Three-dimensional Simulation of Vertical-Cavity Surface-Emitting Lasers

Ph.D. Dissertation

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Preface

When I started the research on semiconductor laser diodes in 2002, I had already had few years of experience in physics-based numerical simulation. In order to succeed in this field, not only the profound understanding of physical processes is necessary, but comparable amount of mathematical and computational skills are essential, as well. The second reason, why I selected this topic, was the strong industrial motivation for a software that can aid the design of optoelectronic devices targeting the commercial market. As the history of vertical-cavity surface-emitting lasers (VCSELs) went back to only about two decades, their simulation also offered the possibility of new academic contribution.

When joining to the simulation team set up by Furukawa Electric Institute of Technology Ltd. (FETI) for this project, the group had already consisted of four members. Nevertheless, all of us could be regarded as relative newcomers to the optoelectronic field, and we must have built up our knowledge base continuously. Looking back from recent days, the outcome of this cooperation was worth the efforts, since we have established a reputation among both our partners and the scientific community, and have developed consecutive software packages, the most recent one called as PhC-VOTES++ (Photonic Crystal VCSEL Optical-Thermal-Electrical Solver +Gain +Dynamics).

Soon after starting the modeling activity, we faced the problem to deal with noncylindrical vertical-cavity surface-emitting lasers (VCSELs). Although the simulation field was fairly covered for perfect rotational symmetry, the discussion of more complicated realistic structures was only in initial phase. Therefore it seemed a profitable idea to invest considerable efforts into this direction. We discovered only in the meantime that these devices could be purposely designed to deviate from the conventional circular geometry in order to achieve particular characteristics, such as laser mode or polarization control. When photonic crystal (PhC) laser diodes entered our perspective, we already had a satisfactory tool at hand for their calculation.

Accordingly, the ultimate goals of this dissertation are the accomplishment of a coupled, real three-dimensional opto-electro-thermal simulation, and its application for the qualitative and quantitative description of advanced VCSELs’ features. To this end, the hierarchical modeling concept is adapted, and I develop appropriate new approaches of increasing complexity in order to investigate sophisticated devices. Important subjects of the analysis are premised briefly as follows. The impact of a square-like optical confinement is modeled on the laser emission, and a special surface relief is used to alter its
behavior. Three-dimensional light scattering is demonstrated on the square- or elliptical-shaped oxide apertures of these lasers. Polarization mode splitting is exposed for VCSELs employing different elliptical windows. Important characteristics of PhC-VCSELs are explained and optimized with the help of computer simulation, such as their threshold current and single-mode operation.

The support of numerous persons is acknowledged below, who assisted in completing this dissertation. First of all, I thank to Prof. Tamás Veszprémi for introducing me into the methods of scientific research and publication, and for the encouraging environment he provided. He proved to be an excellent adviser, in both prosperous and rather difficult circumstances, and also in personal communication. Moreover, he has always been the leader of our team, who smoothes the disputes and emphasizes the common arguments of all contestants.

I am grateful to Dr. Tamás Kárpáti, Zsolt Puskás and Dr. György Zsombok for the huge assistance in developing the software and performing calculations, and also for the valuable ideas in model generation. Their different background often helped to form a challenging atmosphere, in which phenomena were discussed from various aspects.

Dr. Gábor Varga deserves special thanks, being the person who had brought me in connection with numerical simulation when I had been undergraduate student, and later suggested to work on this project. This thesis could not have been carried out if Dr. Naoki Hashizume of Furukawa Electric Corporation Ltd. had not initiated the laser diode simulation in FETI. After coordinating our activity from abroad, we enjoyed the cooperation with him in Budapest for four years. I give my thanks to him for the experience he shared about laser modeling and market with us.

I am also indebted to several Japanese colleagues, without whose experimental feedback this work would have been only an exciting theoretical adventure. They introduced me into the basics of fabrication and characterization processes, and coauthored few patents and conference publications, too. I would like to mention Dr. Takeo Kageyama, Tomofumi Kise, Keishi Takaki and Dr. Akihiko Kasukawa here.

I warmly appreciate the help of Prof. Péter Deák and Dr. László Kocsányi for accommodating me to the Department of Atomic Physics at the Budapest University of Technology and Economics (BUTE), and for reviewing this thesis.

I would like to acknowledge the outstanding help of Dr. Gyula Besztercey, the president of FETI. He did not only guarantee a scholarship when I was a postgraduate student, but followed and supported my scientific achievements regularly, as well.

Finally, I express my heartfelt thanks to my family, friends and colleagues either at the university or in FETI, who ensured a safe and motivating environment that is indispensable to elaborate a similar work.
# Contents

1 Introduction ............................................. 1
  1.1 History and Applications ............................. 1
  1.2 Device Operation ..................................... 3
  1.3 Why Simulation? ...................................... 11
  1.4 Structure of this Dissertation ....................... 12

2 Simulation Background ................................... 13
  2.1 Introduction ........................................ 13
  2.2 Electrical Model ..................................... 13
  2.3 Thermal Model ....................................... 15
  2.4 Optical Mode Calculation .............................. 16
    2.4.1 Effective Index Method .......................... 20
    2.4.2 Weighted Index Method ........................... 22
    2.4.3 Coupled Mode Model .............................. 24
    2.4.4 Finite Element Method ............................ 26
    2.4.5 Comparison of Optical Models .................... 27
  2.5 Rate Equation Approach ............................... 30
  2.6 Description of the Active Region ..................... 34

3 Novel Results ........................................... 36
  3.1 Goals ............................................... 36
  3.2 Semi-Analytical Optical Mode Calculation .............. 37
    3.2.1 Group Theoretical Considerations .................. 37
    3.2.2 Effective Radius-Weighted Index Method .............. 38
    3.2.3 Hybrid Weighted Index Method ...................... 40
    3.2.4 Optical Modes for Square-Like Aperture .......... 42
  3.3 Resonator Modes of Advanced VCSELs .................. 46
    3.3.1 Solution with the Scalar Helmholtz Equation ....... 46
    3.3.2 Vectorial Approach for Helmholtz Equation ......... 48
    3.3.3 Effective Numerical Treatment of Large Matrix Problems ....... 50
    3.3.4 Model Validation ................................ 54
    3.3.5 Elliptical Devices ............................... 56
## CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3.6 Square-Like Aperture</td>
<td>59</td>
</tr>
<tr>
<td>3.3.7 Photonic Crystal VCSEL</td>
<td>59</td>
</tr>
<tr>
<td>3.4 Coupled Opto-Electro-Thermal Simulations</td>
<td>62</td>
</tr>
<tr>
<td>3.4.1 Electrical Model</td>
<td>62</td>
</tr>
<tr>
<td>3.4.2 Thermal Model</td>
<td>63</td>
</tr>
<tr>
<td>3.4.3 Laser Model</td>
<td>64</td>
</tr>
<tr>
<td>3.4.4 Discretization</td>
<td>66</td>
</tr>
<tr>
<td>3.4.5 Self-Consistent Coupling</td>
<td>69</td>
</tr>
<tr>
<td>3.4.6 Non-Circular Oxide Aperture</td>
<td>69</td>
</tr>
<tr>
<td>3.4.7 Triangular Surface Relief</td>
<td>72</td>
</tr>
<tr>
<td>3.4.8 Elliptical Surface Relief</td>
<td>76</td>
</tr>
<tr>
<td>3.5 Design of a Single-Mode PhC-VCSEL</td>
<td>78</td>
</tr>
</tbody>
</table>

### 4 Summary and Outlook

#### A Further Optical Approaches

<table>
<thead>
<tr>
<th>Method</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1 Effective Frequency Method</td>
<td>86</td>
</tr>
<tr>
<td>A.2 Numerical Mode Matching Method</td>
<td>87</td>
</tr>
<tr>
<td>A.3 Eigenmode Expansion with Perfectly Matched Layers</td>
<td>89</td>
</tr>
<tr>
<td>A.4 Method of Lines</td>
<td>89</td>
</tr>
<tr>
<td>A.5 Plane Wave Admittance Method</td>
<td>91</td>
</tr>
<tr>
<td>A.6 Green’s Function Model</td>
<td>92</td>
</tr>
<tr>
<td>A.7 Optimized-Waist Paraxial Eigenmodes Method</td>
<td>93</td>
</tr>
</tbody>
</table>

**List of Publications** 95

**Bibliography** 97
Chapter 1

Introduction

1.1 History and Applications

Vertical-cavity surface-emitting lasers (VCSELs) were invented by K. Iga in 1977 [1, 2]. The first lasing operation was observed in 1979 at 77 K [3], and the first at room-temperature was demonstrated in 1988 [4]. The research was accelerated for reducing the threshold current and increasing efficiencies. Oxide-confined VCSELs provided a record-breaking low threshold currents [5], and high power-conversion efficiencies of over 50% [6]. They reached the commercial market in the late nineties, and looked to meet the third generation of development in 1999, as we entered a new information and technology era [1].

