated as a generalized eigenvalue problem with spatially dependent eigenvectors $(R_1^{j,k}, S_1^{j,k}, R_2^{j,k}, S_2^{j,k}, R_3^{j,k}, S_3^{j,k}, R_1^{j+1,k}, S_1^{j+1,k}, R_2^{j+1,k}, S_2^{j+1,k}, R_3^{j+1,k}, S_3^{j+1,k}, \dots)^t$ and normalized eigenvalues $(\delta + i\alpha)L$. In this work, we assume the following absorbing boundary condition: The field amplitude of the basic waves always starts from zero at the boundaries. This generalizes a similar concept for the 1D distributed feedback laser structure originally proposed by Kogelnik and Shank [65]. The boundary consists of the set of points lying immediately outside but closest to one half of the circular domain on the side opposite to the wave's propagation. As an example, the boundary of R_3 is indicated by black squares in Fig. 5.3(b). We investigated the impact of discretization on the solutions of Eq. (5.19) by varying N and confirmed that well-converged solutions can be obtained at $N = 7$ with a short calculation time (~ 1 minute with a personal computer).

5.2.2 Analysis results for triangular lattice

In this section, we present numerical results of the coupled-wave equations derived above. By solving the coupled-wave Eq. (5.15), we can obtain various properties of interest, including the band structure, radiation constant, threshold gain, field intensity envelope profile within the device, and FFPs. To validate our CWT analysis, we also compare some of the calculated results with experimental observations. Unless otherwise noted in the following examples, the lattice constant $a = 341$ nm, the air-hole shape is circular with air-hole filling factor $f = 0.15$ (corresponding to an r/a ratio of 0.20, where r is the air-hole radius), and the laser vertical structural parameters are described in Ref. [86].

5.2.2.1 Band structure and radiation constant

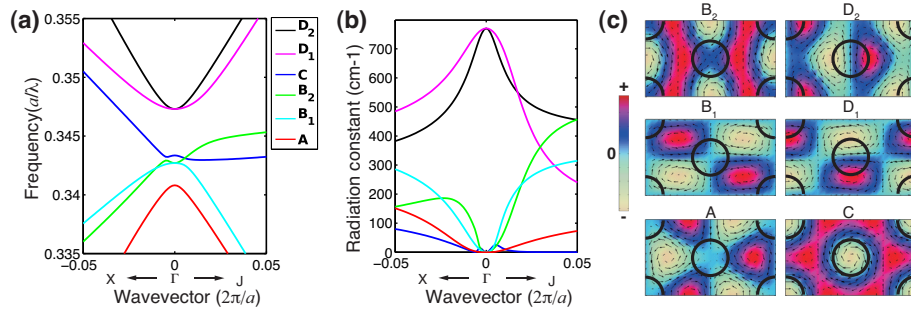


Figure 5.4: Calculated (a) band structure and (b) radiation constant of the eigenmodes in the vicinity of the second-order Γ point for a triangular-lattice PCSEL with circular air holes. Six modes near the Γ point are referred to as modes: A , B_1 , B_2 , C , D_1 , and D_2 , in the order of increasing frequency. Modes B_1 and B_2 , as well as D_1 and D_2 , are doubly degenerate at the Γ point. (c) E-field vector distribution (arrows) and H-field patterns (in color) of the individual band-edge modes. The black circles indicate the air holes. Band-edge modes A and C are known as hexapole and monopole modes, respectively [31]. In the calculations, the lattice constant $a = 341$ nm, and the air-hole filling factor $f = 0.15$.

By considering an infinitely periodic structure, that is, by neglecting the derivative terms in the coupled-wave Eq. (5.15), the band structure in the vicinity of the second-order Γ point can be obtained. The calculated band structure in the two characteristic directions of the triangular lattice (Γ - X and Γ - J directions) is shown in Fig. 5.4(a), where the six eigenmodes are referred to as A , B_1 , B_2 , C , D_1 , and D_2 , respectively, in the order of increasing frequency. The leakiness of these eigenmodes is quantified in terms of the radiation constant α_r ($\alpha_r = 2\alpha$: the modal power loss due to the surface emission) [84, 87]. Figure 5.4(b) shows the calculated radiation constant plotted against the in-plane wavevector. It can be seen from the figure that modes D_1 and D_2 lead to a substantial radiation loss at the band edge (i.e., at the Γ point), whereas modes A , B_1 ,

B_2 , and C are not leaky ($\alpha = 0$). This contrast is closely related with the symmetry of their field patterns with respect to the air holes. Figure 5.4(c) shows the calculated field patterns of the band-edge modes A – D_2 . We note that the electric fields of modes D_1 and D_2 are symmetric with respect to the air holes, and thus, they lead to significant loss. In contrast, the electric fields of modes A , B_1 , B_2 , and C are antisymmetric, leading to zero radiation loss [31, 84]. As a consequence, the antisymmetric (nonradiative) modes are favored for lasing. The lasing mode is determined, as described in the following section, by taking into account the total losses (both the surface emission and in-plane losses) in a finite-size laser structure.

A noteworthy fact is that as the in-plane wavevector is slightly detuned from the band edge, most of the antisymmetric modes start to become significantly more lossy, regardless of the directions, thereby ensuring that band-edge modes keep lasing stably. However, the only exception is mode C , which has a slow-group-velocity region in the Γ – J directions. (We refer to modes in this region as flat-band modes.) Because the radiation constant becomes noticeably small within this region, the flat-band modes may also participate in lasing mode competition. This type of mode competition was reported in Ref. [72], where a multiple-mode lasing action occurring at both the band edge and the flat-band modes in the Γ – J direction was observed.

5.2.2.2 Threshold gain and field intensity envelope

In this section, we solve the coupled-wave Eq. (5.15) in a finite-size system to evaluate the threshold gain of the eigenmodes. We discretize Eq. (5.15) by using the staggered-grid finite-difference method [86]. It is important to note here that, for the triangular-lattice PC configuration, it is crucial to both discretize the computational domain on a hexagonal grid [83] instead of the commonly used square grid and use appropriate boundary conditions (Section 5.2.1.2). We focus our analysis on the antisymmetric band-edge modes mentioned above (i.e., modes A , B_1 , B_2 , and C), which are most likely to be lasing modes. In the following calculations, we assume an absorbing boundary condition and the radius of the circular-shape computational region L is set to be $L = 30 \mu\text{m}$ (Section 5.2.1.2).

For finite-size structures, threshold gain and mode frequency correspond to the imaginary and real parts of the normalized eigenvalue, $(\delta + i\alpha)L$ [86]. As an example, we show in Fig. 5.5(a) a plot of the normalized threshold gain (αL) as a function of deviation from the Bragg condition (δL). Though a large number of modes are found to exist as a result of the numerical calculation, we identify the fundamental modes (indicated by arrows) using the techniques described in Refs. [63, 86]. We note that there exists

an additional mode that has a low threshold comparable to that of the fundamental band-edge modes. We refer to this mode as the W mode. The normalized threshold gains of the low-threshold modes indicated by arrows in Fig. 5.5(a) are listed in Table 5.1. As the lasing action occurs at the mode with the lowest threshold gain (loss), Table 5.1 indicates that mode C [indicated by red arrow in Fig. 5.5(a)] is favored for lasing with a large threshold-gain discrimination of over 20 cm^{-1} against the competing side modes (i.e., modes B_1 and B_2). This fact reveals that stable single-mode operation at mode C can be possibly achieved for triangular-lattice PCSELs.

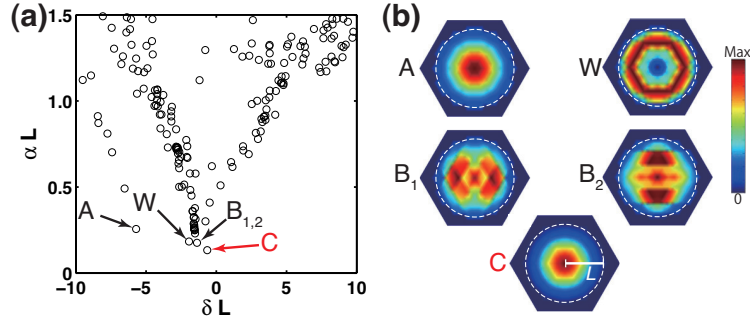


Figure 5.5: (a) Normalized threshold gain (αL) as a function of normalized mode frequency deviation (δL). The fundamental band-edge modes (A , B_1 , B_2 , and C) and an additional mode W are indicated by arrows. (b) Field intensity envelopes of the modes indicated by arrows in (a). The data are calculated by using the same parameters as specified in the caption of Fig. 5.4. Note that the field intensity envelopes are plotted on hexagonal grids with a circular-shape computational domain (dashed circle). The radius of the circular domain, $L = 30 \text{ }\mu\text{m}$, is discretized to span seven grid cells for which the eigenvalues converge well.

Table 5.1: Normalized threshold gain (αL) of the low-threshold modes indicated by arrows in Fig. 5.5(a).

Mode	A	W	$B_{1,2}$	C
αL	0.256	0.184	0.176	0.133

To gain insight into the nature of the modes indicated in Fig. 5.5(a), it is useful to examine their field intensity envelopes throughout the entire laser cavity. The slowly-varying envelope profile (function) modulates the fast-varying Bloch waves in the PC lattice and can be determined by [63, 86]

$$I(x, y) = \sum_{k=1}^3 |R_k(x, y)|^2 + |S_k(x, y)|^2. \quad (5.20)$$

Figure 5.5(b) shows the field intensity envelopes of the individual modes. We note that energy of the fundamental band-edge modes (A , B_1 , B_2 , and C) is relatively confined to the central part of the laser cavity, whereas mode W exhibits a null intensity in the

center. The exact physical interpretation of the origin of mode W is not yet clear. From the character of the doughnut-shape intensity envelope, we suggest that mode W might be a whispering-gallery-like mode that was discussed in Ref. [38]. We also note that the threshold-gain discrimination between the individual modes, otherwise equal to zero in infinitely periodic structures, may result from the differences in their in-plane losses [86]. A closer examination of the field intensities [Fig. 5.5(b)] distributed at the boundary (dashed circle) of the laser cavity reveals that the lowest-threshold mode C possesses the smallest amount of energy that escapes from the boundary (i.e., the in-plane losses). In contrast, mode A exhibits a much higher threshold because of the relatively larger in-plane losses. This intuitive explanation is confirmed by a quantitative study of the in-plane losses based on the formula derived in Ref. [86]. We find that, for the laser structure specified in Fig. 5.5, the in-plane losses dominate the threshold and that the in-plane losses of mode A are a factor of 2.7 larger than those of mode C .

5.2.2.3 Comparison of band structures and FFPs

Figure 5.6(a) shows the measured band structure of a fabricated device with the same structural parameters as specified above. The band structure was mapped out around the Γ point by measuring the angle-dependent spontaneous emission spectra well below the lasing threshold [46]. The threshold current (I_{th}) at room temperature continuous wave (CW) operation was 25 mA. The measurements were performed in the Γ - X and Γ - J directions under a CW current level of $0.9I_{\text{th}}$ and in the measurements the sample was attached on a heat sink. The dashed curves in Fig. 5.6(a) replot the data shown in Fig. 5.4(a) in order to enable a direct comparison with the experimental results. It can be seen that the measured and calculated band structures are in satisfactory agreement. The slight discrepancy may be mainly attributed to the experimental details, such as the change in refractive index owing to carrier injection and thermal effects. We note that in the measured band structure, several additional bands (e.g., bands existing between modes D_1 and C near the Γ point) were also observed. These bands are considered to be TM modes as discussed in Ref. [87]. As the laser structure is not completely symmetric in the vertical direction [86], TM mode usually coexists with TE mode and may derive some optical gain from the multiple quantum-well active layer. However, since the optical gain is greater for the TE mode than for the TM mode [33], the existence of the TM bands rarely becomes an issue for our laser devices. It is also interesting to note that, especially near the Γ point, the intensity of spontaneous emission from the antisymmetric modes A - C is extremely weak compared to that from modes D_1 and D_2 . This is due to the difference in their radiative nature, as presented in Fig. 5.4(b). The lasing spectrum at the Γ point measured at $1.2I_{\text{th}}$ current level is shown in Fig. 5.6(b),

which evidently suggests that single-mode lasing indeed occurs at band-edge mode C (yellow dashed line). This observation is consistent with the lasing mode predicted above.

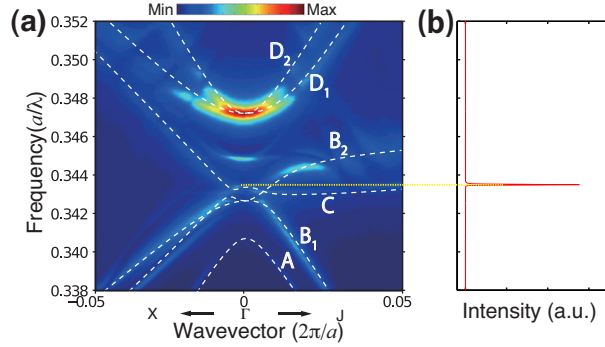


Figure 5.6: (a) Comparison of the measured (in color) and calculated (white dashed curves) band structures. (b) Lasing spectrum measured above the lasing threshold in the direction normal to the PC plane. The threshold current (I_{th}) at room temperature CW operation was 25 mA. Band structure and lasing spectrum were measured at CW current levels of $0.9I_{th}$ and $1.2I_{th}$, respectively. The frequency of the lasing peak in (b) is 0.3434 (a/λ), indicating that the lasing mode is band-edge mode C (yellow dashed line).

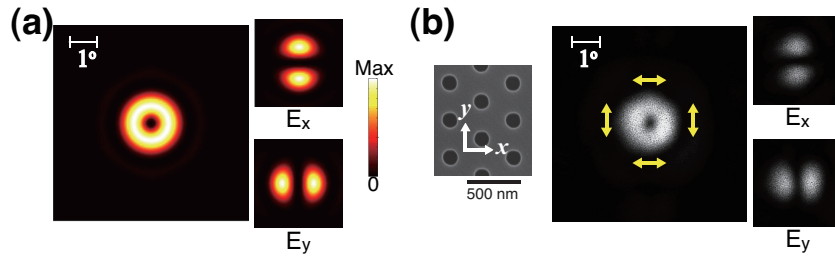


Figure 5.7: (a) Calculated and (b) measured FFPs of mode C . A scanning microscope image of the fabricated PC with $a = 341$ nm and $f = 0.15$ (where the r/a ratio is 0.20 and r is the air-hole radius) is shown in the left inset of (b). E_x (E_y) displayed in the right insets represents the x (y) component of the FFP. Parameters used for the calculations are the same as those shown in the caption of Fig. 5.5. The yellow arrows in (b) indicate the directions of the measured beam polarization. The beam divergence angle of the FFPs for both cases is around 1° , reflecting the large area of coherent oscillation.

Next, we examine the FFP and polarization profile of the lasing mode (see Ref. [86] for details of the calculation method for FFP). Figure 5.7(a) shows the calculated FFP of mode C . A doughnut-shape beam with a divergence angle of around 1° is obtained; this closely matches the measured FFP shown in Fig. 5.7(b). The polarization profiles shown in the insets indicate that mode C exhibits an azimuthal polarization, which stems from the monopolar nature of its field pattern, as depicted in Fig. 5.4(c).

5.2.2.4 Lasing mode control by tuning air-hole size

As has been demonstrated in the previous works on triangular-lattice PCSELs [31, 43], single-mode lasing action may also be achieved at band-edge mode A (i.e., the hexapole mode). Based on our CWT analysis, we find that by tuning some structural parameters, e.g., by varying the air-hole size, mode A may be favored for lasing. As an example, we list in Table 5.2 the normalized threshold gain of the low-threshold modes A – C for air holes with a larger filling factor of $f = 0.26$. The data given in Table 5.2 suggest that mode A is the lasing mode with a threshold-gain discrimination of around 20 cm^{-1} against the competing modes (i.e., modes B_1 and B_2). The calculated FFP and polarization profile of mode A are shown in Fig. 5.8(a). It is seen that mode A exhibits a doughnut-shape pattern with hexagonal symmetry and possesses a characteristic polarization: The electric-field vector is rotated 4π around the circumference of the doughnut beam (instead of 2π for the monopole mode C). The weak side lobes of the calculated FFP result from the radiation field being terminated abruptly in the numerical calculation.

Table 5.2: Normalized threshold gain (αL) of the low-threshold modes A – C . Parameters used for the calculations are the same as those shown in Fig. 5.5 except that a larger air-hole filling factor $f = 0.26$ is used.