VCSELs offer numerous advantages over edge-emitting lasers in the low power regime (few mW). These include the submilliampere threshold current, and high operation-to-threshold current ratio, that allow high-speed modulation. 25 Gbit/s modulation speed was reported for diodes with GaInAs active material [2]. The wavelength and threshold are relatively insensitive against temperature variation for these diodes. The almost circular output beam is emitted from the top or the bottom surface of these lasers, which together enable efficient fiber coupling without expensive coupling optics elements familiar in the case of edge-emitters. Their geometry is well suited for fabricating two-dimensional arrays by fully monolithic processes, that yields very low cost chip production. Wafer level testing is also possible in this configuration. Their use is heavily pursued in parallel fiber-optic communication, where multiple-wavelength arrays are good candidates. They operate in single longitudinal mode due to the short cavity length, while the number of transverse modes can be controlled by the lateral dimensions. In general, most properties of VCSELs can be much easier scaled than those of edge-emitters.

It can be seen on Fig. 1.1 that the two largest fields of laser diode market are optical storage and telecommunication applications [7]. VCSELs are potentially suitable for these fields, but can have contributions only if they offer superior performance or significant cost reduction over the recently installed devices. For conventional diode lasers,
such as in compact disk (CD) players, the technology, production and cost reduction are well developed, therefore displacing them will not be easy. Long-distance telecommunication is covered with expensive distributed feedback (DFB) lasers that realize a precise wavelength control and narrow optical linewidth. Although VCSELs might improve on some aspects, there is little pressure on this low-volume market to drive the development of cheaper optical sources. However, long wavelength single-mode VCSELs could be more promising than the recent Fabry-Perot laser diodes in metropolitan links (500 m to 20 km range) due to better yield, less expensive testing, drive electronics and packaging. In the short-haul links comprising mainly multi-mode fibers, light emitting diodes (LEDs), 780 nm CD lasers and multi-mode VCSELs are the candidates as light sources. LEDs are most common, but suffer from low fiber-coupled efficiency and below-Gbit/s transmission speed. Edge-emitters are either not appropriate for high-speed modulation (CD players) or their temperature sensitivity calls for expensive control electronics and packaging. VCSELs combine the essential advantages of both at somewhat higher price (under $5 packaged) than that of LEDs. As already mentioned, they are suitable for easy array production, moreover, the dispersion limits of the transmitting optical fiber may be circumvented by wavelength-division multiplexing technique [8]. VCSELs can also count on interesting applications, in which LEDs are replaced for better performance. An optical computer mouse with a VCSEL sensor appeared on the market that offers lower power consumption, narrower beam divergence and higher sensitivity.

The target applications for VCSELs at visible wavelengths are generally the same as...
1.2 Device Operation

VCSELs like other lasers comprise an active material responsible for the stimulated emission and mirrors that provide the necessary optical feedback. The structural solutions are, however, partly surprising compared to most conventional lasers, and even to edge-emitting lasers. A VCSEL and a Fabry-Perot laser diode are sketched on Fig. 1.2. The basic differences arise from the fact, that the direction of the emission is axial, and parallel to the current flow.

Since the gain path along the emission direction (referred as axial, longitudinal or vertical direction in the following) is much shorter than in edge-emitters: only few tens or nanometers or less, mirrors with very high reflectivity are required for the optical feedback. Usual reflectivity coefficients should exceed 99% on the output side and 99.9% on the back part. Such mirrors can be fabricated from dozens of quarter-wavelength layers for edge-emitters, and the benefit may come from the array ability to increase system throughput. For example, in high speed, high volume laser printers, the VCSEL array can multiplex several lines simultaneously through the optical system. 650 nm VCSELs may emerge as potential sources for plastic-fiber communication [9, 10]. A unique application can be the so-called VCSEL-based smart pixels for free-space optoelectronic processing, which are electronic processing cells with optical input and output elements arranged in two-dimensional arrays [11]. High-speed massively parallel optical interconnections hold the promise to provide an alternative to silicon-based chips. As the integration of optical interconnections with electronic circuits improves, the interconnection distance shortens, and the parallelism increases, the packaging cost associated with parallel optical fibers will make free-space interconnects more attractive [12].
CHAPTER 1. INTRODUCTION

with alternating refractive indices, and are called distributed Bragg-reflectors (DBRs). They result in the desired reflectivity in a wide wavelength range called the stop-band. The actual value can be easily estimated by multiplying the reflectivity coefficients of single interfaces for lossless layers, however, it reaches a maximum if absorption is present. Therefore it is essential to use materials with large enough index contrast to achieve the necessary feedback level. A second stringent condition on mirror formation is the need for matching the lattice constants to avoid mechanical stress in the DBRs. These two restrictions usually demand quaternary semiconductor compounds \((A_{x}B_{1-x}C_{y}D_{1-y}\text{ or }A_{x}B_{y}C_{1-x-y}D\text{ types})\) for the mirrors, that allow a free variation of one constituent, while the lattice constant can be kept fixed by appropriate scaling of the other. \(Al_{x}Ga_{1-x}As\) is a fortunate ternary compound, which guarantees the lattice matching within almost 0.1% precision, and another alternative way is to employ amorphous materials. In any case, special attention must be paid on the band gap of the semiconductors mirrors, as it must be obviously larger than that of the active material in order to avoid internal band-to-band absorption. This condition may also restrict the acceptable composition range of the compound semiconductors.

The active zone of VCSELs usually contains single or multiple quantum wells (QWs), that are intentionally undoped. They are separated by barriers, and are joined to layers with opposite doping on the two sides. Sometimes the intrinsic region is thicker than just the QWs and barriers, and forms the so-called separate confinement heterostructure (SCH) \([13]\). The p-i-n junction is of center importance for electrically pumped diode lasers, because the carrier recombination is more efficient than it would be in a simple p-n junction. Optical pumping with a shorter wavelength light source offers the second possibility to attain population inversion. The QW and barrier materials should be chosen with respect to the desired operation wavelength, keeping in mind several additional facts. The band gap is larger in thin QWs than in the same bulk material, as discrete subbands evolve between the potential barriers. The peak of the material gain spectrum is usually designed below the passive resonator wavelength at room temperature, because it tends to redshift faster with increasing operation temperature. Perfect matching should be obtained at the typical conditions under laser operation. Most common QW materials facilitating direct transitions include AlGaInN or II-VI compounds for blue and green lasers \([14, 15, 16]\), AlGaInP for red ones \([17]\), GaAs for 850 nm emission \([6]\), strained GaInAs between 980-1200 nm \([18]\), GaAlInAs and GaInNAs for 1300 nm \([19, 20, 21]\), and InGaAsP for 1550 nm \([22]\).

Polarization control is important in noise-free applications like optical telecommunication. Since there is no favored direction in VCSELs possessing perfect rotational symmetry, these devices are extremely vulnerable to polarization switching. Although small anisotropies are always present in real devices, and the fundamental mode is usually polarized along the [011] or [0\overline{1}1] crystal axes due to the electrooptic effect \([23]\), the polarization state easily changes under current injection. To avoid this feature, asymmetries
1.2. DEVICE OPERATION

Figure 1.3: Bottom-emitting etched mesa VCSEL

like off-angle substrate [24], elliptical mesas [25, 26], anisotropic multiple quantum-well regions [27], anisotropic current injection [28, 29], external polarization selection elements [30, 31], or linear surface gratings [32, 33, 34] are often introduced to these lasers.

VCSEL Types

In order to achieve efficient device characteristics, it is essential to confine the optical field as well the population inversion in directions perpendicular to the emitted laser beam (this plane will be referred as lateral or sometimes transverse cross-section). Current and carrier confinements can also be distinguished for electrically injected laser diodes, which are strongly related but not equivalent due to the possibility of lateral carrier diffusion in the QW. Several options have been proposed for the lateral limitation of these quantities.

The simplest structure realizing current confinement is the etched mesa VCSEL (see Fig. 1.3), that is analogous to the edge-emitting ridge waveguide structure [35]. The round or square postlike mesa is usually stopped just above the active layer to avoid surface recombination of carriers, and to prevent significant current spreading [36]. The etched mesa also provides a large lateral index step, and thus strong optical confinement. Multi-mode operation could be therefore expected for all but submicron diameter mesas. However, since the etched surface is imperfect, higher order modes tend to suffer from higher scattering loss, that may stabilize the single-mode output [37]. Nevertheless, the threshold current always increases due to the strong scattering loss. Because of the small dimensions of the etched-mesa top, it is convenient to construct bottom-emitting diodes through a transparent substrate.

The left side of Fig. 1.4 illustrates a simple-to-manufacture, proton-implanted, gain-guided VCSEL [38]. The implant aperture realizes a current confinement, but has practically no direct impact on the optical mode. The modes can be laterally confined by temperature induced refractive index change [39] or by the gain region limited more or less by the injected current (the optical gain can be taken into account as the imaginary part of the complex refractivity). However, the thermal profile in the device may be unstable under modulation. If the implant aperture does not penetrate into the active
region, lateral current spreading may add a significant unproductive shunt current. If it proceeds through the QW, the current is effectively apertured, but the large interface recombination deteriorates the operation.