Mode	A	W	$B_{1,2}$	C
αL	0.294	0.548	0.324	0.400

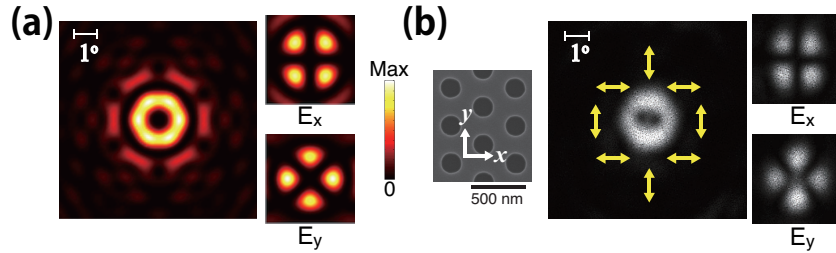


Figure 5.8: (a) Calculated and (b) measured FFPs of mode A . A scanning microscope image of the fabricated PC with $a = 341 \text{ nm}$ and $f = 0.26$ (where $r/a = 0.27$) is shown in the left inset of (b). E_x (E_y) displayed in the right insets represents the x (y) component of the FFP. Parameters used for the calculations are specified in the caption of Table 5.2. The yellow arrows in (b) indicate the directions of the measured beam polarization.

To further demonstrate the predictive power of our CWT analysis, we fabricated another device with $f = 0.26$. By measuring the band structure and the lasing spectrum in the same manner as described for Fig. 5.6, we confirmed that lasing indeed occurs at band-edge mode A . The measured FFP and polarization profile are shown in Fig. 5.8(b), and they are in good agreement with the calculated FFP shown in Fig. 5.8(a). The

slight asymmetry in the measured FFP (e.g., the weak streak in the central part of the doughnut-shape beam) can be attributed to the nonuniform electrical pumping or the asymmetric geometry of the gain region determined by carrier diffusion in practical experimental situations.

5.3 Treating air holes with arbitrary sidewalls and back-side reflection effect

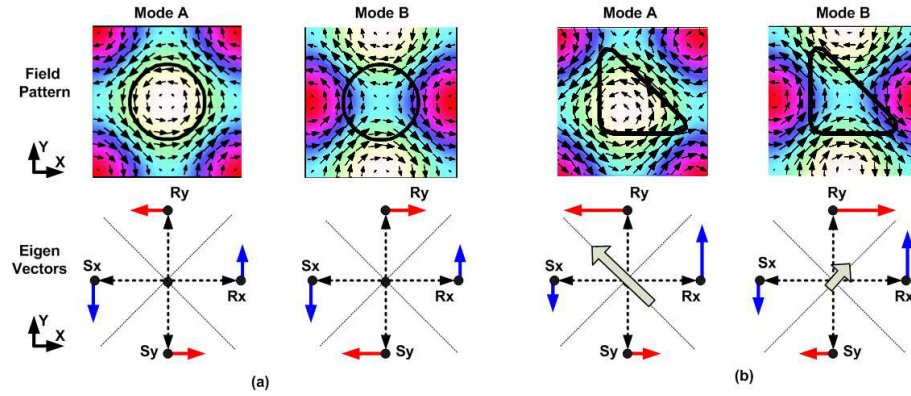


Figure 5.9: Field distribution and eigenvectors of modes A and B, for the: (a) CC air holes, and (b) RIT air holes. The color pattern in the field distribution shows the magnetic field distribution, and the black arrows show the electric field distribution. The eigenvectors of modes A and B are illustrated in coordinate space, with the dashed arrows showing the propagating directions of four basic waves; the red and blue arrows show the amplitudes and polarizations of their electric fields, and the gray arrows show the amplitudes and polarizations of the radiative waves determined by Eqs. (3.20a)-(3.20b).

Figure 5.9 shows the field patterns and eigenvectors of modes A and B for the CC and RIT air holes in real space. The eigenvectors solved from Eq. (3.15) are complex values that represent the amplitudes and phases of the four basic waves, with their polarizations given by Eqs. (3.20a)-(3.20b). For convenience, only the amplitudes are plotted in Fig. 5.9; the lengths of the red and blue arrows indicate the amplitudes, and the arrow directions indicate the electric field polarization of the waves. Because of the perfect symmetry of the CC air holes, the four basic waves have equal amplitudes, while the asymmetric RIT air-hole shape results in different amplitudes between R_x , R_y and S_x , S_y , as shown in Fig. 5.9.

As is evident in Fig. 5.9 and the fact that $\mathbf{E}$ is a vector while $\mathbf{H}$ is a pseudovector, mode A with CC air holes is antisymmetric with respect to the $Y = X$ and $Y = -X$ axes, but mode B is symmetric with respect to the same axes. As a result of these symmetries and the equal amplitudes of the eigenvectors, the combination of these four

basic waves according to Eqs. (3.20a)-(3.20b) leads to complete destructive interference, which minimizes the radiative power and yields a large Q factor for modes A and B, as confirmed by the FDTD simulation [80]. The RIT air holes, on the other hand, break the symmetry in one of the two axes, and as a result, complete destructive interference is no longer applicable but partial constitutive interference appears. Therefore, a high radiation power and a low Q factor are obtained for modes A and B. The symmetries also determine the polarization of the radiative waves. As shown in Fig. 5.9, cancellation of the four basic waves results in the polarization of radiative wave in the $Y = -X$ direction for mode A but in the $Y = X$ direction for mode B.

From this discussion we confirmed that the in-plane asymmetries of the air holes play a crucial role in achieving high-power PCSELs since the asymmetry determines the interference of the individual modal eigenvectors. Partial constructive interference is enhanced by such asymmetries, which can result from in-plane asymmetric air-hole shapes or vertically tilted sidewalls.

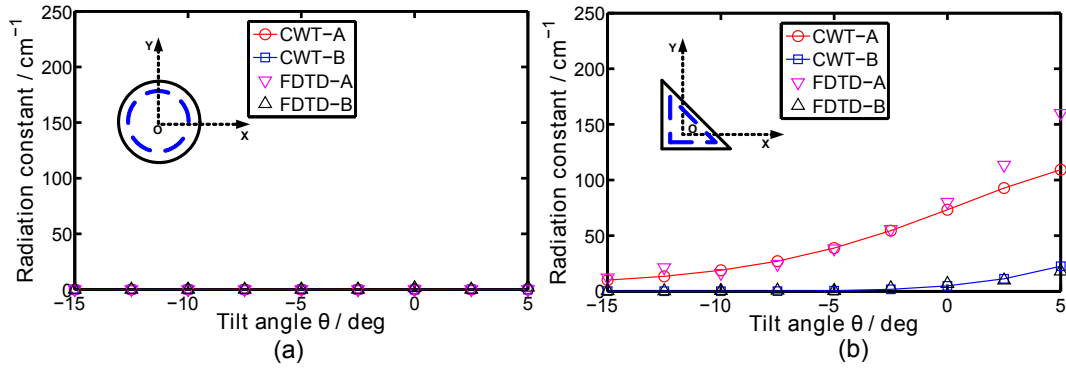


Figure 5.10: Radiation constant vs. tilt angle θ for modes A and B in the tapered case: (a) CC air holes; (b) RIT air holes. The solid and dashed shapes in the insets show the up and down facets of the air holes, respectively; both CWT and FDTD results are plotted.

5.4 Summary

A full 3D CWT was developed for triangular-lattice PCSELs with TE polarization by extending our previous CWT model [84, 86]. When compared to the previous model, the key feature of the extended theory is that six basic waves were introduced in the coupled-wave equation to describe the C_{6v} symmetry of the eigenmodes in the vicinity of the second-order Γ point; additionally, both surface radiation and in-plane losses, which are critical for analyzing the finite-size laser structure, were included. By solving the extended coupled-wave equation, modal properties, including the band structure, radiation constant, threshold gain, field intensity profile, and FFP were studied. Comparison

of the calculated band structure and FFP of the lasing mode with experimental results showed good agreement. Single-mode lasing at the monopole mode C predicted by our threshold gain analysis was confirmed by experimental data. Furthermore, it was shown that the hexapole mode A can be favored for lasing by using a larger air-hole size; this was also confirmed by the experiments.

Another extension of our theory is the inclusion of the refractive index variation in the vertical direction. To investigate the effects of the vertically asymmetric sidewalls on the device output, two kinds of tapered air-hole geometries (circular and RIT) without and with center-of-gravity shifts, are investigated. PCSELs without center-of-gravity shift in the tapered air holes basically exhibit similar output properties as the uniform ones with an effectively averaged air-hole filling fraction. In contrast, PCSELs with center-of-gravity shift in the tapered air holes show remarkably different behaviors. The properties of the radiation constant, threshold gains (mode selectivity), and the FFP profiles can be modified in a fairly different manner depending on the distance and direction of the shift. Particularly, the radiation constant, i.e., the output power, can be improved significantly by intendedly breaking the symmetry of the in-plane field distributions. This suggests that air-holes with appropriate tapered sidewalls might be a promising geometry suitable for single-mode high-power operation.

Although the analyses performed in this chapter were restricted to circular or RIT air holes, the power of our theory lies in the fact that it can be applied to air holes of any arbitrary shape as it inherently incorporates a large number of high-order waves [84]. Moreover, the general coupled-wave equation is applicable not only to triangular lattice but also to centered-rectangular lattices with C_{2v} or C_{4v} symmetry [44, 87], thereby unifying the analysis of the modal properties of PCSELs.

Chapter 6

Above-threshold coupled-wave analysis

6.1 Introduction

As described in Chapter 1, one of the most advantageous features is that PCSELs can potentially achieve single-mode operations with the largest cavity area and the highest output power. Recently, the side length of the laser cavity has been progressively increasing, with the aim of further improving the output power [54–57].

Generally, the output power scales naturally with the square of the cavity side length L . However, the small mode spacing (including both the mode frequency and threshold-gain margin), decreasing with the square of the cavity dimension, fundamentally limits the cavity size for single-mode operations. Moreover, the long cavity length usually tends to result in a highly inhomogeneous profile of the photon density, which in turn induces a spatially nonuniform carrier density. This is so-called spatial hole burning (SHB), which has always been a bottleneck for the family of high-power semiconductor lasers based on one-dimensional (1D) gratings [e.g., DFB (distributed feedback) and DBR (distributed Bragg reflector) lasers] or facing-mirror resonators [e.g., (vertical-cavity surface-emitting lasers) VCSELs] [97]. SHB effects in these conventional laser cavities have been studied extensively [99]–[102]. These studies suggest that spatial inhomogeneity of photon and carrier density, particularly in the strongly coupled case (i.e., a large value of κL , where κ is the coupling coefficient), could lead to decreased output efficiency and mode instability at injection currents above the lasing threshold. As to the 2D PCSELs, theoretical works thus far have been limited to the linear case and are only applicable to the analysis at the threshold [84, 86–88]. An *above-threshold* model is required to understand the impact of SHB to mode stability and its implication in laser design optimization to achieve higher

peak powers. In this chapter, to provide insights into the single-mode lasing range, we first present an analysis of the mode spacing between the main and side modes based on our previous linear theory. Then, we develop an *above-threshold* model by incorporating rate equation into the linear coupled-wave equations. In our new model, we take into account of both the spatially-varying effective refractive index and local gain variation caused by SHB effect. By solving the *nonlinear* coupled-wave equations using a self-consistent technique, we study the impact of SHB on laser stability at various injection currents above threshold. We find that the local gain variation might be the dominant mechanism that degrades the mode stability of large-area PCSEL devices operating at current levels, which well explains the observed experimental data. Our findings present new guidelines for high-power PCSEL designs, in which SHB imposes additional limits on increasing cavity length beyond which laser performance deteriorates.

6.2 Laser behavior above threshold

6.2.1 Spatial hole burning

Below the laser threshold, the stimulated emission term can be neglected in the longitudinal carrier rate equation. In this case, a uniform carrier injection current J causes a uniform carrier distribution N along the laser. However, above the threshold, an optical power distribution builds up and this power distribution is rarely uniform. The stimulated recombination will consequently cause a nonuniform carrier distribution. In other words, areas of strong optical field intensity will show a lower carrier density. This is called spatial hole burning (SHB), and here it occurs in the xy plane.

The place along the laser cavity where SHB occurs is also related to the strength of the coupling of the periodic structure. Basically, three coupling strengths can be distinguished $\kappa L < 1$ or *undercoupling*, $\kappa L \simeq 1$ or *critical coupling*, $\kappa L > 1$ or *overcoupling*. For overcoupling lasers, spatial holes tend to appear in the middle of the periodic structure. For undercoupled lasers, spatial holes tend to appear at the edges of the periodic structure. For critical coupling, the carrier distribution shows less pronounced holes.

6.2.2 Interaction between photons and carriers: laser rate equation

A phenomenological approach is used to describe behaviors of diode lasers through a set of coupled rate equations related to the balances for carriers and photons. The standard equations generally assume uniform longitudinal distributions of carriers and photon densities within the laser cavity. This is, however, not the case in high-power

laser diodes, in which carrier and photon inhomogeneity is significant particularly at high current.

To incorporate the SHB effect, the rate equation for the carrier and photon densities are modified. We assume that only one mode is lasing. Rate equation for the carrier density $N(t)$ (cm^{-3}) and the photon density $P(t)$ (cm^{-3}) can be written as [97]

$$\frac{dN(t)}{dt} = \eta_i \frac{J(t)}{qd} - \frac{N(t)}{\tau_s} - v_g g(N)P(t) + D_n \nabla^2 N(t), \quad (6.1)$$

where

$N(t)$ = electron density (cm^{-3})

η_i = injection quantum efficiency

e = electric charge (1.6×10^{-19} Coulomb)

τ_s = carrier lifetime (s)

$v_g = c/n_g$ = the group velocity of light (cm/s)

$P(t)$ = photon density (cm^{-3})

J = injection current density (A/cm^2)

d = thickness of the active region (cm)

$g(N)$ = the gain coefficient (cm^{-1})

The first term on the right hand side of Eq. (6.1), $\eta_i J/ed$ is the injected number of carriers into the active layer per unit volume per second. The second term accounts for the carrier loss due to the radiative and non-radiative recombinations. The third term $v_g g(n)P$ is the carrier loss due to stimulated emissions. The last term accounts for carrier loss due to carrier diffusion. For simplicity, we neglect the carrier diffusion effect at the laser boundaries because diffusion length of the injected carrier is much smaller than the laser length (e.g., $3 \mu\text{m} \ll 70 \mu\text{m}$).

In the steady state ($dN(t)/dt = 0$), we can derive the net carrier density in the active region as

$$N_n(x, y) = \frac{J_c \tau_s}{ed} - \tau_s v_g g(x, y)P(x, y), \quad (6.2)$$

where we assume that the current is injected to the active region uniformly with a current density of J_c ($J_c = \eta_i J$). The photon density $P(x, y)$ is inhomogeneous particularly at strongly-coupled case (with a large value of κL), as shown in Fig. 6.1(a). When we assume that the current is injected uniformly with current density of J , the net carrier density $N_n(x, y)$ exhibits an inhomogeneous profile as shown in Fig. 6.1(b): The carrier density at the central part of the laser cavity, is reduced due to the relatively larger stimulated recombination rate. This is the illustration of the SHB effect.

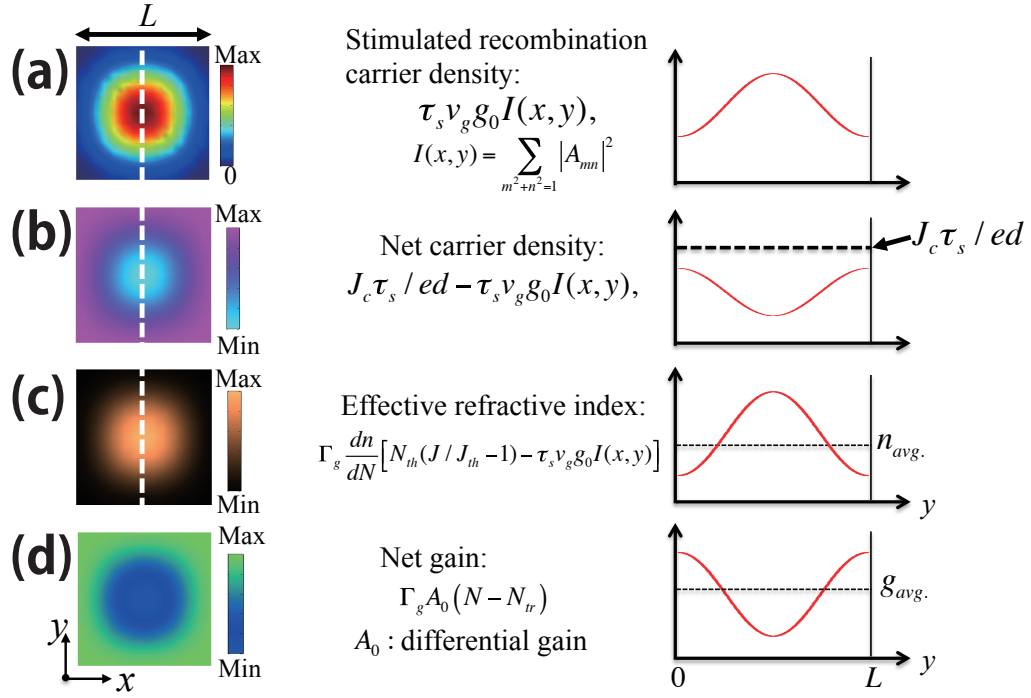


Figure 6.1: Schematics of the (a) photon density distribution, (b) carrier density distribution, (c) refractive index distribution, and (d) gain profile induced by the spatial hole burning effect.

6.2.3 Spatial variation of refractive index

Inhomogeneous carrier density within the active region gives rise to a spatially-varying refractive index. This mechanism was explained by the plasma effect of free electrons in the conduction band or the band-gap change due to the injected carriers. The resultant refractive index $n_1(x, y)$ of the active region can be expressed as

$$n_1(x, y) = n_{10} + (dn/dN)N_n(x, y). \quad (6.3)$$

Here, the carrier induced refractive index is a negative number for GaAs-based semiconductor materials. In Ref. [96], $dn/dN = -(1.9 \pm 0.1) \times 10^{-20} \text{ cm}^3$ was reported for a InGaAs/GaAs quantum-well laser.

The effective refractive index $n_{\text{eff}}(x, y)$ is expressed in terms of the optical confinement factor Γ_g as

$$n_{\text{eff}}(x, y) = \Gamma_g n_1(x, y) + (1 - \Gamma_g) n_2. \quad (6.4)$$

where n_2 is the refractive index contributed by the guide layer and cladding layer. Here, n_2 can be assumed to be constant because its change is much smaller than that of the active layer.

Combining Eqs. (6.2-6.4), we obtain the following equation

$$\begin{aligned}
 n_{\text{eff}}(x, y) &= n_{\text{eff0}} + \Gamma_g(dn/dN) [(J_c\tau_s/ed - \tau_s v_g g(x, y)P(x, y) - N_{\text{th}})] \\
 &= n_{\text{eff0}} + \Gamma_g(dn/dN) [N_{\text{th}}(J_c/J_{\text{th}} - 1) - \tau_s v_g g(x, y)P(x, y)] \\
 &= n_{\text{eff0}} + \Delta n(x, y),
 \end{aligned} \tag{6.5}$$

where n_{eff0} is the effective refractive index at threshold. N_{th} is the threshold carrier density, J_{th} is the threshold current density, and $\Delta n(x, y)$ is the change in the effective refractive index, n_{eff0} and $\Delta n(x, y)$ are given as

$$\begin{aligned}
 n_{\text{eff0}}(x, y) &= \Gamma_g n_{10}(x, y) + (1 - \Gamma_g)n_2 + \Gamma_g(dn/dN)(\tau_s J_{\text{th}}/ed) \\
 &= \Gamma_g n_{10}(x, y) + (1 - \Gamma_g)n_2 + \Gamma_g(dn/dN)\tau_s N_{\text{th}},
 \end{aligned} \tag{6.6}$$

and

$$\Delta n(x, y) = \Gamma_g(dn/dN) [N_{\text{th}}(J_c/J_{\text{th}} - 1) - \tau_s v_g g(x, y)P(x, y)]. \tag{6.7}$$

The schematic of $\Delta n(x, y)$ is depicted in Fig. 6.1(c), showing a bell-shaped profile similar to the photon (optical field) intensity profile $P(x, y)$.

6.2.4 Spatial variation of gain distribution

It should be stressed that the local gain is also a function of the carrier density N . Here, we employ a simplified gain model used by G. P. Agrawal [92], in which the so-called amplitude-gain coefficient α_v (in the coupled-wave equation) is given by

$$\alpha_v = (g - \alpha_{\text{int}})/2 \tag{6.8}$$

where α_{int} accounts for the internal losses and g in the power gain. In the linear-gain approximation, g is related to the carrier density N inside the active region by

$$g(N) = \Gamma_g A_0 (N - N_{\text{tr}}). \tag{6.9}$$

where Γ_g is the confinement factor, $A_0 (= dg/dN)$ is a proportionality constant (differential gain), and N_{tr} is the carrier density required to overcome the intrinsic material loss (transparent carrier density). Therefore, α_v exhibit a reverse-bell-shaped profile as shown in Fig. 6.1(d).

6.2.5 Above-threshold coupled-wave equations

The derived 3D nonlinear coupled-wave equation are expressed in the following form:

$$\begin{aligned}
& \left[\delta_v + i\alpha_v + (1 - \sqrt{m_x^2 + n_y^2})\beta_0 \right] A_{m,n} - i \left(m_x \frac{\partial}{\partial x} + n_y \frac{\partial}{\partial y} \right) A_{m,n} \\
&= \sum_{|r^2+s^2|=1; r \neq m, s \neq n} \kappa_{mn}^{(rs)} A_{r,s} \\
& - \frac{k_0^2}{2\beta_0} \sum_{|m'^2+n'^2| \neq 1} \xi_{m-m', n-n'} \int_{PC} (\rho_{mn} E_{x,m',n'} + \eta_{mn} E_{y,m',n'}) \Theta_0^*(z) dz, \quad (6.10)
\end{aligned}$$

where $\delta_v = \beta_v - \beta_0 = n_{\text{eff}} \frac{\omega}{c} - \beta_0$ is the deviation from the Bragg condition, n_{eff} is the effective refractive index for the fundamental guided mode, α is the modal loss. Here, It should be stressed here that, because of the spatially-varying refractive index due to SHB, both the coupling coefficients $\kappa_{mn}^{(rs)}$ and δ is no longer constants. Here we neglected a spatial dependence of the coupling coefficients. On the other hand, we must take a spatial dependence of δ_v into account. δ is modified as the following equations using $\Delta n(x, y)$ of Eq. (6.7)

$$\begin{aligned}
\delta_v &= (n_{\text{eff}0} + \Delta n) \frac{\omega}{c} - \beta_0 \\
&= \delta + \Delta(x, y)(\delta + \beta_0) \\
&\simeq \delta + \Delta(x, y)\beta_0, \quad (6.11)
\end{aligned}$$

where $\delta = n_{\text{eff}0} \frac{\omega}{c} - \beta_0$ ($\delta \ll \beta_0$), and

$$\begin{aligned}
\Delta(x, y) &= \Delta n(x, y) / n_{\text{eff}0} \\
&= \Gamma_g (dn/dN) [N_{\text{th}}(J_c/J_{\text{th}} - 1) - \tau_s v_g g(x, y) P(x, y)] / n_{\text{eff}0} \quad (6.12)
\end{aligned}$$

Here, $P(x, y)$ represents the photon density.

At lasing, the gain must balance the threshold gain. We applied this requirement to our model with an inhomogeneous gain distribution. The lasing condition is

$$\iint_{\text{cav}} g(x, y) dx dy / L^2 = 2\alpha_0 + \alpha_{\text{loss}}, \quad (6.13)$$

where α_0 is the threshold gain of the lasing mode and α_{loss} is the internal power loss in the laser cavity. In the linear gain approximation, gain is related to the carrier density N inside the active region by

$$\begin{aligned}
g &= \Gamma_g A_0 (N - N_0) \\
&= \Gamma_g (A_0 N - \alpha_{\text{in}}), \quad (6.14)
\end{aligned}$$

where A_0 and α_{in} are constants. $A_0 = dg/dN$ is the material differential gain (typically $A_0 = 3.0 \times 10^{-16} \text{cm}^2$), and N_0 is the transparent carrier density ($1.5 \times 10^{18} \text{cm}^{-3}$) [92].

Rewriting Eq. (6.13) using Eq. (6.2) and Eq. (6.14), we have

$$\iint_{\text{cav}} [\Gamma_g(A_0(J_c\tau_s/ed - \tau_s v_g g(x, y)P(x, y)) - \alpha_{\text{in}})] dxdy/L^2 = 2\alpha_0 + \alpha_{\text{loss}}, \quad (6.15)$$

At threshold, $g_{\text{th}} = \Gamma_g(A_0 N_{\text{th}} - \alpha_{\text{in}})$, thus Eq. (6.13) becomes

$$\iint_{\text{cav}} [\Gamma_g(A_0 N_{\text{th}} - \alpha_{\text{in}})] dxdy/L^2 = 2\alpha_0 + \alpha_{\text{loss}}, \quad (6.16)$$

Combining Eqs. (6.15) and (6.16), we have

$$\iint_{\text{cav}} (J_c\tau_s/ed - N_{\text{th}} - \tau_s v_g g(x, y)P(x, y)) dxdy/L^2 = 0, \quad (6.17)$$

Note that $N_{\text{th}} = J_{\text{th}}\tau_s/ed$, the the injection current is related to the photon density in the active region by

$$\begin{aligned} J_c/J_{\text{th}} - 1 &= \iint_{\text{cav}} \tau_s v_g g(x, y)P(x, y) dxdy / (N_{\text{th}} L^2), \\ &= \tau_s v_g g_0 \iint_{\text{cav}} P(x, y) dxdy / (N_{\text{th}} L^2), \end{aligned} \quad (6.18)$$

where we approximated that $g(x, y)$ is equal to the constant g_0 , and we performed the integration only for $P(x, y)$ because the change in $g(x, y)$ is much smaller than that in $P(x, y)$ [91].

Substituting Eq. (6.18) into Eq. (6.12), we have

$$\begin{aligned} \Delta(x, y) &= \Gamma_g(dn/dN)N_{\text{th}} \left(\tau_s v_g g_0 \iint_{\text{cav}} P(x, y) dxdy / (N_{\text{th}} L^2) \right) / n_{\text{eff}0} \\ &\quad - \Gamma_g(dn/dN)\tau_s v_g g_0 P(x, y) / n_{\text{eff}0} \\ &= \Gamma_g(dn/dN)\tau_s v_g g_0 \left(\iint_{\text{cav}} P(x, y) dxdy / L^2 \right) / n_{\text{eff}0} \\ &\quad - \Gamma_g(dn/dN)\tau_s v_g g_0 P(x, y) / n_{\text{eff}0} \end{aligned} \quad (6.19)$$

The photon density $P(x, y)$ and its integral over the whole laser cavity, are related to the optical field intensity of the lasing mode as follows

$$P(x, y) = I(x, y) \frac{P(L, L/2)}{|R_x(L, L/2)|^2}, \quad (6.20)$$

$$\iint_{\text{cav}} P(x, y) dxdy = \iint_{\text{cav}} I(x, y) dxdy \frac{P(L, L/2)}{|R_x(L, L/2)|^2}, \quad (6.21)$$

where $I(x, y) = |R_x(x, y)|^2 + |S_x(x, y)|^2 + |R_y(x, y)|^2 + |S_y(x, y)|^2$.

By substituting Eqs. (6.20) and (6.21) into Eq. (6.19), $\Delta(x, y)$ can be expressed as

$$\begin{aligned} \Delta(x, y) = & \Gamma_g(dn/dN)\tau_s v_g g_0 P(L, L/2) / (|R_x(L, L/2)|^2 n_{\text{eff}0} L^2) \iint_{\text{cav}} I(x, y) dx dy \\ & - \Gamma_g(dn/dN)\tau_s v_g g_0 P(L, L/2) / (|R_x(L, L/2)|^2 n_{\text{eff}0}) I(x, y), \end{aligned} \quad (6.22)$$

and Eq. (6.18) becomes

$$J_c/J_{\text{th}} - 1 = \tau_s v_g g_0 P(L, L/2) / (|R_x(L, L/2)|^2 N_{\text{th}} L^2) \iint_{\text{cav}} I(x, y) dx dy. \quad (6.23)$$

6.2.6 Self-consistent calculation procedure

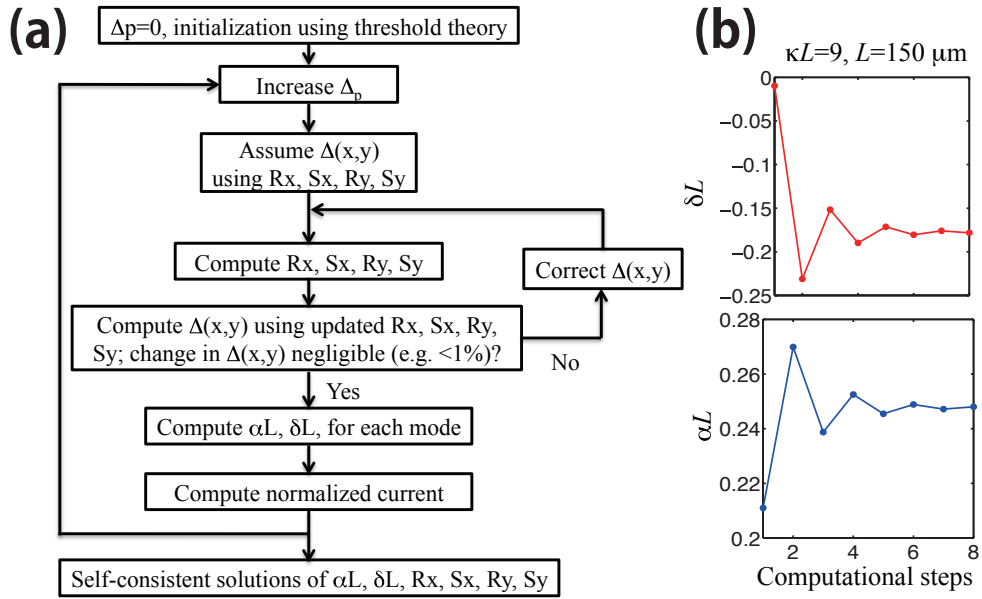


Figure 6.2: (a) Self-consistent calculation procedure for solving the above-threshold coupled-wave equation. (b) Convergence of the eigenvalues calculated for a PC-SEL with circular air holes.

The above-threshold coupled-wave equations derived above need to be solved self-consistently [99]. A flowchart of the calculation procedure is shown in Fig. 6.2(a). For the numerical calculation, we divide $\Delta(x, y)$ into a constant term $\Delta_a(x, y)$ and a spatial dependent term $\Delta_b(x, y)$ as

$$\Delta(x, y) = \Delta_a(x, y) + \Delta_b(x, y), \quad (6.24)$$

where

$$\Delta_a(x, y) = -\Delta_p \iint_{\text{cav}} I(x, y) dx dy / (|R_x(L, L/2)|^2 L^2), \quad (6.25)$$

$$\Delta_b(x, y) = \Delta_p I(x, y) / (|R_x(L, L/2)|^2), \quad (6.26)$$

$$\Delta_p = -\Gamma_g (dn/dN) \tau_s v_g g_0 P(L, L/2) / n_{\text{eff}0} \quad (6.27)$$

By varying the amplitude of $\Delta_p(x, y)$, we can calculate the normalized threshold gain αL and the normalized lasing wavelength δL at any injection current level above threshold. In our calculation, we normalized the field intensity as follows

$$\iint_{\text{cav}} I(x, y) dx dy / L^2 = 1. \quad (6.28)$$

When we express the injection current, we introduced the normalized injection current density

$$-\Gamma_g (dn/dN) N_{\text{th}} (J_c / J_{\text{th}} - 1) = -n_{\text{eff}0} \Delta_a \quad (6.29)$$

A typical example showing convergence of eigenvalues at a normalized injection current of 2.0×10^{-4} (corresponding to a 3.7 times of threshold current) is shown in Fig. 6.2(b).