A VCSEL utilizing a dielectric aperture is shown on the right half of Fig. 1.4. It is generally fabricated by selective oxidation of a high aluminum content AlGaAs layer [40, 41]. Its first purpose is to block the shunt current that would otherwise flow between the p- and n-regions, and is superior compared to the proton-implantation. If the oxide aperture is formed on the null of the axial standing wave pattern that evolves in the DBR, it has little effect of the optical mode [42], but an oxide on the maximum guides several lateral modes. The most attractive feature of the dielectric aperture is therefore the great flexibility of the design. Of course, carrier confinement is still missing, unless some lateral potential barrier is provided in the layer of the QW. It may occur that the oxide aperture was not ideally circular due to manufacturing reasons. If oxidation speed were ideally isotropic, the aperture shape would be the exact replica of the mesa geometry. It has already been reported that the oxidation could proceed faster in the [1 0 0] direction compared to the [1 1 0] direction [40], and the final aperture may differ from the transverse mesa shape. It is also possible to position the electric contacts just above and below the cavity to avoid carrier-induced absorption and also conduction through the mirrors, which can reduce the series resistance and Joule-heating. This option is referred as intra-cavity contacts.

A buried heterostructure VCSEL sketched on Fig. 1.5 combines the confinement of current, carriers and optical field in a single structure, if the regrown current-blocking material surrounding the etched pillar has larger band gap and lower refractivity than the inner one. Although this behavior seems very promising, the fabrication faces serious difficulties [43]. The direct regrowth over a deeply etched mesa containing high Al-content region is difficult, as well as and the integration with epitaxial or fused mirrors. There may be some problems with circular instead of square active regions, since the many crystal planes exposed in a circular geometry causes havoc for uniform regrowth. No technique stabilizing the surface has been found either [44].
1.2. DEVICE OPERATION

Figure 1.5: The buried heterostructure VCSEL (left figure) and the buried tunnel junction VCSEL (right) offer alternative current paths.

An important advantage of buried tunnel junction VCSEL (see Fig. 1.5) is the elimination of p-doped semiconductors, that suffer from higher free-carrier absorption than their n-doped counterparts. They utilize a single, very thin layer with strong p-doping located on the optical node, followed by a highly n-doped one, which create a tunnel junction [45, 46]. It provides holes via quantum-mechanical tunneling even if the device has n-type contacts on both sides [47]. Similar series resistance can be achieved with a low-resistance tunnel junction as in oxide-confined VCSELs. It also results in an effectively limited current injection through the QW. The difficulties arise again from the control of etching and regrowth when fabricating the tunnel junction, similar to the buried heterostructure laser diode.

A vertical external cavity surface-emitting laser (VECSEL, see Fig. 1.6) utilizes optical injection to achieve and maintain the population inversion in the QWs [48]. The DBR is missing from one side of this laser in order to illuminate the active region directly with a shorter wavelength light source, typically with another laser diode. However a high

Figure 1.6: VCSEL with external concave mirror
CHAPTER 1. INTRODUCTION

Figure 1.7: Promising VCSELs for single-mode laser operation: the photonic crystal structure and the laser incorporating a surface relief.

reflectivity external concave mirror or an external DBR is used to provide the necessary feedback. Since the distance between the QWs and the external mirror can be varied, this laser is tunable within a wide wavelength range [49]. Since no lateral index change is built in the resonator, it is essentially a gain-guided device, and its dimensions are defined by the spot size of the incoming light.

The next two structures do not offer exclusive injection schemes or current paths, but affect directly only the optical modes. VCSELs incorporating photonic crystals (PhC) have been studied extensively for about five years [50, 51, 52]. The common method is to create deep holes arranged in a regular pattern with the help of reactive ion etching (Fig. 1.7), and to leave few positions intact. These form the central defect zone, where the optical modes are confined. The holes have relatively weak guiding contribution compared to other index-guided solutions, and act as scattering centers for the light, which may result in single mode operation. A VCSEL with only one ring of deep triangular holes was also studied [53]. An alternative procedure is to create shallow PhC patterns close the active region before depositing the DBR mirrors [54]. The holes possess only obvious blocking effects on the current path in both cases.

Etching a shallow surface relief is a popular method to introduce mode-selective losses [55]. It has been reported that the mirror reflectivity diminished drastically if a quarter-wavelength layer (half of a mirror pair) was removed from or added to the completed DBR, and the mirror loss increased roughly by one magnitude [56]. This can be exploited as a filter if the layer is only partly modified, where the undesired modes exhibit considerably intensity. This approach is depicted on Fig. 1.7, where the topmost layer was removed outside of a circle that is smaller in diameter than the oxide aperture. Besides of mode selection, it can be also adopted for polarization control, if the relief exhibits an asymmetric shape, such as an ellipse [57] or a linear grating [32, 33, 34].

Quantitative Characteristics

It is essential to summarize some basic relationships before turning our attention to the motivation for comprehensive simulation. These equations serve as a fundamental
1.2. DEVICE OPERATION

guideline for device design, and can be derived from the rate equation approach [13], which is analyzed in details later (see Section 2.5). They apply for electrical injected VCSELs, which are the subject of most research and commercial development. The important laser diode properties cover the threshold current, the initial slope of the light power versus current curve, the modulation bandwidth and the related relaxation oscillation frequency, and the thermal stability marked by the rollover point.

The laser diode operates as a poor LED below threshold. Carriers are transported from the contacts to the active region through semiconductor layers, and most of them are involved in various recombination processes in the QWs. The current injection efficiency is denoted by $\eta$, while the remaining carriers contribute to the current leakage. Stimulated emission is negligible below threshold, the active processes are radiative, defect-induced and Auger-type nonradiative recombinations. All of them can be taken into account in an effective electronic lifetime $\tau_n$.

The laser threshold is determined by the balance of modal loss and gain: $\Gamma g(n_{thr}) = \alpha_{tot}$, where $g$ labels the material optical gain as a function of threshold carrier density $n_{thr}$, and $\alpha_{tot}$ is the total resonator loss. $\Gamma$ denotes the optical confinement factor of the normalized laser mode profile for the region under population inversion, and is typically few percents for VCSELs. With the help of the volume of the QW under injection ($V_{QW}$) and the unit charge $e$, the laser threshold current can be written as follows:

$$I_{thr} = \frac{eV_{QW} n_{thr}}{\eta \tau_n} = \frac{eV_{QW}}{\eta \tau_n} \eta^{-1} (\alpha_{tot}/\Gamma). \quad (1.1)$$

If the the current and the laser mode are confined effectively to the same small area, the current injection efficiency is close to unity, the recombination processes are slow, and the diode exhibits small optical loss (corresponding to long photon lifetime), low threshold current can be expected.

The modal gain is clamped at the level of the modal loss above threshold. Apart from the gain saturation at high optical intensity, it results in constant free carrier density, since any excess carriers would undergo stimulated emission and convert into photons. The steady-state photon number ($S$) can be obtained from the balance between excess injection current and the stimulated emission term:

$$S = \frac{1}{v_g \Gamma g(n_{thr})} \eta (I - I_{thr}) = \frac{1}{v_g \alpha_{tot}} \eta (I - I_{thr}) = \frac{\eta \tau_p}{e} (I - I_{thr}) \quad (1.2)$$

with the introduction of the group velocity $v_g$ and the photon or resonator lifetime $\tau_p$. The emitted optical power is derived as follows. In the absence of pumping, the photon number would decay at a rate of the inverse photon lifetime. However, only some photons contribute to the emitted laser beam, since there are several loss sources. The light leaving the resonator is taken account as the mirror loss, which can be further separated for the useful output ($\alpha_{m1}$, either the top or the bottom mirror) and for the other ($\alpha_{m2}$). Unintentional absorption and scattering inside the laser diode contribute to the internal
losses summarized in $\alpha_{\text{int}}$. Finally, every photon accounts for $\hbar \nu$ energy, where $\nu$ labels the frequency of the laser. The useful power of the laser thus reads:

$$P_{\text{light}} = \frac{S}{\tau_p} \frac{\alpha_m}{\alpha_{\text{tot}}} \hbar \nu = \eta \frac{\alpha_m}{e \alpha_{\text{tot}}} \hbar \nu (I - I_{\text{thr}}). \quad (1.3)$$

An alternating energy exchange takes place between the carrier and the photon reservoirs under harmonic current modulation. An above-average driving current starts to overload the carrier density, that will result in higher optical gain and stimulated emission. As the optical intensity strengthens, the stimulated emission rate further increases, and the carriers begin to deplete. The ratio of this oscillation’s amplitude and the current modulation’s amplitude depends on the frequency of the input signal. It reaches a maximum at the relaxation oscillation frequency, which varies with the steady-state stimulated emission rate:

$$f_R = \frac{1}{2\pi} \sqrt{\frac{v_g \Gamma S}{\tau_p V_{\text{QW}}} \frac{\partial g}{\partial n}}_{n_{\text{thr}}} = \frac{1}{2\pi} \sqrt{\eta \frac{v_g \Gamma V_{\text{QW}}}{\tau_p V_{\text{QW}}} \frac{\partial g}{\partial n}}_{n_{\text{thr}}} (I - I_{\text{thr}}). \quad (1.4)$$

The -3 dB modulation bandwidth is about $1.55 f_R$, provided that damping and parasitics are not too large [13]. Therefore it is sometimes referred as the intrinsic modulation bandwidth of the QW. Since the gain is a sublinear function of the free carrier density, it is desirable to have low threshold carrier density to maximize the differential gain.