6.3 Above-threshold analysis

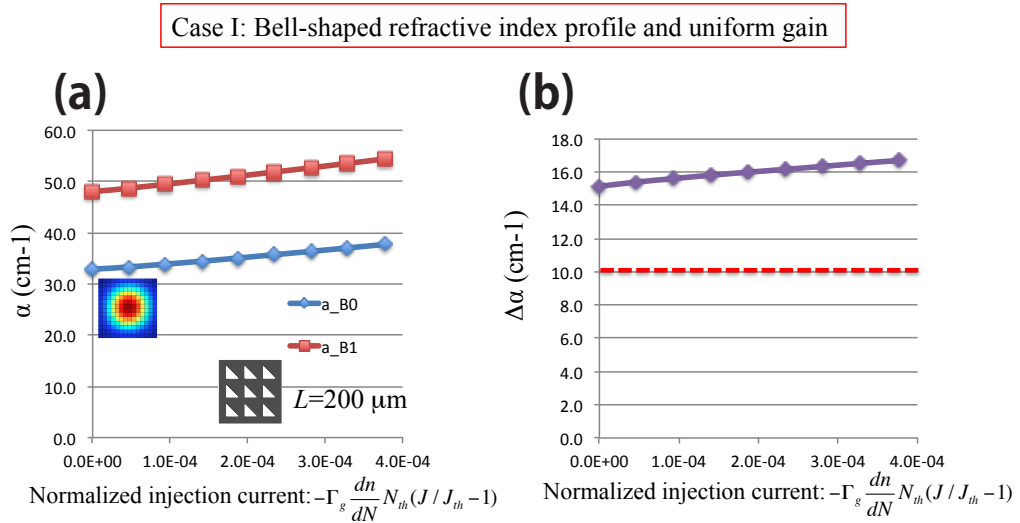


Figure 6.3: Threshold gains (α) of the fundamental mode B_0 and the next competing mode B_1 versus the normalized injection current. (b) The threshold-gain margin ($\Delta\alpha$) of mode B_0 and B_1 versus the normalized injection current. The cross-point the dashed red line indicates single-mode lasing condition: $\Delta\alpha = 10 \text{ cm}^{-1}$. In the calculations, the the air-hole filling factor $f = 0.20$ and the device length $L = 200 \mu\text{m}$.

By self-consistently solving the above-threshold couple-wave equations, we can calculate the modal properties at any injection current level above threshold. The threshold gains of the fundamental mode B_0 and the next competing mode B_1 , as well as their threshold gain margin, are plotted as a function of the normalized current injection $[-\Gamma_g(dn/dN)N_{th}(J_c/J_{th} - 1)]$, in Figs. 9(a) and (b), respectively. In the calculation, we assumed a bell-shaped refractive index profile and a uniform local gain profile. The PC structure (inset) consists of square-lattice right-angled triangles with filling factor $f = 0.20$, coupling coefficient $\kappa_3=454 \text{ cm}^{-1}$, $L = 200 \text{ }\mu\text{m}$, and lattice constant $a = 295 \text{ nm}$.

From Fig. 6.3, it is found that threshold gain of the individual mode slightly increases with the increasing injection current and their threshold margin. The physical explanation of the increased modal threshold gains and the threshold margins is very interest. When the refractive index in the laser cavity exhibits a bell-shaped profile as shown in Fig. 6.1(c), the band gap between the symmetric modes (C and D) and anti-symmetric modes (A and B) shifts and forms a V-shaped well for photons. This implies that the effective reflectivity induced by the band edges is decreased, which makes the modes (anti-symmetric modes) much more leaky in the in-plane directions. Therefore, as the injection current increases, threshold gain is steadily increased. Overall, the resultant threshold-gain margin is increased around 2 cm^{-1} when the injection current is increased around 3.7 times. Therefore, inhomogeneous refractive index profile due to SHB cannot explained the two-mode operation observed experimentally in Fig. 4.12.

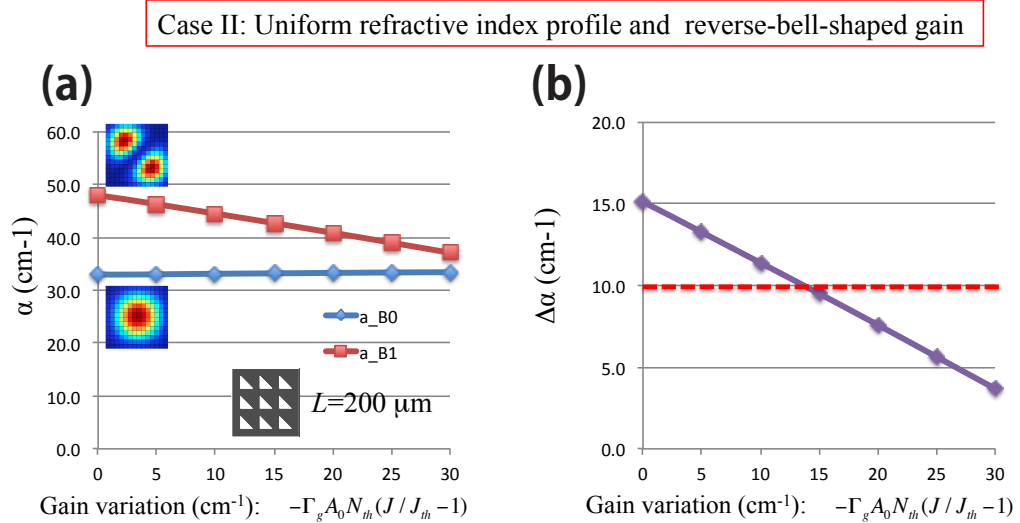


Figure 6.4: (a) Threshold gains (α) of the fundamental mode B_0 and the next competing mode B_1 versus the local gain variation. (b) The threshold-gain margin ($\Delta\alpha$) of mode B_0 and B_1 versus the normalized injection current. The cross-point the dashed red line indicates single-mode lasing condition: $\Delta\alpha=10 \text{ cm}^{-1}$. In the calculations, the the air-hole filling factor $f = 0.20$ and the device length $L=200 \text{ }\mu\text{m}$.

Next, we assume a uniform refractive index profile and a reverse-bell-shaped gain profile. The calculated threshold gains of modes B_0 and B_1 and their threshold gain margin are shown in Figs. 6.4(a) and (b), respectively. We find that modes B_0 and B_1 exhibit totally different behavior: Threshold gain of the fundamental mode B_0 is slightly increased, whereas mode B decreases remarkably with increasing gain variation (which is proportional to the injection current). Consequently, the threshold gain margin significantly decreases from 15 cm^{-1} to 4 cm^{-1} . This indicates that the single-mode operation can be obtained near threshold, but two-mode operation with modes B_0 and B_1 occurs at high current levels (i.e., output power), which well explains our experimental observation presented in Fig. 4.12. The above results in Fig. 6.4 can be understood with fundamental laser physics. In any laser structure the overlap factor between the gain spatial distribution and that of the modal intensity is crucial and proportionate. In semiconductor lasers, once the pump power is strong enough to induce the population inversion, the medium starts to amplify light. The lasing threshold is determined by equating the modal loss with the modal gain; and the modal gain is proportional to the overlap integral between the spatial distribution of the gain and that of the modal intensity. Therefore if one assumes that, to the first order as in Eq. (6.9), the gain is proportional to the carrier density over the transparency, then the overlap between the spatial distribution of the gain and that of the fundamental mode (B_0) intensity (Fig. 6.1(d)) is reduced, therefore giving rise to a higher threshold. In contrast, the overlap between the gain and the high-order mode (B_1) is enhanced and finally could efficiently excite the high-order side mode.

Case III: Uniform refractive index profile and bell-shaped gain

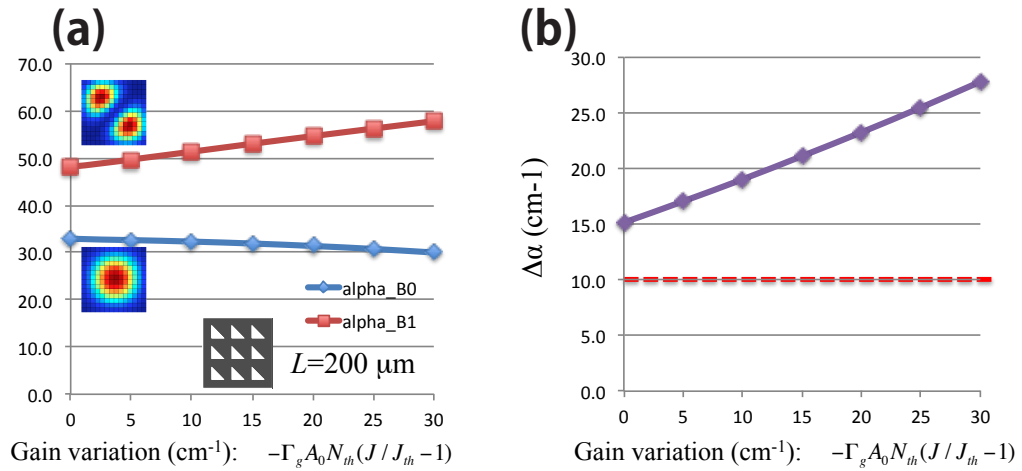


Figure 6.5: (a) Threshold gains (α) of the fundamnet B_0 and the next competing mode B_1 versus the the local gain variation. (b) Threshold-gain margin ($\Delta\alpha$) of mode B_0 and B_1 versus the normalized gain. The cross-point the dashed red line indicates single-mode lasing condition: $\Delta\alpha=10 \text{ cm}^{-1}$. In the calculations, the air-hole filling factor $f = 0.20$ and the device length $L=200 \text{ } \mu\text{m}$.

Finally, to confirm our intuitive understanding of the effect of gain profile on threshold-gain margin, we assume a bell-shaped gain profile (which has a peak gain near the center of the laser cavity). This kind of nonuniform gain profile can be realized by using separated p-side electrodes similar to the one-dimensional scheme proposed in Ref. [108]. As demonstrated in Fig. 6.5, this nonuniform gain profile gives rise to an improved mode stability even at high current levels.

6.4 Summary

In summary, we have performed an above-threshold 3D CWT analysis of the modal properties of the band-edge modes in PCSEs by incorporating rate equation into the linear couple-wave theory. In particular, we focused our analyses on the threshold-gain variation and threshold gain margin, as well as their dependence on the device length L and injection currents. Two critical issues that may greatly affect the single-mode high-power operation of the laser cavity are presented and discussed. The first issue is the limitation of increasing L to achieve high-power operation. Based on the linear theory, we find that the threshold-gain margin between the lowest threshold (fundamental) modes and the next high-order modes steadily decreases with a increasing device length. This threshold degeneracy may limit the increase of L for high-power operation, particularly at extremely large- L regimes. The second issue is the degraded mode stability encountered at high injection current levels. When the inhomogeneous photon and carrier density caused by spatial hole burning (SHB) are taken into account, the threshold-gain margin between the fundamental modes and the high-order modes, which determines the mode stability of the extremely large- L devices, becomes much smaller. The agreement between the theoretical prediction and experiments supports the hypothesis that modified gain profile is the dominant mechanism that accounts for the high-order mode lasing observed at high current levels.

Future investigation will be devoted to improvement of the *nonlinear* (above-threshold) CWT model by incorporating the more complicated nonlinear effects such as gain saturation, carrier diffusion, and thermal effects. Meanwhile, further analysis based on the present model will be performed to optimize the PC structures for higher power operation and improved mode selectivities.

Chapter 7

Conclusions

7.1 Summary

In this thesis we have presented a 3D CWT model for PCSELs. Instead of simply extending the previous 2D CWT model, we built up a new 3D model which analytically describes the complex wave interaction in a full 3D system. The capability of our 3D model is far beyond the previous 2D model and the conventional numerical computer simulation methods such as plane-wave expansion method (PWEM) and finite-difference time-domain method (FDTD). Our theory is now able to treat PC geometries of any arbitrary shape in the PC plane, any lattice structures that enables 2D resonance (i.e., the generalized centered-rectangular lattice), and arbitrary sidewalls in the direction normal to the PC plane. We have demonstrated that our theory provides an efficient, accurate, and reliable analysis of a variety of modal properties of interest by comparing with the numerical computer simulations and experimental results. Moreover, the modal properties that can be treated are not limited to the threshold condition but have been extended to the above-threshold regime. The results included in this thesis are summarized below.

Chapter 1 described the background of PCSELs by giving an overview of their recent progress and breakthrough. Motivation of this thesis was presented after emphasizing the importance of developing an analytical tool for PCSELs.

Chapter 2 started with a brief description of the basic laser structure to be investigated and the lasing principles. The conceptual coupling diagram in reciprocal lattice space was introduced to explain how a 2D cavity mode can be formed. Next, conventional theoretical methods: 2D PWEM, FDTD and 2D CWT model were described; and limitation of each method was pointed out. In particular, we reviewed the previous

2D CWT model in more detail. We found that the previous CWT is not able to treat general PC air-hole shapes because of its limited number of wave vectors included in the coupling diagram. More importantly, a 2D structure was assumed in the coupled-wave formulation, which intrinsically restricted its application to the realistic 3D laser structure. To overcome drawbacks of the previous 2D CWT model, a full 3D model must be developed.

Chapter 3 established the framework of the 3D CWT. Starting with the E -field based Maxwell's equation, we derived a full 3D coupled-wave equation by including a large number of high-order wave vectors and carefully treating the vertical field profile of each wave vector in a full 3D structure. The new 3D CWT is capable of treating arbitrarily-shaped air holes; moreover, the surface emission, which determines the device output, can be directly calculated. To further emphasize the fundamental difference between the new 3D and previous 2D, we investigated the electric field profile of the individual waves and the mode gaps induced by the wave couplings. Next, the accuracy and the validity of the 3D CWT was confirmed by comparison with 3D-FDTD simulations. The computational time which typically takes ~ 4 h for 3D-FDTD on a paralleled supercomputer system was significantly reduced to less than 1 s.

Chapter 4 presented the main body of the analysis results for square-lattice PCSELs and several important experimental demonstrations. First, the coupled-wave equation was extended for finite-size structures by including the slowly-varying envelopes of the resonant modes. Differing from the infinitely periodic structures, the finite-size analysis includes both the surface radiation loss and the in-plane loss leaking from the laser cavity boundaries. Therefore, the laser threshold gain and the far-field pattern (FFP) can be evaluated. Two kinds of air-hole designs: circular and equilateral triangular shapes were studied by analyzing their threshold gains and FFPs. Both of these analysis results are in good agreement with the experiments. Interestingly, we revealed that the in-plane loss plays an important role in enabling the stable single-mode operation, which could provide a large threshold-gain discrimination of over 20 cm^{-1} . By further investigating the threshold gain dependence on laser cavity length L , we found that the lasing mode could be switched by changing L . This kind of mode selectivity is provided by the balance of the in-plane loss and the surface emission loss. Next, we experimentally demonstrated this mode selectivity behavior by fabricating samples with different cavity lengths with $L = 50 \text{ }\mu\text{m}$ and $L = 200 \text{ }\mu\text{m}$. With increased L , clearly lasing mode switching from band-edge mode A to B was observed by measuring the band structure and the lasing spectrum. Further investigation of the threshold gains in larger-area PSEL devices lets us notice the single-mode stability issue resulted from the high-order band-edge modes. In the final part of this chapter, we studied single-mode stability in large-area ($L > 150 \text{ }\mu\text{m}$) PCSELs. We experimentally observed clear mode competition above the laser

threshold within large-area samples which initially exhibited single-mode operation. The physical mechanisms of this mode competition were found to be attributed to decreased threshold gain margin between the fundamental lasing mode and high-order band-edge modes, as well as the spatial hole burning effect due to the highly inhomogeneous modal field intensity distribution. These findings presents new insights into designing single-mode high-power PCSELs where strategy of suppressing these high-order modes much be considered.

Chapter 5 presented an extended CWT model that is able to treat more generalized PC geometries. Two important extensions were realized. First was the lattice structures. In contrast to the square-lattice with C_{4v} symmetry, a triangular lattice with higher symmetry C_{6v} was considered. A generalized coupled-wave equation was derived by introducing six basic waves into the coupled-wave model for both Γ -point and non- Γ -point modes. The key point is the careful treatment of the more complicated overlaps between the polarized fields. The derived coupled-wave equation actually is applicable to any type of centered-rectangular lattice with C_{2v} by simply replacing the basic wave terms. By solving the derived finite-size coupled-wave equation on a hexagonal grid, we studied the band structure, radiation constant, threshold gain, field intensity profiles, and FFP of the resonant modes. Comparison with experiments confirms the accuracy and the validity of our theoretical analysis. Furthermore, we also demonstrated the lasing monopole mode can be switched to the hexapole mode by using a larger air-hole size. The second part presented extension for air-hole geometry with arbitrary sidewalls. In other words, the refractive index of the air holes within the PC layer are not restricted to the perfectly uniform case and instead can be nonuniform along the vertical direction. To realize this purpose, we modified the 3D coupled-wave equation by incorporating the refractive index distribution in the vertical direction. Then, as an example, we studied tapered sidewalls with both symmetric and asymmetric in-plane air-hole shapes. We found that the surface emission properties can be significantly modified by appropriately introducing the vertical asymmetry. Accordingly, the FFPs and the polarization profiles of the output beam can be engineered in a larger freedom. These findings well explained the most recently experimental results of PCSELs fabricated using MOCVD or MBE methods.