It can be seen that all important parameters of the VCSEL improve if the threshold current is low. This can be basically achieved if the modal loss is small enough. As the internal loss usually cannot be cut back infinitely, because it tends to be determined by the absorption in extrinsic semiconductors close to the active region, low mirror losses would also be required. On the contrary, high emitted laser power would require high mirror-to-internal loss ratio, and these two conditions cannot be fulfilled simultaneously. It depends on the application whether high power or quick response is the primary priority.

The thermal effects have been neglected so far. Many parameters of the diode lasers degrade with increasing temperature, though a deliberate misalignment of the gain from the mode at room temperature can be used to partially compensate them within a limited range. Nevertheless, the threshold current usually increases, and the light power and modulation bandwidth hang behind those predicted by Eqs. (1.3) and (1.4) after exceeding some critical temperature in the QW. Therefore it is attempted to minimize the series resistance of the device responsible for Joule heating, as well as its thermal resistance. The latter can be roughly estimated as:

$$R_{\text{th}} \approx \begin{cases} \frac{\hbar}{4\kappa r^2 \pi} & \text{for quasi-axial heat flow,} \\ \frac{1}{4\kappa r} & \text{for three-dimensional heat flow} \end{cases} \quad (1.5)$$

where $\kappa$ is an average thermal conductivity, and $r$ is the radius of an assumed homogeneous heat source [13]. The first approximation can be valid for a VCSEL flip-chip
bonded to a heat sink, whose QWs are located in $h$ distance from the heat sink. The second one holds for a small VCSEL with thick substrate. A power-law fitting versus the active radius for realistic devices usually yields an exponent between -1 and -2.

1.3 Why Simulation?

Few basic relationships have been outlined that can be useful for initial design. However, they do obviously not offer a complete description of the variables involved in practical device development, which requires lots of compromises among competing figures of merit. Physics-based comprehensive modeling is essential to make these decisions. The development period of future products can be shortened using such a tool, and costs may be reduced. Of course, experimental work is still indispensable to provide the input material parameters, as well as for the evaluation and validation of the numerical findings. Technology computer aided design (TCAD) was introduced more than a decade ago for microelectronic devices based on silicon, and has become widely accepted in the meantime. The physical processes in optoelectronic devices are, in turn, more complex, and only few commercial softwares are available, but their applicability is limited.

It is essential to give some examples of the trade-off decisions, that are easier to make using sophisticated simulation. The contradiction between the low threshold current and the high outcoupling efficiency has already been mentioned. The doping concentration of the extrinsic semiconductor layers is another interesting property of diode lasers. Strong impurity doping would result in good electric conductivity, and thus low electric resistance and Joule heating, at the expense of high free-carrier absorption and internal loss in the relevant layers. It is also easier to achieve high free carrier density in a thinner QW, but the band structure becomes quantized, and therefore the transition energies and the density of state changes.

One of the most important design issues is the placing of the oxide aperture in single-mode VCSELs. Forming it on the node of the optical field would filter out higher order modes, but the confinement of the fundamental mode also decreases. Therefore somewhat higher threshold current is needed to start the lasing effect. The mode guiding can be quantitatively described with the help of the transverse confinement factor. It is defined as the normalized integral of the lateral intensity distribution for the active area, which corresponds to the current aperture in electrically injected laser diodes if current spreading is negligible. It has been found that, as a rule of thumb, single-mode operation could be expected if the transverse confinement factor of the fundamental mode was higher than 75%, and the confinement factors of the higher modes were at least smaller by 15% than that of the fundamental mode [58]. However, weak built-in index-guiding can easily be surpassed by thermal lensing, which carries the possibility of dynamic instabilities.

The above-mentioned examples can all be treated with axisymmetric two-dimensional (2-D) solvers. However, recently investigated devices like PhC-VCSELs and those incor-
porating other noncylindrical shapes call for three-dimensional (3-D) solutions. Although some of these devices have already been studied with their proper axisymmetric substitutes, it seems to be advantageous to incorporate them into an unified framework, and this is the main objective of this thesis. This demand is backed by the following interesting problems. A square-like oxide aperture results in the splitting of some lateral modes, and they can be observed as new distinct peaks on the spectrum. How does the polarization suppression ratio depend on the eccentricity of an elliptical oxide aperture or surface relief? A third question arises for PhC-VCSELs utilizing either proton-implanted or a nodal oxide aperture, when the sizes of the distinct optical and electrical apertures is to be optimized.

1.4 Structure of this Dissertation

This thesis is organized as follows:

**Chapter 1: Introduction.** The history and fundamentals of VCSELs are exposed, and the motivation for the numerical simulation is given.

**Chapter 2: Simulation Background.** The physics of VCSELs is summarized based on already published works, with particular attention on the calculation of laser resonator modes. The existing optical models are classified from various aspects.

**Chapter 3: Novel Results.** New methods are proposed for the solution of the Helmholtz equation in index-guided VCSELs. An efficient algorithm is presented to deal with the resulting large-scale sparse algebraic problem. A generalization of a coupled opto-electro-thermal solution for 3-D is also exposed. Simulation results are shown for noncylindrical VCSELs involving square-like and elliptical oxide apertures, triangular and elliptical surface reliefs, and a deep etched PhC pattern.

**Chapter 4: Summary and Outlook.** The major results of this dissertation are emphasized, and the pros and cons of the developed models are discussed in the perspective of the hierarchical modeling concept. The possible future model extensions and interest close the thesis.

**Appendix A: Further Optical Approaches.** The review of laser mode simulation is consummated with the description of seven more methods.
Chapter 2
Simulation Background

2.1 Introduction

The simulation of vertical-cavity surface-emitting lasers is a very complex task, but it can be appropriately partitioned into separate physical subproblems. The coupling among these parts may be carried out in a self-consistent way, if necessary. In order to predict the characteristics of typical operation of semiconductor lasers, one should consider at least optical, thermal and electrical aspects of the device. Additionally, the active material must be discussed at an appropriate level. The closely coupled thermal and electrical processes are often modeled within the frame of a single thermodynamic model. On the other hand, optics and electronics share a strong interaction only due to stimulated emission, while the individual laser mode patterns depend weakly on the carrier and current profiles. Therefore the optical simulation can be separated into two tasks, to the calculation of the laser modes, and to the estimation of modal intensities under static or dynamic conditions. A deeper theoretical explanation will be given later. Existing simulation methods are reviewed in this chapter, with special focus on the optical mode calculation, as it is the main subject of this study.

2.2 Electrical Model

The electrical simulation for VCSELs aims several purposes. First, one would like to estimate the current-voltage (I-V) characteristics of the device in order to have a knowledge about its power consumption. Since it consists of mainly semiconductor materials with varying dopant profiles, the theoretical formulation and the multidimensional realization can be very difficult. It is sometimes enough to approximate the nonlinear behavior with a simple broken-line model parameterized with a threshold voltage and an above-threshold differential resistance. Related topic is the calculation of the Joule-heat power density distribution inside the mirrors, which should be incorporated into the thermal description. The third purpose is to estimate the current density impinging on the active region
CHAPTER 2. SIMULATION BACKGROUND

that maintains the population-inversion. Non-uniform current distribution can lead to different overlaps with the laser modes, and affect remarkably their intensities.