Chapter 6 was dedicated to developing an above-threshold laser model. In the above-threshold regime, an inhomogeneous spatial distributions of photon density induces a nonuniform carrier density, and therefore the refractive index and spatial gain. This so-called spatial hole burning (SHB) in turn modifies the optical modal field profile and may critically influence the mode stability of the laser cavity above the laser threshold. To model this SHB effect, we incorporated the laser rate equations into the 3D coupled-wave equation in which a spatially-varying effective refractive index and gain

were considered. The derived coupled-wave equation was a nonlinear equation and can be solved self-consistently. Next, by solving the nonlinear coupled-wave equation, we investigate the evolution of the field intensity distributions and threshold gain of the fundamental lasing mode. We found that the field intensity distribution is flattened with increasing increasing current and the total effective threshold gain also increased due to the increased in-plane loss. By further performing the similar analysis for the high-order band-edge modes, we also found that threshold gain of the high-order modes was reduced because of the enhanced spatial overlap between these modes and the modified spatial gain. This finally degraded the single-mode stability and resulted in multimode lasing. These quantitative study of the above-threshold behavior well explained the mode competition observed experimentally in the end of chapter 4. Finally, several promising methods for mitigating SHB effects are suggested and discussed.

7.2 Perspectives on future work

The theory developed in this work not only provides analytical insights into complex wave interaction inside PCSELs, but also can be applied to further optimizing the design of PCSELs for various applications. Though we have limited our attention to the case of TE polarization, the extension to TM polarization is straightforward. By incorporating the SHB effect, the CWT theory has now evolved into a more practical laser solver. Yet, a laser diode is a fairly complex system in which electrical, electro-optic, and thermal phenomena constantly interact in a nonlinear way. Describing all these phenomena in full detail may lead to a theoretical model that is far too complex to work with. On the other hand, introducing too much simplification may degrade the accuracy and validity of a laser model. Therefore, the right trade-off is required. This also depends on the laser characteristic being investigated. For high-power PCSELs, further investigation of thermal effects, carrier diffusion, and gain saturation is necessary. To this end, our basic methodology developed for the nonlinear CWT can be adopted and further exploited to combine new physical processes.

As a new type of semiconductor laser born in the late 1990s, PCSELs have experienced several breakthroughs which underpin its promising potential to realize various functionalities that conventional semiconductor lasers can not. There are still a wide range of choices for PC geometries that can be explored to realize other totally new functionalities and further optimization. The 3D CWT described in this thesis enables us to investigate PC structures in a large design space. Systematic study of the effects of various PC geometries on the output of the device might open new directions of future research for improving the device performance.

Appendix A

Energy conservation theorem for PCSELS

The coupled-wave Eqs. (4.15-4.18) can be rewritten as

$$-i(\delta + i\alpha)R_x = \partial R_x / \partial x - i(C_{11}R_x + C_{12}S_x + C_{13}R_y + C_{14}S_y), \quad (\text{A1})$$

$$-i(\delta + i\alpha)S_x = -\partial S_x / \partial x - i(C_{21}R_x + C_{22}S_x + C_{23}R_y + C_{24}S_y), \quad (\text{A2})$$

$$-i(\delta + i\alpha)R_y = \partial R_y / \partial y - i(C_{31}R_x + C_{32}S_x + C_{33}R_y + C_{34}S_y), \quad (\text{A3})$$

$$-i(\delta + i\alpha)S_y = -\partial S_y / \partial y - i(C_{41}R_x + C_{42}S_x + C_{43}R_y + C_{44}S_y), \quad (\text{A4})$$

where $C_{ij}(1 \leq i, j \leq 4) = C_{1D,ij} + C_{rad,ij} + C_{2D,ij}$ [see Eqs. (3.31)-(3.33)]. Multiplying Eq. (A1) by R_x^* , Eq. (A2) by S_x^* , Eq. (A3) by R_y^* , and Eq. (A4) by S_y^* , and adding the four equations and their conjugates, we obtain

$$\begin{aligned} 2\alpha(|R_x|^2 + |S_x|^2 + |R_y|^2 + |S_y|^2) = & \frac{\partial}{\partial x}(|R_x|^2 - |S_x|^2) + \frac{\partial}{\partial y}(|R_y|^2 - |S_y|^2) \\ & + 2\kappa_{v,i}(|\xi_{-1,0}R_x + \xi_{1,0}S_x|^2 + |\xi_{0,-1}R_y + \xi_{0,1}S_y|^2), \end{aligned} \quad (\text{A5})$$

where the $C_{1D,ij}$ and $C_{2D,ij}$ terms have vanished due to their Hermitian property, and only the term $\kappa_{v,i} = -Im\{\frac{k_0^4}{2\beta_0} \iint_{PC} G(z, z')\Theta_0(z')\Theta_0^*(z)dz'dz\}$ which is closely associated with the out-of-plane coupling remains [see Eq. (3.34)]. In order to model the power flow in the 2D PCSELS, we integrate Eq. (A5) over the whole laser cavity area, i.e.,

$0 \leq x, y \leq L$. Then we have

$$\begin{aligned}
2\alpha \int_0^L \int_0^L (|R_x|^2 + |S_x|^2 + |R_y|^2 + |S_y|^2) dx dy = \\
\int_0^L \int_0^L \left[\frac{\partial}{\partial x} (|R_x|^2 - |S_x|^2) + \frac{\partial}{\partial y} (|R_y|^2 - |S_y|^2) \right] dx dy \\
+ 2\kappa_{v,i} \int_0^L \int_0^L (|\xi_{-1,0}R_x + \xi_{1,0}S_x|^2 + |\xi_{0,-1}R_y + \xi_{0,1}S_y|^2) dx dy.
\end{aligned} \tag{A6}$$

For a laser structure with boundary condition given by Eq. (4.22), the field amplitudes of basic waves at the four edges can be expressed as

$$\begin{aligned}
R_x(0, y) &= 0, \quad S_x(0, y) = S_{ex}(y), \\
R_x(L, y) &= R_{ex}(y), \quad S_x(L, y) = 0, \\
R_y(x, 0) &= 0, \quad S_y(x, 0) = S_{ey}(x), \\
R_y(x, L) &= R_{ey}(x), \quad S_y(x, L) = 0.
\end{aligned} \tag{A7}$$

Then Eq. (A6) can be written as

$$P_{stim} = P_{edge} + P_{rad}, \tag{A8}$$

if we define

$$P_{stim} = 2\alpha \int_0^L \int_0^L (|R_x|^2 + |S_x|^2 + |R_y|^2 + |S_y|^2) dx dy, \tag{A9}$$

$$P_{edge} = \int_0^L (|R_{ex}|^2 + |S_{ex}|^2) dy + \int_0^L (|R_{ey}|^2 + |S_{ey}|^2) dx, \tag{A10}$$

$$P_{rad} = 2\kappa_{v,i} \int_0^L \int_0^L (|\xi_{-1,0}R_x + \xi_{1,0}S_x|^2 + |\xi_{0,-1}R_y + \xi_{0,1}S_y|^2) dx dy. \tag{A11}$$

Here, P_{stim} describes the total stimulated power inside the laser structure, P_{edge} represents the power escaping from the edges of the laser cavity (i.e. the in-plane loss), and P_{rad} represents the radiation power emitted from the device surface [note that this quantity is proportional to the intensity of the radiative waves described by Eqs. (3.20a-3.20b)], respectively. Equation (A8) states the fact that the power generated inside the laser structure is equal to the sum of the power escaping from the edges of the structure and the surface radiation power.

Appendix B

Solutions of radiative and high-order waves within triangular lattice PCs

The radiative and high-order waves [i.e., $E_{x,m',n'}$ and $E_{y,m',n'}$ in Eq. (5.15)] can be solved in a manner similar to that described in our previous works [84, 87]. The major difference is that the number of basic waves that serve as sources to excite radiative and high-order waves are six in this case, instead of four. Therefore, we shall only show the final analytical solutions.

The radiative waves (for which $m = n = 0$) can be expressed as

$$\begin{pmatrix} \Delta E_x \\ \Delta E_y \end{pmatrix} = k_0^2 \int_{PC} G(z, z') \Theta_0(z') dz' \cdot \begin{pmatrix} \xi_{-1,0}\rho_{1,0} & \xi_{1,0}\rho_{-1,0} & \xi_{0,-1}\rho_{0,1} & \xi_{0,1}\rho_{0,-1} & \xi_{-1,-1}\rho_{1,1} & \xi_{1,1}\rho_{-1,-1} \\ \xi_{-1,0}\eta_{1,0} & \xi_{1,0}\eta_{-1,0} & \xi_{0,-1}\eta_{0,1} & \xi_{0,1}\eta_{0,-1} & \xi_{-1,-1}\eta_{1,1} & \xi_{1,1}\eta_{-1,-1} \end{pmatrix} \cdot \mathbf{V}, \quad (\text{B1})$$

where $G(z, z') = -i/2\beta_z \cdot e^{-i\beta_z|z-z'|}$ is an approximated Green's function [84, 85], $\beta_z = k_0 n_0(z)$, and $\mathbf{V} = (R_1, S_1, R_2, S_2, R_3, S_3)^t$.

The integrals of high-order waves (for which $|m^2 + n^2| > 1$) included in the second term of the right-hand side of the coupled-wave Eq. (5.15) can be expressed as

$$\begin{aligned}
 & \begin{pmatrix} \int_{PC} E_{x,m,n}(z) \Theta_0^*(z) dz \\ \int_{PC} E_{y,m,n}(z) \Theta_0^*(z) dz \end{pmatrix} \\
 &= \frac{1}{m_x^2 + n_y^2} \begin{pmatrix} n_y & m_x \\ -m_x & n_y \end{pmatrix} \begin{pmatrix} \mu_{m,n}^{(1,0)} & \mu_{m,n}^{(-1,0)} & \mu_{m,n}^{(0,1)} & \mu_{m,n}^{(0,-1)} & \mu_{m,n}^{(1,1)} & \mu_{m,n}^{(-1,-1)} \\ \nu_{m,n}^{(1,0)} & \nu_{m,n}^{(-1,0)} & \nu_{m,n}^{(0,1)} & \nu_{m,n}^{(0,-1)} & \nu_{m,n}^{(1,1)} & \nu_{m,n}^{(-1,-1)} \end{pmatrix} \cdot \mathbf{V} \\
 &\equiv \begin{pmatrix} \varsigma_{x,m,n}^{(1,0)} & \varsigma_{x,m,n}^{(-1,0)} & \varsigma_{x,m,n}^{(0,1)} & \varsigma_{x,m,n}^{(0,-1)} & \varsigma_{x,m,n}^{(1,1)} & \varsigma_{x,m,n}^{(-1,-1)} \\ \varsigma_{y,m,n}^{(1,0)} & \varsigma_{y,m,n}^{(-1,0)} & \varsigma_{y,m,n}^{(0,1)} & \varsigma_{y,m,n}^{(0,-1)} & \varsigma_{y,m,n}^{(1,1)} & \varsigma_{y,m,n}^{(-1,-1)} \end{pmatrix} \cdot \mathbf{V}, \quad (\text{B2})
 \end{aligned}$$

where

$$\mu_{mn}^{(rs)} = k_0^2 \iint_{PC} \xi_{m-r, n-s} (n_y \rho_{rs} - m_x \eta_{rs}) G_{m,n}(z, z') \Theta_0(z') \Theta_0^*(z) dz' dz, \quad (\text{B3})$$

$$\nu_{mn}^{(rs)} = - \int_{PC} \frac{1}{n_0^2} \xi_{m-r, n-s} (m_x \rho_{rs} + n_y \eta_{rs}) |\Theta_0(z)|^2 dz, \quad (\text{B4})$$

$$G_{m,n}(z, z') = \frac{1}{2\beta_{z,m,n}} e^{-\beta_{z,m,n}|z-z'|}, \quad \beta_{z,m,n} = \sqrt{(m_x^2 + n_y^2)\beta_0^2 - k_0^2 n_0^2(z)}. \quad (\text{B5})$$

As a consequence, the overlap integrals appearing on the right-hand side of Eq. (5.15) can be replaced by terms only associated with basic waves. Finally, a coupled-wave equation for infinite periodic structures [for which the derivative terms in Eq. (5.15) are neglected] can be written in the matrix form as

$$(\delta + i\alpha)\mathbf{V} = \mathbf{C}\mathbf{V}, \quad (\text{B6})$$

where $\mathbf{C}$ is a 6×6 matrix. The matrix elements of $\mathbf{C}$ can be written as

$$\mathbf{C} = \mathbf{d}\mathbf{k}_{0,mn} + \mathbf{C}_b + \mathbf{C}_r + \mathbf{C}_h, \quad (\text{B7})$$

where

$$\mathbf{d}\mathbf{k}_{0,mn} = \begin{pmatrix} dk_{0;1,0} & 0 & 0 & 0 & 0 & 0 \\ 0 & dk_{0;-1,0} & 0 & 0 & 0 & 0 \\ 0 & 0 & dk_{0;0,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & dk_{0;0,-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & dk_{0;1,1} & 0 \\ 0 & 0 & 0 & 0 & 0 & dk_{0;-1,-1} \end{pmatrix}, \quad (\text{B8})$$

$$\mathbf{C}_b = \begin{pmatrix} 0 & \kappa_{1,0}^{(-1,0)} & \kappa_{1,0}^{(0,1)} & \kappa_{1,0}^{(0,-1)} & \kappa_{1,0}^{(1,1)} & \kappa_{1,0}^{(-1,-1)} \\ \kappa_{-1,0}^{(1,0)} & 0 & \kappa_{-1,0}^{(0,1)} & \kappa_{-1,0}^{(0,-1)} & \kappa_{-1,0}^{(1,1)} & \kappa_{-1,0}^{(-1,-1)} \\ \kappa_{0,1}^{(1,0)} & \kappa_{0,1}^{(-1,0)} & 0 & \kappa_{0,1}^{(0,-1)} & \kappa_{0,1}^{(1,1)} & \kappa_{0,1}^{(-1,-1)} \\ \kappa_{0,-1}^{(1,0)} & \kappa_{0,-1}^{(-1,0)} & \kappa_{0,-1}^{(0,1)} & 0 & \kappa_{0,-1}^{(1,1)} & \kappa_{0,-1}^{(-1,-1)} \\ \kappa_{1,1}^{(1,0)} & \kappa_{1,1}^{(-1,0)} & \kappa_{1,1}^{(0,1)} & \kappa_{1,1}^{(0,-1)} & 0 & \kappa_{1,1}^{(-1,-1)} \\ \kappa_{-1,-1}^{(1,0)} & \kappa_{-1,-1}^{(-1,0)} & \kappa_{-1,-1}^{(0,1)} & \kappa_{-1,-1}^{(0,-1)} & \kappa_{-1,-1}^{(1,1)} & 0 \end{pmatrix}, \quad (\text{B9})$$

$$\mathbf{C}_r = \begin{pmatrix} \zeta_{1,0}^{(1,0)} & \zeta_{1,0}^{(-1,0)} & \zeta_{1,0}^{(0,1)} & \zeta_{1,0}^{(0,-1)} & \zeta_{1,0}^{(1,1)} & \zeta_{1,0}^{(-1,-1)} \\ \zeta_{-1,0}^{(1,0)} & \zeta_{-1,0}^{(-1,0)} & \zeta_{-1,0}^{(0,1)} & \zeta_{-1,0}^{(0,-1)} & \zeta_{-1,0}^{(1,1)} & \zeta_{-1,0}^{(-1,-1)} \\ \zeta_{0,1}^{(1,0)} & \zeta_{0,1}^{(-1,0)} & \zeta_{0,1}^{(0,1)} & \zeta_{0,1}^{(0,-1)} & \zeta_{0,1}^{(1,1)} & \zeta_{0,1}^{(-1,-1)} \\ \zeta_{0,-1}^{(1,0)} & \zeta_{0,-1}^{(-1,0)} & \zeta_{0,-1}^{(0,1)} & \zeta_{0,-1}^{(0,-1)} & \zeta_{0,-1}^{(1,1)} & \zeta_{0,-1}^{(-1,-1)} \\ \zeta_{1,1}^{(1,0)} & \zeta_{1,1}^{(-1,0)} & \zeta_{1,1}^{(0,1)} & \zeta_{1,1}^{(0,-1)} & \zeta_{1,1}^{(1,1)} & \zeta_{1,1}^{(-1,-1)} \\ \zeta_{-1,-1}^{(1,0)} & \zeta_{-1,-1}^{(-1,0)} & \zeta_{-1,-1}^{(0,1)} & \zeta_{-1,-1}^{(0,-1)} & \zeta_{-1,-1}^{(1,1)} & \zeta_{-1,-1}^{(-1,-1)} \end{pmatrix}, \quad (\text{B10})$$

$$\mathbf{C}_h = \begin{pmatrix} \chi_{1,0}^{(1,0)} & \chi_{1,0}^{(-1,0)} & \chi_{1,0}^{(0,1)} & \chi_{1,0}^{(0,-1)} & \chi_{1,0}^{(1,1)} & \chi_{1,0}^{(-1,-1)} \\ \chi_{-1,0}^{(1,0)} & \chi_{-1,0}^{(-1,0)} & \chi_{-1,0}^{(0,1)} & \chi_{-1,0}^{(0,-1)} & \chi_{-1,0}^{(1,1)} & \chi_{-1,0}^{(-1,-1)} \\ \chi_{0,1}^{(1,0)} & \chi_{0,1}^{(-1,0)} & \chi_{0,1}^{(0,1)} & \chi_{0,1}^{(0,-1)} & \chi_{0,1}^{(1,1)} & \chi_{0,1}^{(-1,-1)} \\ \chi_{0,-1}^{(1,0)} & \chi_{0,-1}^{(-1,0)} & \chi_{0,-1}^{(0,1)} & \chi_{0,-1}^{(0,-1)} & \chi_{0,-1}^{(1,1)} & \chi_{0,-1}^{(-1,-1)} \\ \chi_{1,1}^{(1,0)} & \chi_{1,1}^{(-1,0)} & \chi_{1,1}^{(0,1)} & \chi_{1,1}^{(0,-1)} & \chi_{1,1}^{(1,1)} & \chi_{1,1}^{(-1,-1)} \\ \chi_{-1,-1}^{(1,0)} & \chi_{-1,-1}^{(-1,0)} & \chi_{-1,-1}^{(0,1)} & \chi_{-1,-1}^{(0,-1)} & \chi_{-1,-1}^{(1,1)} & \chi_{-1,-1}^{(-1,-1)} \end{pmatrix}, \quad (\text{B11})$$

and

$$dk_{0;m,n} = (\sqrt{m_x(m,n)^2 + n_y(m,n)^2} - 1)\beta_0, \quad (\text{B12})$$

$$\zeta_{mn}^{(rs)} = -\frac{k_0^4}{2\beta_0} \iint_{PC} \xi_{m,n} \xi_{-r,-s} (\rho_{mn} \rho_{rs} + \eta_{mn} \eta_{rs}) G(z, z') \Theta_0(z') \Theta_0^*(z) dz' d\mathbf{x} \quad (\text{B13})$$

$$\chi_{mn}^{(rs)} = -\frac{k_0^2}{2\beta_0} \sum_{\sqrt{m'^2+n'^2} > 1} \xi_{m-m', n-n'} (\rho_{mn} \zeta_{x,m',n'}^{(rs)} + \eta_{mn} \zeta_{y,m',n'}^{(rs)}). \quad (\text{B14})$$

Here, a large number of high-order waves are included by truncating the summation terms in Eq. (B14) at $|m', n'| \leq 10$ [84]. Note that the matrix $\mathbf{dk}_{0,mn}$ represents the variation of the in-plane wavenumbers resulting from deviation of the individual basic wave vectors from the second-order Γ point, and $\mathbf{C}_b$, $\mathbf{C}_r$, and $\mathbf{C}_h$ correspond to the coupling effects of basic, radiative, and high-order waves, respectively.

Bibliography

- [1] T. H. Maiman, “Stimulated optical radiation in ruby,” *Nature (London)* **187**, 493 (1960).
- [2] M. Yano, H. Nishi, and M. Takusagawa, “Theoretical and experimental study of threshold characteristics in InGaAsP/InP DH lasers,” *IEEE J. Quantum Electron.* **15**, 571-579 (1979).
- [3] H. Kogelnik and C. V. Shank, “Stimulated emission in a periodic structure,” *Appl. Phys. Lett.* **18**, 152 (1971).
- [4] K. Aiki, M. Nakamura, J. Umeda, A. Yariv, A. Katzir, and H. W. Yen, “GaAs-GaAlAs distributed-feedback diode lasers with separate optical and carrier confinement,” *Appl. Phys. Lett.*, **27**, 145 (1975).
- [5] K. Utaka, K. Akiba, K. Sakai, and Y. Matsushima. “Room-temperature CW operation of distributed-feedback buried-heterostructure InGaAsP/InP lasers emitting at $1.57\text{ }\mu\text{m}$,” *Electron. Lett.*, **17**, 961-963, (1981).
- [6] C. H. Henry, R. F. Kazarinov, R. A. Logan, and R. Yen, “Observation of destructive interference in the radiation loss of second-order distributed feedback lasers,” *IEEE J. Quantum Electron.* **21**, 151–154 (1985).
- [7] K. Kojima, S. Noda, K. Mitsunaga, K. Kyuma, and K. Hamanaka, “Continuous wave operation of a surface-emitting AlGaAs/GaAs multiquantum well distributed Bragg reflector laser,” *Appl. Phys. Lett.* **50**, 1705 (1987).
- [8] S. H. Macomber, J. S. Mott, R. J. Noll, G. M. Gallatin, E. J. Gratrix, S. L. O’Dwyer, and S. A. Lambert, “Surface-emitting distributed feedback semiconductor laser,” *Appl. Phys. Lett.* **51**, 472-474 (1987).
- [9] K. Iga, “Surface-emitting laser—its birth and generation of new optoelectronics field,” *IEEE J. Sel. Top. Quant. Electron.*, **6**, 1201-1215 (2000).
- [10] F. Koyama, “Recent advances of VCSEL photonics,” *J. Lightwave Technol.*, **24**, 4502-4513, (2006).

- [11] R. M. Michalzik (ed.) *VCSELs: Fundamentals, Technology, and applications of Vertical-Cavity Surface-Emitting Lasers* (Springer, 2013).
- [12] S. L. McCall, A. F. J. Levi, R. E. Slusher, S. J. Pearton, and R. A. Logan. “Whispering-gallery mode microdisk lasers,” *Appl. Phys. Lett.*, **60**, 289-291, (1992).
- [13] C. Gmachl, F. Capasso, E. E. Narimanov, J. U. Nockel, A. D. Stone, J. Faist, D. L. Sivco, and A. Y. Cho, “High-power directional emission from microlasers with chaotic resonators,” *Science*, **280**, 1556-1564, (1998).
- [14] J. Wiersig and M. Hentschel, “Combining directional light output and ultralow loss in deformed microdisks,” *Phys. Rev. Lett.*, **100** 033901, (2008).
- [15] M. Fujita and T. Baba, “Microgear laser,” *Appl. Phys. Lett.*, **80**, 2051-2053, (2002).
- [16] Y. Zhang, C. Hamsen, J. T. Choy, Y. Huang, J. H. Ryou, R. D. Dupuis, and M. Loncar, *Opt. Lett.*, **36**, 2704-2706, (2011).
- [17] A. J. Danner, T. S. Kim, and K. D. Choquette, “Single fundamental mode photonic crystal vertical cavity laser with improved output power,” *Electron. Lett.*, **41**, 325-326 (2005).
- [18] K. H. Lee, J. H. Baek, I. K. Hwang, Y. H. Lee, G. H. Lee, J. H. Ser, H. D. Kim, and H. E. Shin, “Square-lattice photonic-crystal vertical-cavity surface-emitting lasers,” *Opt. Express* **12**, 4136-4143 (2004).
- [19] K. D. Choquette, D. F. Siriani, A. M. Kasten, M. P. Tan, J. D. Sulkin, P. O. Leisher, J. J. Raftery Jr., and A. J. Danner, “Single mode photonic crystal vertical cavity surface emitting lasers,” *Advances in Optical Technologies*, 280920 (2012).
- [20] M. C. Y. Huang, Y. Zhou, and C. J. Chang-Hasnain, “A surface-emitting laser incorporating a high index- contrast subwavelength grating,” *Nat. Photonics* **1**, 119-122 (2007).
- [21] H. Yang, D. Zhao, S. Chuwongin, J-H. Seo, W. Yang, Y. Shuai, J. Berggren, M. Hammar, Z. Ma, and W. Zhou, “Transfer-printed stacked nanomembrane lasers on silicon,” *Nat. Photonics* **6**, 615-620 (2012).
- [22] O. Painter, R. K. Lee, A. Scherer, A. Yariv, J. D. O’ Brien, P. D. Dapkus, and I. Kim, “Two-dimensional photonic band-gap defect mode laser,” *Science* **284**, 1819-1821 (1999).
- [23] H. G. Park, S. H. Kim, S. H. Kwon, Y. G. Ju, J. K. Yang, J. H. Baek, S. B. Kim, and Y. H. Lee, “Electrically driven single-cell photonic crystal laser,” *Science* **305**, 1444-1447 (2004).

- [24] B. Ellis, M. A. Mayer, G. Shambat, T. Sarmiento, J. Harris, E. E. Haller, and J. Vuckovic, "Ultralow-threshold electrically pumped quantum-dot photonic-crystal nanocavity laser," *Nat. Photonics* **5**, 297-300 (2011).
- [25] S. Matsuo, A. Shinya, T. Kakitsuka, K. Nozaki, T. Segawa, T. Sato, Y. Kawaguchi, and M. Notomi, "High-speed ultracompact buried heterostructure photonic-crystal laser with 13 fJ of energy consumed per bit transmitted," *Nat. Photonics* **4**, 648-654 (2010).
- [26] K. Takeda, T. Sato, A. Shinya, K. Nozaki, W. Kobayashi, H. Taniyama, M. Notomi, K. Hasebe, T. Kakitsuka, and S. Matsuo, "Few-fJ/bit data transmissions using directly modulated lambda-scale embedded active region photonic-crystal lasers," *Nat. Photonics* **7**, 569-575 (2013).
- [27] M. Imada, S. Noda, A. Chutinan, T. Tokuda, M. Murata, and G. Sasaki, "Coherent two-dimensional lasing action in surface-emitting laser with triangular-lattice photonic crystal structure," *Appl. Phys. Lett.* **75**, 316 (1999).
- [28] M. Meier, A. Mekis, A. Dodabalapur, A. Timko, R. E. Slusher, J. D. Joannopoulos, and O. Nalamasu, *Appl. Phys. Lett.* **74**, 7 (1999).
- [29] S. Noda, M. Yokoyama, M. Imada, A. Chutinan, and M. Mochizuki, "Polarization mode control of two-dimensional photonic crystal laser by unit cell structure design," *Science* **293**, 1123-1125 (2001).
- [30] M. Notomi, H. Suzuki, and T. Tamamura, "Directional lasing oscillation of two-dimensional organic photonic crystal lasers at several photonic band gaps," *Appl. Phys. Lett.* **78**, 1325 (2001).
- [31] M. Imada, A. Chutinan, S. Noda, and M. Mochizuki, "Multidirectionally distributed feedback photonic crystal lasers," *Phys. Rev. B* **65**, 195306 (2002).
- [32] G. A. Turnbull, P. Andrew, W. L. Barnes, and I. D. W. Samuel, "Operating characteristics of a semiconducting polymer laser pumped by a microchip laser," *Appl. Phys. Lett.* **82**, 313 (2003).
- [33] I. Vurgaftman and J. R. Meyer, "Design optimization for high-brightness surface-emitting photonic-crystal distributed-feedback lasers," *IEEE J. Quantum Electron.* **39**, 689-700 (2003).
- [34] D. Ohnishi, T. Okano, M. Imada, and S. Noda, "Room temperature continuous wave operation of a surface-emitting two-dimensional photonic crystal diode laser," *Opt. Express* **12**, 1562-1568 (2004).

- [35] E. Miyai, K. Sakai, T. Okano, W. Kunishi, D. Ohnishi, and S. Noda, "Lasers producing tailored beams," *Nature (London)* **441**, 946 (2006).
- [36] M. Kim, C. S. Kim, W. W. Bewley, J. R. Lindle, C. L. Canedy, I. Vurgaftman, and J. R. Meyer, "Surface-emitting photonic-crystal distributed-feedback laser for the midinfrared," *Appl. Phys. Lett.* **88**, 191105 (2006).
- [37] L. Sirigu, R. Terazzi, M. I. Amanti, M. Giovannini, and J. Faist, "Terahertz quantum cascade lasers based on two-dimensional photonic crystal resonators," *Opt. Express* **16**, 5206-5217 (2008).
- [38] Y. Chassagneux, R. Colombelli, W. Maineult, S. Barbieri, H. E. Beere, D. A. Ritchie, S. P. Khanna, E. H. Linfield, and A. G. Davies, "Electrically pumped photonic-crystal terahertz lasers controlled by boundary conditions," *Nature (London)* **457**, 174-178 (2009).
- [39] L. Mahler and A. Tredicucci, "Photonic engineering of surface-emitting terahertz quantum cascade lasers," *Laser Photonics Rev.* **5**, 647-658 (2011).
- [40] H. Matsubara, S. Yoshimoto, H. Saito, Y. Jianglin, Y. Tanaka, and S. Noda, "GaN photonic-crystal surface-emitting laser at blue-violet wavelengths," *Science* **319**, 445-447 (2008).
- [41] T. C. Lu, S. W. Chen, L. F. Lin, T. T. Kao, C. C. Kao, P. Yu, H. C. Kuo, and S. C. Wang, "GaN-based two-dimensional surface-emitting photonic crystal lasers with AlN/GaN distributed Bragg reflector," *Appl. Phys. Lett.* **92**, 011129 (2008).
- [42] Y. Kurosaka, S. Iwahashi, Y. Liang, K. Sakai, E. Miyai, W. Kunishi, D. Ohnishi, and S. Noda, "On-chip beam-steering photonic-crystal lasers," *Nat. Photonics* **4**, 447-450 (2010).
- [43] S. Iwahashi, Y. Kurosaka, K. Sakai, K. Kitamura, N. Takayama, and S. Noda, "Higher-order vector beams produced by photonic-crystal lasers," *Opt. Express* **19**, 11963-11968 (2011).
- [44] S. Iwahashi, K. Sakai, Y. Kurosaka, and S. Noda, "Centered-rectangular lattice photonic-crystal surface-emitting lasers," *Phys. Rev. B* **85**, 035304 (2012).
- [45] M. Yokoyama and S. Noda, "Polarization mode control of two-dimensional photonic crystal laser having a square lattice structure," *IEEE J. Quantum Electron.* **39**, 1074-1080 (2003).
- [46] K. Sakai, E. Miyai, T. Sakaguchi, D. Ohnishi, T. Okano, and S. Noda, "Lasing band-edge identification for a surface-emitting photonic crystal laser," *IEEE J. Sel. Areas Commun.* **23**, 1335-1340 (2005).