Thermodynamic Model

A sophisticated electro-thermal transport model comprises the Poisson-equation for the electric potential ($\Phi$), the continuity equation for the density of electrons ($n$) and holes ($p$), and the heat diffusion equation [59]. Its main prerequisite is the assumption of a local thermal equilibrium between the charge carriers and the crystal lattice.

\[-\nabla(\varepsilon \nabla \Phi) = e(p - n + N_D^+ - N_A^-) \]  
\[-e \frac{\partial n}{\partial t} = -\nabla j_n + eR \]  
\[ e \frac{\partial p}{\partial t} = -\nabla j_p - eR \]  
\[ c_p \frac{\partial T}{\partial t} = -\nabla q + \rho_{\text{heat}} \]

Here $e$ denotes the unit charge, $N_D^+$ and $N_A^-$ the ionized donor and acceptor concentrations, respectively. $R$ is the recombination rate of electron-hole pairs, $c$ is the specific heat, $\rho$ denotes the mass density, $T$ the temperature, and $\rho_{\text{heat}}$ the total heat power density. The electron ($j_n$), hole ($j_p$) and heat current densities ($q$) include diffusion and cross-terms, extended with drift currents for the first two as follows:

\[ j_n = -e(\mu_n n \nabla \Phi - D_n \nabla n + \mu_n n P_n \nabla T), \]  
\[ j_p = -e(\mu_p p \nabla \Phi + D_p \nabla p + \mu_p p P_p \nabla T), \]

\[ q = -\kappa \nabla T + \nabla [j_n (P_n T + \Phi_n)] - \nabla [j_p (P_p T + \Phi_p)], \]

with $\mu_{n,p}$ mobilities, $D_{n,p}$ diffusion coefficients, $P_{n,p}$ thermoelectric powers and $\Phi_{n,p}$ quasi-Fermi potentials, respectively. The subscripts $n$ and $p$ refer to electrons and holes. The diffusion coefficients are related to the mobilities according to Einstein-relationship. It is also possible to apply a hydrodynamic model if one assumes different lattice and charge carrier temperatures. Heterojunctions are described using a thermionic emission model [60], and QWs are treated as scattering centers [61], resulting in additional carrier capture rates in Eqs. (2.2) and (2.3).

Simplified Approach

The implementation of the above thermodynamic equations is, however, a very complex task. A drastically simplified model can also be suitable to estimate the above-threshold conditions in VCSELs with semiconductor mirrors. The current flow and the differential resistance are mainly determined by the mirrors and contact resistances in these devices.
2.3 Thermal Model

The following description provides the current profile through the QWs, as well as Joule-heating in the broken-line limit, but cannot capture the nonlinear semiconductor behavior.

The thermodynamic equations are simplified on the basis of several assumptions. When an ordinary VCSEL is modulated at not higher than about 10 Gbit/s bit rate, the transport of carriers to the active region is almost quasistationary, because the relaxation time of the carrier flow perturbation is typically in the order of 0.01-0.1 ps [62]. Thus time derivatives of the carrier densities can be omitted on slower time scale. Charge neutrality is assumed in the semiconductor mirrors as well as in the QWs, implying that the density of free carriers equals to that of the ionized donors, and free electron concentration equals to free hole concentration in the (intrinsic) QWs. Only majority currents are taken into account on the two sides of the active region, electron current on the n-doped side, and hole current on the p-doped side. Diffusion terms may be neglected, provided that the layers have piecewise constant doping levels, and all impurities are ionized. Electron-hole recombination is practically zero outside the QWs. Omitting temperature-gradient induced cross-terms finally leads to the simple continuity equation:

\[ 0 = -\nabla j = \nabla (\sigma \nabla \Phi), \]  

where

\[ \sigma = \begin{cases} 
\varepsilon \mu_e N_D & \text{for n-doped semiconductors} \\
\varepsilon \mu_p N_A & \text{for p-doped semiconductors} 
\end{cases} \]  

(2.8)

(2.9)

gives the electric conductivity. The heterojunctions can be modeled by an anisotropic diagonal conductivity tensor, in which the component perpendicular to the interface is decreased [62, 63, 64].

Appropriate boundary conditions must be assigned to the Laplace-equation. The simplest choice is to impose constant potential at the metal contacts (Dirichlet-type), and zero normal derivatives elsewhere (Neumann-type). A mixed boundary condition \( \Phi - r \sigma \hat{n} \cdot \nabla \Phi = \Phi_0 \) describes an alternative contact with \( \Phi_0 \) fixed potential and \( r \) metal-semiconductor sheet resistivity, and \( \hat{n} \) denotes the normal unit vector of the interface.

The resulting equations can be solved after numerical discretization. The finite volume method (FVM), sometimes also referred as box method [59], is the most intuitive option, which involves expressions of outgoing fluxes from every element, and leads to an equivalent network representation of the system. It can be easily formulated for simple polyhedra, such as straight hexahedra and prisms, or tetrahedra. Finite difference method (FDM) can also be implemented for orthogonal grids, while finite element method (FEM) can be adopted for arbitrary geometry.

2.3 Thermal Model

The most important purpose of thermal modeling is the estimation of the thermal resistance of the VCSEL. This global parameter is defined as the linear coefficient relating
the maximal temperature increase and the total dissipated heat power for small input powers. The main laser parameters such as wavelengths and losses of the modes, and the optical gain peak depend on the thermal resistance within the frame of a simple lumped element representation, and it should be minimized to achieve high thermal stability. A more sophisticated description given by Eqs. (2.4) and (2.7) involves spatially distributed material parameters and temperature profile. It is rewritten without cross-terms as follows:

\[ c_p \frac{\partial T}{\partial t} = \nabla (\kappa \nabla T) + \rho_{\text{heat}}, \tag{2.10} \]

where the distributed heat source constitutes several factors. The two largest ones are nonradiative recombination in the QWs and the Joule-heating inside the mirrors. Minor contributions emerge from free-carrier absorption of photons, and from Peltier-heating.

The thermal time constant due to perturbations in the heat sources can be calculated using the above time-dependent equation. The temperature change under typical modulation at few Gbit/s is negligible, if long 0 or 1 sequences are avoided, because the thermal time constant of a VCSEL is in the order of microseconds. One can use the static version of the above equation with averaged heat sources in this situation.

The selection of boundary conditions is similar to the electronic problem. Constant temperature is often assumed at the heat sink (Dirichlet-type), and homogeneous Neumann-condition elsewhere. One may also want to use a mixed boundary condition \( T - \kappa \alpha^{-1} \hat{n} \cdot \nabla T = T_0 \) at the heat sink and at the metal contacts, which impose finite heat transfer characterized by \( \alpha \) coefficient to a fixed temperature \( (T_0) \) reservoir. The numerical solution is carried out employing FVM/FDM/FEM discretization, and yields the temperature distribution inside the VCSEL. The local values can then be incorporated into most material parameters, with which temperature-dependent device characteristics can be simulated.

2.4 Optical Mode Calculation

Modes of Open Cavities

The most challenging simulation task for VCSELs is the accurate calculation of resonator eigenmodes. One difficulty comes from the fact that the laser diode is, in contrast to the familiar closed cavities known from classical electrodynamics or quantum mechanics, an open system from which a portion of light escapes through a partially transmitting mirror.

There are two options to circumvent this difficulty. First is to consider the laser cavity plus its infinite surroundings (called as the “universe”) as a conservative system, and to calculate the eigenmodes of this set. This approach would result in a continuum of modes of the universe besides the interesting cavity modes, which form an orthogonal basis together, but the description of the laser operation would be extremely uneconomic.
The second approach postulates a non-hermitian Hamiltonian for only the open cavity, whose left and right eigenfunctions form a biorthogonal basis, and defines a new inner product [67]. Mode orthogonality and completeness holds for only the cavity modes with respect to this inner product, and the usual methods can be utilized later. There are two prerequisites of this theory: 1. the discontinuity condition forcing a truncation of the cavity (by a step in the index of refraction, for example), and 2. the "no-tail" condition ensuring that outgoing waves are not scattered back (for instance, by constant refractivity outside the cavity) [68].

Establishing the Problem

The laser mode problem is specified, supposed that the refractive index is known in the whole laser diode, in the substrate and in the air. The background (nominal) index may be changed due to several effects, which must be incorporated as correction terms. These include temperature- and carrier-induced change in the real part of the refractivity, birefringence due to electrooptic or elastooptic phenomena resulting in an anisotropic tensor, gain and free-carrier absorption modifying the imaginary part, etc. Note that the real and imaginary parts cannot be changed independently, and corrections in one would give rise appropriate modifications of the other, as known from Kramers-Kronig relations [66]. Nevertheless, some terms might be neglected for practical calculations. The simulation for nonlinear relationship between the electric displacement ($D$) and electric field ($E$), or for that possessing temporal hysteresis is out of the scope of this thesis.

The resonator modes are usually calculated under two conditions. The cold cavity model assumes an unbiased diode without pumping in the QWs. As a consequence, any initial excitation decays exponentially with time due to cavity losses. Three origins of losses can be distinguished, first mirror loss due to the finite reflectivity of DBRs that is required for light emission. On the other hand, absorption loss inside the mirrors, as well as scattering loss caused by a dielectric aperture inevitably decrease the laser efficiency through increased threshold gain and diminished outcoupling factor.

The second approach deals with an active cavity pumped either by current injection or optically to compensate the losses and maintain stationary laser light power. The second unknown in this model besides the modal wavelength is the critical pumping level or the threshold gain, at which the laser intensity is neither attenuated nor amplified. In fact, the injection mechanism does not only affect the gain of the active material but changes the refractive index distribution due to heating, and influences the properties of the optical modes. This secondary effect can be taken into account in both models. The cold and active cavity descriptions are obviously inherently related, and their relationship is further discussed in Section 2.5.