- [47] E. Miyai and S. Noda, "Phase-shift effect on a two-dimensional surface-emitting photonic-crystal laser," *Appl. Phys. Lett.* **86**, 111113 (2005).
- [48] Y. Kurosaka, K. Sakai, E. Miyai, and S. Noda, "Controlling vertical optical confinement in two-dimensional two-dimensional surface-emitting photonic-crystal lasers by shape of air holes," *Opt. Express*, **16**, 18485 (2008).
- [49] Y. Kurosaka, K. Hirose, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, "Effects of non-lasing band in two-dimensional photonic-crystal lasers clarified using omnidirectional band structure," *Opt. Express*, **19**, 21773 (2012).
- [50] M. Nishimoto, K. Ishizaki, K. Maekawa, K. Kitamura, and S. Noda, "Air-Hole retained growth by molecular beam epitaxy for fabricating GaAs-based photonic-crystal lasers," *Appl. Phys. Express* **6**, 042002 (2013).
- [51] W. Kunishi, D. Ohnishi, E. Miyai, K. Sakai, and S. Noda, "High-power single-lobed surface-emitting photonic-crystal laser," in *Proceedings of The Conference on Lasers and Electro-Optics (CLEO), 2006*. CMKK1, Long Beach, May, 2006.
- [52] K. Otsuka, K. Sakai, Y. Kurosaka, J. Kashiwagi, W. Kunishi, D. Ohnishi, and S. Noda, in *Proceedings of the Lasers and Electro-Optics Society, 2007. LEOS 2007*. pp.562-563, Lake Buena Vista, FL, USA, 21-25 Oct. 2007.
- [53] T. Sakaguchi, W. Kunishi, S. Arimura, K. Nagase, E. Miyai, D. Ohnishi, K. Sakai, and S. Noda, "Surface-emitting photonic-crystal laser with 35W peak power," in *Proceedings of The Conference on Lasers and Electro-Optics (CLEO), 2009*. CTuH1, Baltimore, June, 2009.
- [54] K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, in *Proceedings of the Conference on Lasers and Electro-Optics Pacific Rim (CLEO-PR), 2013*, ThI1-4, Kyoto, Japan, 30 June-4 July 2013.
- [55] K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, "High power photonic crystal surface emitting lasers under CW Condition," 14a-B1-2, JSAP, Fall (2012).
- [56] K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, "High power photonic crystal surface emitting lasers," 28p-C1-18, JSAP, Spring (2013).
- [57] K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, "High power photonic crystal surface emitting lasers," 18p-A3-10, JSAP, Fall (2013).
- [58] K. Sakai, *Two dimensional coupled-wave theory for two-dimensional photonic-crystal lasers*. PhD thesis, Kyoto University, Kyoto, Japan. 2007.

- [59] J. Kashiwagi, *Study on high-power operation of two-dimensional photonic-crystal lasers*. Master thesis, Kyoto University, Kyoto, Japan. 2008.
- [60] K. Otsuka, *Study on lasing area enlargement and stability of two-dimensional photonic-crystal lasers*. Master thesis, Kyoto University, Kyoto, Japan. 2009.
- [61] M. Toda, “Proposed cross grating single-mode DFB laser,” *IEEE J. Quantum Electron.* **28**, 1653-1662, (1992).
- [62] K. Sakai, E. Miyai, and S. Noda, “Coupled-wave model for square-lattice two-dimensional photonic crystal with transverse-electric-like mode,” *Appl. Phys. Lett.* **89**, 021101 (2006).
- [63] K. Sakai, E. Miyai, and S. Noda, “Coupled-wave theory for square-lattice photonic crystal lasers with TE polarization,” *IEEE J. Quantum Electron.* **46**, 788-795 (2010).
- [64] M. Koba and P. Szczepanski, “The threshold mode structure analysis of the two-dimensional photonic crystal lasers,” *Prog. Electromagn. Res.* **125**, 365–389 (2012).
- [65] H. Kogelnik and C. V. Shank, “Coupled-wave theory of distributed feedback lasers,” *J. Appl. Phys.* **43**, 2327-2335 (1972).
- [66] W. Streifer, D. R. Scifres and R. D. Burnham, “Coupled wave analysis of DFB and DBR lasers” *IEEE J. Quantum Electron.* **13**, 134-141 (1977).
- [67] R. F. Kazarinov and C. H. Henry, “Second-order distributed feedback lasers with mode selection provided by first-order radiation losses,” *IEEE J. Quantum Electron.* **21**, 144-150 (1985).
- [68] W. Streifer, D. R. Scifres, and R. Burnham, “Analysis of grating-coupled radiation in GaAs: GaAlAs lasers and waveguides-I,” *IEEE J. Quantum Electron.* **12**, 422-428 (1976).
- [69] D. Rosenblatt, A. Sharon, and A. Friesem, “Resonant grating waveguide structures,” *IEEE J. Quantum Electron.* **33**, 2038 (1997).
- [70] K. Sakoda, “Symmetry, degeneracy, and uncoupled modes in two-dimensional photonic lattices,” *Phys. Rev. B* **52**, 7982 (1995).
- [71] R. J. P. Engelen, D. Mori, T. Baba, and L. Kuipers, “Subwavelength structure of the evanescent field of an optical Bloch wave,” *Phys. Rev. Lett.* **102**, 023902 (2009).
- [72] K. Forberich, M. Diem, J. Crewett, U. Lemmer, A. Gombert, and K. Busch, “Lasing action in two-dimensional organic photonic crystal lasers with hexagonal symmetry,” *Appl. Phys. B* **82**, 539–541 (2006).

- [73] W. H. Weber, S. L. McCarthy, and G. W. Ford, "Perturbation Theory Applied to Gain or Loss in an Optical Waveguide," *Applied Optics*, **13**, 715 (1974).
- [74] M. J. Bergmann and H. C. Casey, "Optical-field calculations for lossy multiple-layer Al_xGa_{1-x}N/In_xGa_{1-x}N laser diodes," *J. Appl. Phys.* **84**, 1196 (1998).
- [75] M. Plihal and A. A. Maradudin, "Photonic band structure of two-dimensional systems: The triangular lattice," *Phys. Rev. B* **44**, 8565 (1991).
- [76] M. Plihal, A. Shambrook, and A. A. Maradudin, "Two-dimensional photonic band structures," *Opt. Commun.* **80**, 199 (1991).
- [77] S. Fan and J. D. Joannopoulos, "Analysis of guided resonances in photonic crystal slabs," *Phys. Rev. B* **65**, 235112 (2002).
- [78] H. Y. Ryu, M. Notomi, and Y. H. Lee, "Finite-difference time-domain investigation of band-edge resonant modes in finite-size two-dimensional photonic crystal slab," *Phys. Rev. B* **68**, 045209 (2003).
- [79] M. Yokoyama and S. Noda, "Finite-difference time-domain simulation of two-dimensional photonic crystal surface-emitting laser," *Opt. Express* **13**, 2869–2880 (2005).
- [80] A. F. Oskooi, D. Roundy, M. Ibanescu, P. Bermel, J. Joannopoulos, and S. G. Johnson, "Meep: A flexible free- software package for electromagnetic simulations by the FDTD method," *Comp. Phys. Commun.* **181**, 687 (2010).
- [81] K. S. Yee, *IEEE Trans. Antennas Propag.* **14**, 302 (1966).
- [82] D. H. Sheen, K. Tuncay, C. E. Baag, and P. J. Ortoleva, "Parallel implementation of a velocity-stress staggered-grid finite-difference method for 2-D poroelastic wave propagation," *Comput. Geosci.* **32**, 1182-1191 (2006).
- [83] A. Taflov and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed. (Artech House, Norwood, 2005).
- [84] Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, "Three-dimensional coupled-wave model for square-lattice photonic-crystal lasers with transverse electric polarization: A general approach," *Phys. Rev. B* **84**, 195119 (2011).
- [85] C. Peng, Y. Liang, K. Sakai, S. Iwahashi, and S. Noda, "Coupled-wave analysis for photonic-crystal surface-emitting lasers on air-holes with arbitrary sidewalls," *Opt. Express* **19**, 24672-24686 (2011).

- [86] Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, “Three-dimensional coupled-wave analysis for square-lattice photonic-crystal lasers with transverse electric polarization: Finite-size effects,” *Opt. Express* **20**, 15945–15961 (2012).
- [87] C. Peng, Y. Liang, K. Sakai, S. Iwahashi, and S. Noda, “Three-dimensional coupled-wave theory analysis of centered-rectangular lattice photonic crystal with transverse-electric-like mode,” *Phys. Rev. B* **86**, 035108 (2012).
- [88] Y. Liang, C. Peng, K. Ishizaki, S. Iwahashi, K. Sakai, Y. Tanaka, K. Kitamura, and S. Noda, “Three-dimensional coupled-wave analysis for triangular-lattice photonic-crystal surface-emitting lasers with transverse-electric polarization,” **21**, 565–580 (2013).
- [89] Fundamentally, radiation fields emitted from the center of the laser cavity have similar properties to those emitted from an infinite periodic structure described in Ref. [84]. Unlike CC air holes, Fourier coefficients ($\xi_{m,n}$) of the dielectric function $\epsilon(\mathbf{r})$ for ET air holes are complex numbers. Therefore, the radiation field intensity is proportional to $|\xi_{-1,0}R_x + \xi_{1,0}S_x|^2$ [see Eqs. (3.20a-3.20b)]. These complex Fourier coefficient terms multiplied to basic waves may change the phase difference of the waves diffracted vertically, resulting in a suppression of the destructive interference.
- [90] H. A. Haus, “Gain saturation in distributed feedback lasers,” *Appl. Opt.* **14**, 2650-2652 (1975).
- [91] H. Soda, Y. Kotaki, H. Sudo, H. Ishikawa, S. Yamakoshi, and H. Imai, “Stability in single longitudinal mode operation in GaInAsP/InP phase-adjusted DFB lasers,” *IEEE J. Quantum Electron.*, **23**, 804-814, (1987).
- [92] G. P. Agrawal and A. H. Bobech, “Modeling of distributed feedback semiconductor lasers with axially-varying parameters,” *IEEE J. Quantum Electron.*, **24**, 2407-2414, (1988).
- [93] J. E. A. Whiteaway, G. H. B. Thompson, A. J. Collar, and C. J. Armistead, “The design and assessment of $\lambda/4$ phase-shifted DFB laser structures,” *IEEE J. Quantum Electron.*, **25**, 1261-1279, (1989).
- [94] J. E. A. Whiteaway, B. Garrett, G. H. B. Thompson, A. J. Collar, C. J. Armistead, and M. J. Fice, “The static and dynamic characteristics of single and multiple phase-shifted DFB laser structures,” *IEEE J. Quantum Electron.*, **28**, 1277, (1992).
- [95] S. H. Macomber, “Nonlinear analysis of surface-emitting distributed feedback lasers,” *IEEE J. Quantum Electron.* **26**, 2065-2074 (1990).

- [96] A. A. Ukhanov, A. Stintz, P. G. Eliseev, and K. J. Malloy, "Comparison of the carrier induced refractive index, gain, and linewidth enhancement factor in quantum dot and quantum well lasers," *Appl. Phys. Lett.* **84**, 1058 (2004).
- [97] A. Yariv, *Quantum Electronics*, 3rd ed., Wiley, New York, 1989.
- [98] S. L. Chuang, *Physics of Optoelectronic Devices*, 2nd ed., Wiley, New York, 2009.
- [99] M. C. Wu, Y. Lo, and S. Wang, "Linewidth broadening due to longitudinal spatial hole burning in a long distributed feedback laser," *Appl. Phys. Lett.* **52**, 1119 (1988).
- [100] W. Fang, A. Hsu, S. L. Chuang, T. Tanbun-Ek, and A. M. Sergent, "Measurement and modeling of distributed-feedback lasers with spatial hole burning," *IEEE J. Select. Topics Quantum Electron.*, **3**, 547-554, (1997).
- [101] S. F. Yu, L. M. Zhang, R. G. S. Plumb, and J. E. Carroll, "Effect of external reflectors on radiation profile of grating coupled surface emitting lasers," *IEEE Proceedings-J.* **140**, 30-38 (1993).
- [102] W. Fang, C. Bethea, Y. Chen, and S. Chuang, "Longitudinal spatial inhomogeneities in high-power semiconductor lasers," *IEEE J. Select. Topics Quantum Electron.*, **1**, 117-128 (1995).
- [103] W. Fang, C. Bethea, Y. Chen, and S. Chuang, "Measurement and modeling of distributed-feedback lasers with spatial hole-burning," *IEEE J. Select. Topics Quantum Electron.*, **3**, 547-554 (1997).
- [104] S. L. Chuang, James O'Gorman, and A. F. J. Levi, "Amplified spontaneous emission and carrier pinning in laser diodes," *IEEE J. Quantum Electron.* **29**, 1631-1639 (1993).
- [105] F. Rinner, J. Rogg, P. Friedmann, M. Mikulla, and G. Weimann, "Longitudinal carrier density measurement of high power broad area laser diodes," *Appl. Phys. Lett.* **80**, 19-21 (2002).
- [106] Z. Chen, L. Bao, J. Bai, M. Grimshaw, R. Martinsen, M. Devito, J. Haden, and P. Leisher "Performance limitation and mitigation of longitudinal spatial hole burning in high-power diode lasers," *Proc. SPIE*, **8277**, 19-21 (2002).
- [107] S. Hasuo and T. Ohmi, "Spatial distribution of the light intensity in the injection lasers," *Jap. J. Appl. Phys.* **13**, 1429-1434, 1974.
- [108] M. Usami and S. Akiba, "Suppression of longitudinal spatial hole-burning effect in $\lambda/4$ -shifted DFB lasers by nonuniform current distribution," *IEEE J. Quantum Electron.* **25**, 1245-1253 (1989).

- [109] X. Sun and A. Yariv, “Surface-emitting circular DFB, disk-, and ring- Bragg resonator lasers with chirped gratings: a unified theory and comparative study,” *Opt. Express*, **16**, 9155 (2008).
- [110] X. Sun and A. Yariv, “Surface-emitting circular DFB, disk-, and ring- Bragg resonator lasers with chirped gratings. II: nonuniform pumping and far-field patterns,” *Opt. Express*, **17**, 1 (2009).
- [111] P. Zhou and G. S. Lee, “Mode selection and spatial hole burning suppression of a chirped grating distributed feedback laser,” *Appl. Phys. Lett.* **56**, 1400 (1990).

Acknowledgments

I would first like to thank my supervisor, Professor Susumu Noda, for his support. I am extremely grateful to him for the freedom that he extended to me during my thesis work. His intuitive understanding and charismatic leadership with regards to research form an excellent environment in which new paths could be explored and new ideas brought to fruition. His extraordinary insights of approaching and solving problems, and contagious enthusiasm will greatly influence my further scientific career.

I would also like to thank my dissertation committee, Professors Yoichi Kawakami and Shizuo Fujita for their patient participation and helpful advices on my thesis. I am grateful to Professors Masao Kitano and Mitsuru Funato, who acted as co-advisors during my doctoral study. Their insightful discussions and helpful comments stimulate my research.

I have been a research member of Noda lab for over five and a half years and during this period I have benefited enormously from the excellent environment and a group of gifted people. I am grateful to Professor Takashi Asano, who patiently supervised my research throughout my PhD study and answered my many unconventional questions.

I am also grateful to Dr. Kyosuke Sakai at Hokkaidou Univerisity, whose fundamental work on 2D CWT is the foundation of this thesis. I thank for this stimulating discussion during his stay at Kyoto University and after going back to Hokkaidou. Without his dedicated instruction and guidance this thesis would not have been possible. I am grateful to have Dr. Chao Peng as a friend and colleague. Although there was only two years's overlapped stay between our stays at Kyoto University, I feel that we have been friends for many years and I treasure our friendship. Much of the inspiration for this thesis came from the frequent discussion with him. I must also thank Dr. Seita Iwahashi for his patience in teaching me the fundamental knowledge of PCSEs when I joined Noda lab and keeping discussing issues related to this work. I am grateful to Dr. Ardavan Oskooi who helped in the numerical calculation and for the enlightening discussions.

While at Noda Lab I am fortunate to work with a group of talented colleagues, special mention goes to Assistant Professor Kenji Ishizaki, Assistant Professor Kyoko Kitamura, Assistant Professor Yoshinori Tanaka, Assistant Professor Kazunobu Kojima, Dr. Makoto Yamaguchi, Dr. Menaka Chaminda, Dr. Jeremy Upham, Dr. Shota Yamada, Tatsuya Nakamura, Yoonsik Lee, Ryotaro Konoike, Takuya Inoue, Tsuyoshi Okino, Masaya Nishimoto. They provide an exciting and fun atmosphere in which to work.

I gratefully acknowledge the generous financial support by the research fellowships of Japan Society for the Promotion of Science (JSPS) during my doctoral study at Noda lab.

Finally, I would like to thank my parents, Xinzhong Liang and Ailan Zhu, and my wife, Haining Meng. Without your unconditional love and support I could not have made it this far.

List of publications

Scientific articles in international journals

1. Y. Kurosaka, S. Iwahashi, Y. Liang, K. Sakai, E. Miyai, W. Kunishi, D. Ohnishi, and S. Noda, “On-chip beam-steering photonic-crystal lasers,” *Nat. Photonics* **4**, 447-450 (2010).
2. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, “Three-dimensional coupled-wave model for square-lattice photonic crystal lasers with transverse electric polarization: A general approach,” *Phy. Rev. B* **84**, 195119 (2011).
3. C. Peng, Y. Liang, K. Sakai, S. Iwahashi, and S. Noda, “Coupled-wave analysis for photonic-crystal surface-emitting lasers on air-holes with arbitrary sidewalls,” *Opt. Express* **19**, 24672-24686 (2011).
4. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, “Three-dimensional coupled-wave analysis for square-lattice photonic-crystal lasers with transverse electric polarization: finite-size effects,” *Opt. Express* **20**, 15945-15961 (2012).
5. C. Peng, Y. Liang, K. Sakai, S. Iwahashi, and S. Noda, “Three-dimensional coupled-wave theory analysis of a centered-rectangular lattice photonic crystal laser with a transverse-electric-like mode,” *Phys. Rev. B* **86**, 035108 (2012).
6. Y. Kurosaka, K. Hirose, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, “Effects of non-lasing band in two-dimensional photonic-crystal lasers clarified using omnidirectional band structure,” *Opt. Express* **20**, 21773- 21783 (2012).
7. Y. Liang, C. Peng, K. Ishizaki, S. Iwahashi, K. Sakai, Y. Tanaka, K. Kitamura, and S. Noda, “Three-dimensional coupled-wave analysis for triangular-lattice photonic-crystal surface-emitting lasers with transverse-electric polarization,” *Opt. Express* **21**, 565-580 (2013).

8. Y. Liang, T. Okino, K. Kitamura, K. Ishizaki, C. Peng, and S. Noda, "Mode stability in photonic-crystal surface-emitting lasers with large $\kappa_{1D}L$," *Appl. Phys. Lett.*, (submitted).
9. K. Hirose, Y. Liang, Y. Kurosaka, A. Watanabe, T. Sugiyama, and S. Noda, "Watt-class high power and high beam quality photonic-crystal lasers operated under room-temperature continuous-wave condition," *Nat. Photonics*, (submitted).

International conferences

1. S. Iwahashi, K. Sakai, Y. Kurosaka, Y. Liang, W. Kunishi, D. Ohnishi and S. Noda, "Two-Dimensional Photonic-Crystal Lasers with Centered-Rectangular Lattice Structure," *The 22nd Annual Meeting of the IEEE Photonics Society*, WH2, Ela Quality Resort, Belek-Antalya, Turkey, October 2009.
2. Y. Liang, K. Sakai, S. Iwahashi, Y. Kurosaka, C. Peng, E. Miyai, W. Kunishi, D. Ohnishi and S. Noda, "Two-dimensional Photonic Crystal Surface-Emitting Lasers," *The International Workshop of Next Generation Photonics, California Institute of Technology*, Pasadena, California, USA, February 2010.
3. Y. Kurosaka, S. Iwahashi, Y. Liang, K. Sakai, E. Miyai, W. Kunishi, D. Ohnishi and S. Noda, "On-Chip Beam-Steering Photonic-Crystal Lasers," *The Conference on Lasers and Electro-Optics and the International Quantum Electronics Conference (CLEO)*, CTu03, California, USA, May 2010. (invited)
4. C. Peng, Y. Liang, K. Sakai, S. Iwahashi, E. Miyai and S. Noda, "Improved coupled-wave theory for two-dimensional photonic-crystal surface emitting lasers," *5th International Conference on Nanophotonics (ICNP)*, Fudan University, Shanghai, China, May 2011.
5. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, "Three-dimensional coupled-wave analysis of photonic-crystal surface-emitting lasers," *The 5th GCOE International Symposium on Photonics and Electronics Science and Engineering*, P11, Kyoto University, Japan, March 2012.
6. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, "Three-dimensional coupled-wave model for photonic-crystal surface-emitting lasers," *The Conference on Lasers and Electro-Optics and the International Quantum Electronics Conference (CLEO)*, CTu1N, California, USA, May 2012.

7. Y. Liang, C. Peng, K. Ishizaki, S. Iwahashi, K. Sakai, Y. Tanaka, K. Kitamura, and S. Noda, “Modeling photonic crystal surface emitting lasers with a coupled-wave approach,” *The 13th International OSA Network of Students Conference (IONS-13)*, ETH Zurich and EPFL Lausanne, Switzerland, January 2013.
8. Y. Liang, C. Peng, K. Ishizaki, S. Iwahashi, K. Sakai, Y. Tanaka, K. Kitamura, and S. Noda, “Modeling triangular-lattice photonic-crystal surface-emitting lasers with a three-dimensional coupled-wave theory,” *The 6th GCOE International Symposium on Photonics and Electronics Science and Engineering*, P5, Kyoto University, Japan, March 2013.
9. Y. Liang, C. Peng, S. Iwahashi, Y. Tanaka, K. Ishizaki, and S. Noda, “Three-dimensional coupled-wave theory for centered-rectangular lattice photonic crystal lasers,” *The 7th International Conference on Nanophotonics (ICNP) and the 3rd Conference on Advances in Optoelectronics and Micro/Nano Optics (ICNP/AOM 2013)*, Hong Kong, China, May 2013.
10. Y. Liang, C. Peng, K. Ishizaki, S. Iwahashi, K. Sakai, Y. Tanaka, K. Kitamura, and S. Noda, “Three-dimensional coupled-wave theory for triangular-lattice photonic-crystal lasers,” *The 10th Conference on Lasers and Electro-Optics Pacific Rim and the 18th OptoElectronics and Communications Conference / Photonics in Switching 2013 (CLEO-PR&OECC/PS 2013)*, ThI1-6, Kyoto, Japan, July 2013.

Domestic conferences

1. S. Iwahashi, Y. Liang, Y. Kurosaka, K. Sakai, W. Kunishi, E. Miyai, D. Ohnishi, and S. Noda, “Supercell analysis of photonic-crystal laser consisting of different periodic complex resonators,” *The 56th Spring Meeting of The Japanese Society of Applied Physics Conference*. 31a-ZN-5, University of Tsukuba, Tsukuba, Japan (2009).
2. Y. Kurosaka, S. Iwahashi, Y. Liang, K. Sakai, E. Miyai, D. Ohnishi, W. Kunishi, and S. Noda, “Introduction of long period perturbation in 2D photonic crystal laser consisting of square and rectangular lattice VI,” *The 70th Fall Meeting of The Japanese Society of Applied Physics Conference*. 8p-B-9, University of Toyama, Toyama, Japan (2009).
3. S. Iwahashi, Y. Liang, Y. Kurosaka, K. Sakai, E. Miyai, W. Kunishi, D. Ohnishi, and S. Noda, “Lasing properties of centered rectangular lattice photonic crystal laser,” *The 70th Fall Meeting of The Japanese Society of Applied Physics Conference*. 8p-B-15, University of Toyama, Toyama, Japan (2009).

4. Y. Liang, K. Sakai, S. Iwahashi, Y. Kurosaka, E. Miyai, D. Ohnishi, W. Kunishi, and S. Noda, “Coupled-wave analysis for two-dimensional photonic-crystal lasers I: Air-hole shape and vertical radiation constant,” *The 57th Spring Meeting of The Japanese Society of Applied Physics Conference*. 19a-M-5, Tokai University, Tokyo, Japan (2010).
5. S. Iwahashi, Y. Kurosaka, K. Sakai, Y. Liang, E. Miyai, W. Kunishi, T. Sakaguchi, D. Ohnishi, and S. Noda, “Lasing properties of Centered-Rectangular-Lattice Photonic Crystal Laser II,” *The 57th Spring Meeting of The Japanese Society of Applied Physics Conference*. 19a-M-2, Kanagawa, Japan (2010).
6. Y. Kurosaka, S. Iwahashi, Y. Liang, T. Nobuoka, K. Sakai, E. Miyai, D. Ohnishi, W. Kunishi, and S. Noda, “On-chip Beam-steering Photonic-crystal Lasers,” *The 57th Spring Meeting of The Japanese Society of Applied Physics Conference*. 19a-M-6, Kanagawa, Japan (2010).
7. Y. Liang, K. Sakai, S. Iwahashi, Y. Kurosaka, and S. Noda, “Coupled-wave analysis of two-dimensional photonic-crystal lasers,” *The 29th Electronic Materials Symposium (EMS29)*, We3-3, Shizuoka, Japan, July (2010).
8. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, E. Miyai, D. Ohnishi, W. Kunishi, and S. Noda, “Coupled wave analysis for two dimensional photonic crystal lasers II: High-order coupled-wave model and vertical radiation constants,” *The 71th Fall Meeting of The Japanese Society of Applied Physics Conference*. 16p-J-14, Nagasaki University, Nagasaki, Japan (2010).
9. C. Peng, Y. Liang, K. Sakai, S. Iwahashi, E. Miyai, D. Ohnishi, W. Kunishi, and S. Noda, “Coupled wave analysis for two dimensional photonic crystal lasers III: Radiation constants for the case with vertical reflective interface,” *The 71th Fall Meeting of The Japanese Society of Applied Physics Conference*. 16p-J-15, Nagasaki University, Nagasaki, Japan (2010).
10. S. Iwahashi, Y. Kurosaka, K. Sakai, Y. Liang, E. Miyai, W. Kunishi, T. Sakaguchi, D. Ohnishi, and S. Noda, “Lasing properties of centered rectangular lattice photonic crystal laser III,” *The 71th Fall Meeting of The Japanese Society of Applied Physics Conference*. 16p-J-12, Nagasaki University, Nagasaki, Japan (2010).
11. Y. Liang, C. Peng, K. Sakai, S. Iwahashi and S. Noda, “Coupled-wave Analysis for Two-Dimensional Photonic-Crystal Lasers: Analysis of the resonant mode characteristics of laser cavity,” *The 58th Spring Meeting of The Japanese Society of Applied Physics Conference*. 25p-KA-10, Kanagawa Institute of Technology, Kanagawa, Japan (2011).

12. C. Peng, Y. Liang, K. Sakai, S. Iwahashi and S. Noda, “Coupled wave analysis for two dimensional photonic crystal Lasers: Analysis on the air-hole shapes with tilted walls,” *The 58th Spring Meeting of The Japanese Society of Applied Physics Conference*. 25p-KA-9 Kanagawa Institute of Technology, Kanagawa, Japan (2011).
13. S. Iwahashi, T. Nobuoka, Y. Liang, K. Sakai, Y. Kurosaka, E. Miyai, and S. Noda, “Lasing properties of centered-rectangular-lattice photonic crystal laser IV,” *The 58th Spring Meeting of The Japanese Society of Applied Physics Conference*. 25p-KA-2, Kanagawa Institute of Technology, Kanagawa, Japan (2011).
14. T. Nobuoka, S. Iwahashi, Y. Kurosaka, Yong Liang, K. Sakai, and S. Noda, “Composite photonic-crystal lasers (VII),” *The 58th Spring Meeting of The Japanese Society of Applied Physics Conference*. 25p-KA-3, Kanagawa Institute of Technology, Kanagawa, Japan (2011).
15. Y. Liang, C. Peng, K. Sakai, S. Iwahashi and S. Noda, “Coupled-wave analysis for two-dimensional photonic-crystal lasers (VI) -Analysis of non- Γ -point modes-,” *The 72th Fall Meeting of The Japanese Society of Applied Physics Conference*. 1p-ZR-1, Yamagata University, Yamagata, Japan (2011).
16. C. Peng, Y. Liang, K. Sakai, S. Iwahashi and S. Noda, “Coupled-wave analysis for two-dimensional photonic-crystal lasers (VII) -Symmetry & Asymmetry of air holes and radiation constant-,” *The 72th Fall Meeting of The Japanese Society of Applied Physics Conference*. 1p-ZR-2, Yamagata University, Yamagata, Japan (2011).
17. T. Nobuoka, S. Iwahashi, Y. Kurosaka, Y. Liang, K. Sakai, and S. Noda, “Composite photonic-crystal lasers (VIII),” *The 72th Fall Meeting of The Japanese Society of Applied Physics Conference*. 1a-ZR-9, Yamagata University, Yamagata, Japan (2011).
18. S. Iwahashi, T. Nobuoka, Y. Liang, C. Peng, and S. Noda, “Lasing properties of centered-rectangular-lattice photonic crystal laser,” *The 72th Fall Meeting of The Japanese Society of Applied Physics Conference*. 1a-ZR-7, Yamagata University, Yamagata, Japan (2011).
19. Y. Liang, C. Peng, K. Sakai, S. Iwahashi, and S. Noda, “Coupled-wave analysis for two-dimensional photonic-crystal lasers (VIII) -Analysis of triangular lattice-,” *The 59th Spring Meeting of The Japanese Society of Applied Physics Conference*. 16a-E5-4, Waseda University, Tokyo, Japan (2012).
20. Y. Liang, K. Ishizaki, C. Peng, K. Sakai, S. Iwahashi and S. Noda, “Coupled-wave analysis for photonic-crystal surface-emitting lasers (IX) -Finite-size effects

- on modal properties-,” *The 73th Fall Meeting of The Japanese Society of Applied Physics Conference*. 13a-PA5-10, Ehime University and Matsuyama University, Ehime, Japan (2012).
21. K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, “High Power Photonic Crystal Surface Emitting Lasers under CW Condition,” *The 73th Fall Meeting of The Japanese Society of Applied Physics Conference*. 14a-B1-2, Ehime University and Matsuyama University, Ehime, Japan (2012).
 22. Y. Liang, K. Ishizaki, K. Kitamura, M. Nishimoto, and S. Noda, “Three-dimensional analysis method of photonic-crystal lasers,” *The 5th Joint Symposium of Consortium for Photon Science and Technology Programs (C-PhoST)*. P-50, National Museum of Emerging Science and Innovation, Tokyo, Japan, January (2013).
 23. Y. Liang, K. Ishizaki, T. Okino, K. Kitamura, T. Tanaka, M. Nishimoto, and S. Noda, “Coupled-wave analysis for photonic-crystal surface-emitting lasers (X) -Above-threshold analysis-,” *The 60th Spring Meeting of The Japanese Society of Applied Physics Conference*. 29p-PA7-15, Kanagawa Institute of Technology, Kanagawa, Japan (2013).
 24. T. Okino, Y. Liang, K. Kitamura, and S. Noda, “Beam-direction control by modulated photonic-crystal lasers,” *The 60th Spring Meeting of The Japanese Society of Applied Physics Conference*. 28p-C1-17, Kanagawa Institute of Technology, Kanagawa, Japan (2013).
 25. K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, and S. Noda, “High-Power Photonic-Crystal Surface Emitting Lasers,” *The 60th Spring Meeting of The Japanese Society of Applied Physics Conference*. 28p-C1-18, Kanagawa Institute of Technology, Kanagawa, Japan (2013).
 26. A. Watanabe, K. Hirose, Y. Kurosaka, T. Sugiyama, Y. Liang, and S. Noda, “SHG Using PCSEL Device as Light Source,” *The 60th Spring Meeting of The Japanese Society of Applied Physics Conference*. 28p-C1-20, Kanagawa Institute of Technology, Kanagawa, Japan (2013).
 27. Y. Liang, T. Okino, K. Kitamura, K. Ishizaki, and S. Noda, “Coupled-wave analysis for photonic-crystal surface-emitting lasers (XI) -Nonuniformity of gain profile-,” *The 74th Fall Meeting of The Japanese Society of Applied Physics Conference*. 18p-A3-9, Doshisha University, Kyoto, Japan (2013).
 28. T. Okino, Y. Liang, K. Kitamura, and S. Noda, “Beam-direction control of photonic-crystal lasers with modulated crystalline structures,” *The 74th Fall Meeting of The*

- Japanese Society of Applied Physics Conference*. 18p-A3-7, Doshisha University, Kyoto, Japan (2013).
29. K. Hirose, Y. Kurosaka, A. Watanabe, T. Sugiyama, Y. Liang, S. Noda, “High-Power ($>1\text{W}$) Photonic-Crystal Surface Emitting Lasers (2),” *The 74th Fall Meeting of The Japanese Society of Applied Physics Conference*. 18p-A3-10, Doshisha University, Kyoto, Japan (2013).
30. M. Nishimoto, K. Ishizaki, K. Maekawa, Y. Liang, K. Kitamura, and S. Noda, “Fabrication of Photonic-Crystal Laser Structures by MBE growth II,” *The 74th Fall Meeting of The Japanese Society of Applied Physics Conference*. 17a-PA, Doshisha University, Kyoto, Japan (2013).