Numerous methods have been published to simulate the optical mode properties of VCSELs [69]. Although they all are claimed to be three-dimensional (3-D) models, most of them can be applied only to axisymmetric devices, in which the azimuthal degree of
freedom can be eliminated by a well-known analytical dependence. In order to distinguish clearly among the theories, they will be referred as two-dimensional (2-D) ones, as a function with two independent spatial variables is to be calculated. This step is usually introduced in different places in the literature, either postulating it immediately when setting the problem, later narrowing the discussion to the special structures of interest, or only due to computational difficulties. Further simplification is the assumption of separable solution in some cases, which are labeled here as one-plus-one-dimensional (1+1-D) methods.

**Vectorial and Scalar Descriptions**

The laser resonator modes are calculated on the basis of classical electromagnetic theory, since the number of photons inside the cavity is usually large enough when the stimulated emission dominates. The derivation starts from the time-dependent, source-free Maxwell’s equations for materials with possibly anisotropic complex permittivity ($\varepsilon$) and an isotropic permeability that equals unity:

\[
\nabla (\varepsilon_0 \varepsilon E) = 0, \quad \nabla (\mu_0 H) = 0, \quad \nabla \times E = -\mu_0 \frac{\partial H}{\partial t}, \quad \nabla \times H = \varepsilon_0 \frac{\partial (\varepsilon E)}{\partial t},
\]

with the magnetic field $H$. The charge density acts as a source of the electrostatic field as indicated in Eq. (2.1), and it can be omitted in the case of high-frequency optical fields. One can exploit that the permittivity does not change on the optical time scale of the order of $10^{-15}$ s, therefore it can be taken out of the time-derivative in the forth equation. The equations hold in the space regions, where the permittivity is continuous, and are subject to the well-known boundary conditions at material discontinuities. The tangential components of $E$ and $H$, and the normal components of $\varepsilon E$ and $H$ (since $\mu \equiv 1$) must be continuous.

The finite-difference time-domain (FDTD) approach follows the evolution of the fields on the fastest time-scale after an initial excitation was imposed on the system [70]. The optical modes can be extracted afterwards, provided that their decay times are considerably different. Modes with high losses disappear rapidly, and only the mode with the longest decay time remains after long enough period. The next mode can be separated using the same method after subtracting the first from the fields.

Other approaches convert the problem into the frequency domain according to the adiabatic approximation. It holds if the maximum frequency at which the laser is modulated, is small compared to the inverse photon round-trip time within the laser cavity [71]. The time dependent electromagnetic fields are expanded on the basis of modes that exhibit varying amplitudes. Every mode is characterized by $\exp(i\omega t)$ time dependence under passive conditions, where $\omega = \omega' + i\omega''$ denotes its complex angular frequency. Taking the curl of the third Maxwell’s equation and substituting it into the fourth, one
2.4. OPTICAL MODE CALCULATION

gets the vectorial Helmholtz equation:

\[ \nabla \times (\nabla \times \mathbf{E}) - \frac{\omega^2}{c_0^2} \mathbf{E} = 0, \quad (2.12) \]

with the introduction of the speed of light in vacuum \( c_0 = \sqrt{\varepsilon_0 \mu_0} \). This equation or an equivalent formulation serve as common starting point of most optical methods.

The scalar version for isotropic materials can be derived by employing the identity

\[ \nabla \times (\nabla \times \mathbf{E}) = \nabla (\nabla \cdot \mathbf{E}) - \Delta \mathbf{E}, \]

and utilizing the first Maxwell’s equation:

\[ \nabla (\nabla \cdot \mathbf{E}) = \nabla \left[ \nabla \left( \frac{\mathbf{D}}{\varepsilon} \right) \right] = -\nabla \left( \frac{\nabla \cdot \mathbf{E}}{\varepsilon} \right) \times \mathbf{E} - \left( \frac{\nabla \cdot \mathbf{E}}{\varepsilon} \right) \mathbf{E} \times \frac{\nabla \cdot \mathbf{E}}{\varepsilon} - (\mathbf{E} \nabla) \frac{\nabla \cdot \mathbf{E}}{\varepsilon}. \]

If the dielectric profile varies only weakly, that is \( |\nabla \epsilon| \ll \epsilon/\lambda \) and \( \partial^2 \epsilon/\partial x_i \partial x_j \ll \epsilon/\lambda^2 \) where \( \lambda = 2\pi c_0/(\omega' \sqrt{\varepsilon}) \) is the wavelength in the material, these terms may be neglected compared to \( \Delta \mathbf{E} \) and to the last one in Eq. (2.12). Furthermore, VCSELs usually emit linearly polarized light in one transverse direction. The longitudinal component is usually smaller at least by one order of magnitude, which can be justified by comparing the spatial variation of the electric field components according to the first Maxwell’s equation in a homogeneous layer. One can recognize that the relative magnitudes of the components must agree with the ratio of the respective characteristic lengths. While \( E_z \) increases from zero to maximum in a quarter wavelength layer, the transverse components only in the range of the aperture radius. One reaches finally to the scalar Helmholtz equation for the dominant transverse component \( (E_x \text{ or } E_y) \) denoted by \( \Psi \):

\[ \Delta \Psi + \frac{\omega^2}{c_0^2} \epsilon \Psi = 0. \quad (2.14) \]

Continuous variation of the field is assumed at every material interfaces. Although the scalar treatment is valid only for small index contrast or weak spatial variation, many researchers use it regularly for VCSEL simulation due to its simplicity and reduced computational efforts. In fact, even the vectorial Helmholtz equation is often solved assuming simplified continuous variation for all electric field components. The scalar version is believed to predict inaccurate results mostly for small apertures.

Perfectly Matched Layers

It belongs to the common problems of computational electrodynamics to deal with open cavities. It is obvious that the infinite space cannot be modeled numerically, but any truncation of the calculation domain that enforces zero fields (or field component) could be considered as an arbitrary manipulation to the system. For example, radiated waves would be completely reflected back to the structure from a metallic wall. In order to alleviate this, an absorbing boundary condition should be applied. Contrary to traditional absorbers, a perfectly matched layer (PML) allows the reflectionless attenuation of incident waves in a wide range of wavelength and direction, regardless of polarization.

19
Thus, if the physical domain is covered by PML and closed with homogeneous Dirichlet-condition or with a perfect electric conductor (PEC) outside, the reflected waves decay to almost zero before arriving back to the important region.

PML has been interpreted several ways. The original theory [72, 73] split all electric and magnetic field components into two pieces, resulting in a total of twelve time-dependent scalar equations from two curl-type Maxwell’s equations, and introduced magnetic conductivities that are “impedance-matched” to electrical ones. Alternative descriptions employed either anisotropic lossy mapping of space with complex coordinate stretching [74, 75, 76], or modified complex anisotropic $\varepsilon$ and $\mu$ tensors [77]. The simplest formulation proceeds probably with the complex coordinates, which are used in the covering PML region. In the direction normal to the PML interface, let us say along the $z$-axis, the coordinate is changed to $z' = s_z(z)z$ with $s_z(z) = 1 - i\sigma_z(z)/(\omega_0\varepsilon)$, where $\sigma_z(z)$ is an appropriate stretching function. The same transformation is applied at the other sides for the $x$- and $y$-coordinates. The original and modified coordinates must be identical in the physical domain.

The Maxwell’s equations are modified by replacing the $\nabla$ operator with

$$\nabla_s = \frac{1}{s_x} \frac{\partial}{\partial x} \hat{x} + \frac{1}{s_y} \frac{\partial}{\partial y} \hat{y} + \frac{1}{s_z} \frac{\partial}{\partial z} \hat{z},$$

where unit vectors pointing along the Descartes-coordinate axes are introduced. It can be easily shown that a plane wave (let us label its wavevector by $k$) with an electric field $E \exp(-ikr)$ satisfies the modified Maxwell’s equations in the PML having uniform dielectric constant, only if the dispersion relation $(k_x/s_x)^2 + (k_y/s_y)^2 + (k_z/s_z)^2 = \varepsilon(\omega/c_0)^2$ is fulfilled. If the wavevector forms an angle $\vartheta$ with the $z$-axis, it can be expressed as $E \exp(-ikr) \sim \exp(-is_z \cos \vartheta \sqrt{\varepsilon \omega/c_0}z) = \exp(s'_z \cos \vartheta \sqrt{\varepsilon \omega/c_0}z) \exp(-is'_z \cos \vartheta \sqrt{\varepsilon \omega/c_0}z)$, and is therefore attenuated. If a Dirichlet boundary condition embodying a perfect metal wall is specified at distance $L$ from the inner border of the PML, the theoretical reflection coefficient after back and forth propagation is

$$R = \exp\left[2\cos \vartheta \sqrt{\frac{\varepsilon \omega}{c_0}} \int_0^L s''_z(z)dz\right];$$

and it can be small enough in a wide frequency and direction range, if $s''_z(z)$ is negative. The numerical reflection coefficient after discretization can be larger, if the PML consists of only few cells or the stretching function $\sigma_z(z)$ varies rapidly [78].

The most relevant procedures aiming the determination of the resonator modes are reviewed in details below, further ones exposed in Appendix A complete their list, and they are summarized at the end of this section.

### 2.4.1 Effective Index Method

Effective index method (EIM) is well established for the approximate determination of the waveguide modes in edge-emitting lasers [79]. The 2-D transverse plane is separated into
2.4. OPTICAL MODE CALCULATION

one-dimensional (1-D) equations for the horizontal and vertical directions, respectively. The horizontal solutions in layers without vertical variations yield horizontal mode profiles and averaged effective indices to the vertical solution.

EIM was the first model for the calculation of optical modes in VCSELs [80]. The light propagates perpendicular and not parallel to the layers. A separable solution is searched in the longitudinal and transverse coordinates. First standing wave type eigenfunctions are found for layer stacks representing the lateral regions, assuming that they extend laterally to infinity. With these eigenfunctions one calculates effective refractive indices, with which waveguide modes of equivalent optical fibers are obtained.

A solution of the scalar Helmholtz equation is assumed to have the separable form

\[ \Psi_j(r, z, \phi) = \psi_j(z) \phi(r) \exp(i m \phi) \]

in each radial region (indexed by \( j \)), and \( m = 0, 1, 2, \ldots \) determines the azimuthal pattern of the mode. The modes with \( m > 0 \) are doubly degenerate with sinusoidal and cosinoidal distributions.

The axial standing wave consists of forward and backward propagating plane waves in each layer, namely

\[ \psi_{j,k}(z) = a^{+}_{j,k} \exp(i \beta_{j,k} z) + a^{-}_{j,k} \exp(-i \beta_{j,k} z) \]

in the \( k \)th layer, where \( \beta_{j,k} = (1 - \xi_{j}/2) \sqrt{\varepsilon_{j,k} \omega_0 / c_0} \) denotes the propagation constant and \( a^{+}_{j,k} \) and \( a^{-}_{j,k} \) the amplitudes of forward and backward waves. The nominal angular frequency is given by \( \omega_0 \), and \( \xi_{j} \) is a yet unknown small complex correction factor. The layer solutions must be joined at the interfaces to respect the boundary conditions. Since \( \Psi \) represents the dominant transverse component, \( \psi_j(z) \) must be continuous. The second condition for \( D_z \) requires the continuity of the

\[ \frac{a^{+}_{j,k} \exp(i \beta_{j,k} z)}{\beta_{j,k}} - \frac{a^{-}_{j,k} \exp(-i \beta_{j,k} z)}{\beta_{j,k}} \]

expressions. These lead to a linear relationship given by a 2 × 2 transfer matrix between the forward and backward amplitudes in the adjacent layers. The chain product of these matrices yields the effective transfer matrix \( T_j(\xi_{j}) \) of the stack as a function of the complex parameter \( \xi_{j} \). Since there is no energy input to cold-cavity resonators, only outgoing waves are allowed from the bottom (denoted by subscript \( b \)) and top (\( t \)) surfaces, thus \( a^{+}_{j,b} = 0 \) and \( a^{-}_{j,t} = 0 \). This constraints the transfer matrix to have \( T_j^b(\xi_{j}) = 0 \) element, which selects the allowed resonance frequencies of the stack; and the amplitudes of the standing wave can be then calculated recursively staring from the substrate. It should be stressed that the root finding on a complex plane was not a trivial numerical task.

The effective dielectric constant of the \( j \)th lateral region is obtained by

\[ \langle \varepsilon_j \rangle \approx \frac{\int_{z_0}^{z_N} \psi_j^*(z) \varepsilon_j(z) \psi_j(z) dz}{\int_{z_0}^{z_N} \psi_j^*(z) \psi_j(z) dz} \],

(2.18)

where \( z_0 \) and \( z_N \) refers to the coordinates of the bottom and top surfaces of the diode. The equivalent waveguide problem is set up as follows. Given an optical fiber with regions of \( \langle \varepsilon_j \rangle \) dielectric constants and \( R_j \) radii, and free space propagations constants of \( \beta_j = (1 - \xi_{j}/2 \omega_0 / c_0) \). Then the scalar Helmholtz equation transforms to a radial
CHAPTER 2. SIMULATION BACKGROUND

Bessel-equation
\[ \frac{\partial^2 \phi(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \phi(r)}{\partial r} - \frac{m^2}{r^2} \phi(r) = - \left( \langle \varepsilon_j \rangle \frac{\omega^2}{c_0^2} - \beta_j^2 \right) \phi(r) = -\kappa_j^2 \phi(r) \]  
(2.19)
introducing the radial wavevector component \( \kappa_j \). The solutions are conventional and modified Bessel-functions of the first and second kind, the latter also called Hankel-functions. For an idealized step-index fiber consisting of a core and an infinite cladding, \( \phi(0) \) must be finite and the field must vanish at infinity, thus only the first order Bessel-function \( J_m(\kappa_1 r) \) obeys the solution in the core, and the first order asymptotically decaying Hankel-function \( H_m(\kappa_2 r) \) in the outermost cladding. The continuity of \( \phi(r) \) at the core-cladding interface yields the dispersion relation
\[ \kappa_1 J_{m+1}(\kappa_1 R_1) = \kappa_2 H_{m+1}(\kappa_2 R_1) \]  
(2.20)
which is satisfied only for a discrete set of \( \omega \) complex eigenvalues and the associated \( \phi(r) \) \exp(\text{im}\varphi) \) lateral mode patterns. The obtained linearly polarized modes are labeled as \( \text{LP}_{cmn} \), where \( m = 0, 1, 2, ... \) characterizes the azimuthal variation, \( n \) is the number of nodes along the radius, and \( c (s) \) refers to the even (odd) symmetry with respect to x-axis if \( m > 0 \). All modes have another twofold degeneracy because x- and y-polarizations are not resolved by the scalar description.

Some papers publish \( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \) \phi'(x, y) = \kappa_j^2 \phi'(x, y) \) without the separation in \( r \) and \( \varphi \) coordinates instead of Eq. (2.19), but still use the simplification when solving the dispersion relation. There exists yet another EIM formulation, which allows slow time dependence (\( \tau \gg 10^{-15} \) s) of the field besides the optical frequency, and results in a time-dependent equation for an unknown quantity \( \phi''(x, y, \tau) \) [63, 62]:
\[ \frac{\partial \phi''}{\partial \tau} = \frac{ic_0^2}{2\omega_0 \langle \varepsilon_j \rangle} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\omega^2}{c_0^2} \xi_j \langle \varepsilon_j \rangle \right) \phi''. \]  
(2.21)
Its stationary solution provides equivalent results with those obtained by waveguide analysis, of course. The advantage is that further correction terms caused by changes in the temperature, carrier density, or optical gain may be incorporated into the braced expression.

2.4.2 Weighted Index Method

The weighted index method provides the best separable solution of the optical fields in the \( (r, z, \varphi) \)-coordinates for cylindrically symmetric VCSELs [81, 82]. It is available in vectorial formulation, and takes into account the polarization of the light. As a consequence, it resolves the twofold polarization degeneracy that is hidden in scalar descriptions. The vectorial solutions of optical fibers, which also appear in the separable approximation of VCSEL modes, can be classified to transverse electric (TE_{0n}) modes with their electric field vector pointing exactly to the tangential direction, transverse magnetic (TM_{0n}) ones...
of dominantly radial electric field, and doubly degenerated hybrid (HE_{mn} and EH_{mn}) modes, which exhibit nonvanishing longitudinal components in both electric and magnetic fields. The subscripts refer to their azimuthal and radial variations (number of node surfaces). There is a correspondence relationship between linearly polarized scalar and vectorial fields [79].

Before turning our attention to the vectorial description, the simpler scalar model shall be briefly outlined. The dominant electric field of \( \Psi(r, z, \varphi) = \psi(z)\phi(r) \exp(i m \varphi) \) component is substituted into Eq. (2.14), yielding

\[
\frac{\partial^2 \psi(z)}{\partial z^2} \phi(r) + \left[ \frac{\partial^2 \phi(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \phi(r)}{\partial r} - \frac{m^2}{r^2} \phi(r) \right] \psi(z) + \varepsilon(r, z) \frac{\omega^2}{c_0^2} \psi(z) \phi(r) = 0 \tag{2.22}
\]

after simplifications. By multiplying with \( \psi^*(z) \) and integrating against \( z \) from the lower to the upper boundary planes of the VCSEL; and multiplying with \( \phi^*(r) \) and integrating against \( r \) from zero to infinity, one gets two coupled equations:

\[
\begin{align*}
\left[ \frac{\langle \psi^*(z) \frac{\partial^2 \psi(z)}{\partial z^2} \rangle}{\langle \psi^*(z) \psi(z) \rangle} + \frac{\omega^2}{c_0^2} \frac{\langle \psi^*(z) \varepsilon(r, z) \psi(z) \rangle}{\langle \psi^*(z) \psi(z) \rangle} \right] \phi(r) + \left[ \frac{\partial^2 \phi(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \phi(r)}{\partial r} - \frac{m^2}{r^2} \phi(r) \right] \psi(z) & = 0, \\
\left\{ \left[ \frac{\langle \phi^*(r) \frac{\partial^2 \phi(r)}{\partial r^2} \rangle}{\langle \phi^*(r) \phi(r) \rangle} + \frac{1}{r} \frac{\partial \phi(r)}{\partial r} - \frac{m^2}{r^2} \phi(r) \right] + \frac{\omega^2}{c_0^2} \frac{\langle \phi^*(r) \varepsilon(r, z) \phi(r) \rangle}{\langle \phi^*(r) \phi(r) \rangle} \right\} \psi(z) + \frac{\partial^2 \psi(z)}{\partial z^2} & = 0, \tag{2.23}
\end{align*}
\]

where the brackets denotes the integrals. If one assumes forward and backward traveling waves with \( \beta_k \) propagation constant in the \( k \)th layer, the first term of Eq. (2.23) simplifies to the negative of the weighted squared propagation constant \( \langle \beta_k^2 \rangle \), and the second quotient to weighted permittivities \( \langle \varepsilon_j \rangle \) in each radial region. Using the same arguments for Bessel-functions in the radial direction, the average of the squared radial wave vector component \( \langle \kappa^2 \rangle \) and layerwise weighted permittivities \( \langle \varepsilon_k \rangle \) appear in Eq. (2.24). In order to obtain these quantities, the following iterative procedure is carried out. The first guess of the complex angular frequency and the radial wavenumbers knowing the first guess for \( \langle \beta^2 \rangle \). Then the axial problem is corrected by the calculated \( \langle \kappa^2 \rangle \), etc. The iteration stops after these quantities do not change significantly.

The vectorial treatment is very similar except that two independent scalar functions are required to express all field components. These can be selected as the axial components of the electric \( (A_z) \) and magnetic \( (F_z) \) vector potentials, from which the fields can be easily calculated according to

\[
E = -\frac{ie_0}{\omega \varepsilon_0 \varepsilon} \nabla \times \nabla \times (\hat{z} A_z) - \nabla \times (\hat{z} F_z), \tag{2.25}
\]
\[ \mathbf{H} = \nabla \times (\hat{z} A_z) - \frac{i c_0}{\omega \mu_0} \nabla \times \nabla \times (\hat{z} F_z), \]  
(2.26)

where \( \hat{z} \) stands for longitudinal unit vector. Separable solutions \( A_z(r, z, \varphi) = Q(z) P(r) \exp(i m \varphi) \) and \( F_z(r, z, \varphi) = S(z) R(r) \exp(i m \varphi) \) are substituted into the scalar Helmholtz equation (which is valid in piecewise homogeneous domains), and decoupled for axial and radial problems. Interesting feature is that for pure transverse electric and magnetic modes either \( Q(z) \equiv 0 \) or \( S(z) \equiv 0 \) applies, and therefore the solution proceeds as for the scalar case; but for hybrid modes they are coupled when formulating the radial boundary conditions. In this case one gets a \( 4 \times 4 \) radial transfer matrix transforming the coefficients of the Bessel-components of \( P(r) \) and \( R(r) \) from the core to the outermost region. The condition, that they should be finite at the center, and vanish in radial infinity, enforces two coefficients to be zero on both sides, which is satisfied only if a \( 2 \times 2 \) subdeterminant approaches zero. The best separable solution and the related eigenfrequency is refined by axial and radial iterations for each resonator modes of interest.

2.4.3 Coupled Mode Model

This vectorial approach originates from the description of dielectric waveguides, in which deviations from the ideal geometry results in energy exchange between the modes. Typical structural imperfections include the variation of the core diameter, the ellipticity of the core-cladding interface and fiber bending. The mode mixing can be examined by expressing the electromagnetic fields into modes with longitudinally varying amplitudes. One can select the basis as the guided and radiation modes of an ideal optical fiber, or as modes of locally equivalent fibers, whose cross-sections correspond to the actual geometry along the propagation direction. It is not difficult to recognize the analogy of the layer modes of aforementioned methods to local modes, while the coupled mode model (CMM) uses global modes for the field expansion.

The stationary electromagnetic field is expanded on the complete and continuous basis of the TE and TM modes of an infinite passive cavity material [83, 84]:

\[ \mathbf{E}(r, z, \varphi) = \sum_{m,l,p,\alpha} \int_{\kappa} a_{\kappa,m,l,p}^\alpha(z) \mathbf{E}_{\kappa,m,l,p}^\alpha(r, \varphi) d\kappa, \]  
(2.27)

where \( \kappa \) denotes the radial wave component, \( m \) the azimuthal periodicity of the mode, \( l \) the parity with respect to the x-axis, \( p \) labels the TE or TM distributions, and \( \alpha \) the forward and backward travel directions. The radial variation of the basic modes is given by terms of continuous Bessel-functions for each component of the electric field. The continuous \( \kappa \) variable is numerically discretized using steps \( \Delta \kappa \), and the five parameters can be abbreviated as \( \zeta \). According to coupled mode equations, the longitudinal variation of the expansion coefficients (arranged in vector \( \mathbf{a} \)) is governed by

\[ \frac{d\mathbf{a}}{dz} = (\mathbf{B} + \mathbf{K} \Delta \kappa) \mathbf{a}, \]  
(2.28)
where $B_{\zeta'} = -is_{\alpha}\beta\delta_{\zeta'}$ denotes a diagonal matrix characterizing the propagation in the absence of coupling, $s_{\alpha} = \pm 1$ for forward and backward waves, $\beta = \sqrt{(\varepsilon_{\text{ref}}\omega^2/c_0^2 - \kappa^2)}$ the propagation constant, and $\varepsilon_{\text{ref}}$ gives the dielectric constant of a reference material. The coupling matrix $K$ depends on the deviation of the tensorial permittivity from the isotropic reference material, and its elements read as

$$K_{\zeta\zeta'} = -\frac{i\omega}{C_\zeta} \int \left\{ \mathbf{E}_{\zeta t} \left[ \frac{(\Delta \varepsilon E_{\zeta'})_t}{\varepsilon_{\text{ref}} + \Delta \varepsilon_{zz}} - \frac{(\Delta \varepsilon E_{\zeta'})_z}{\varepsilon_{\text{ref}} + \Delta \varepsilon_{zz}} \right] + \frac{E_{\zeta z}\varepsilon_{\text{ref}}}{\varepsilon_{\text{ref}} + \Delta \varepsilon_{zz}} (\Delta \varepsilon E_{\zeta'})_z \right\} dx dy. \quad (2.29)$$

The subscripts $t$ and $z$ stand for the tangential and longitudinal components, respectively, and $C_\zeta$ is a lengthy normalization constant. The expression can be split for transverse and longitudinal contributions for isotropic materials. If the perturbation is a step function with a simple contour in the transverse plane, the integrals can be evaluated analytically.

The amplitudes of forward and backward propagating waves must match the reflection coefficients at the bottom and top surfaces of the VCSEL, where the geometry is planar. Thus $a^+(0) = R_{\text{bottom}} a^-(0)$ and $a^-(L) = R_{\text{top}} a^+(L)$, where the reflection matrices are diagonal and consists of the scalar reflection coefficients at a given frequency. A global transfer matrix composed from the chain product of single layer matrices $T = \prod_k \exp[(B + K\Delta \kappa)L_k]$ relates the coefficients at the top and bottom positions:

$$[a^+(L)] = \begin{bmatrix} T^{++} & T^{+-} \\ T^{-+} & T^{--} \end{bmatrix} \begin{bmatrix} a^+(0) \\ a^-(0) \end{bmatrix}. \quad (2.30)$$

It follows that $(R_{\text{top}}T^{++}R_{\text{bottom}} + R_{\text{top}}T^{+-} - T^{-+}R_{\text{bottom}} - T^{--})a^-(0) = 0$, which can be fulfilled only for discrete complex frequencies.

It is desirable to reformulate this condition by introducing gain into the active material. The imaginary part of its refractive index should possess a preselected profile and unknown magnitude that compensates the cavity loss and yields real frequency. Since the QWs are thin, their active contribution to the global transfer matrix can be approximated up to linear order instead of exponential, and the transfer matrix is split into passive and active contributions: $T = T_{\text{passive}} + i\Omega T_{\text{active}}$, where the real $\Omega$ parameters is proportional to the magnitude of the gain. Simple manipulation of the equations leads to an eigenvalue problem with $\Omega^{-1}$ as eigenvalue and $a^-(0)$ as eigenvector. Finally an appropriate frequency range should be scanned, in which only (nearly) real eigenvalues and the related distributions are accepted as stationary laser modes.

CMM has been proved successful in describing polarization characteristics of several VCSELs incorporating distorted apertures, and surface patterns of comparable or larger size then the free space wavelength [85, 57, 33]. However, the finite expansion basis does not permit to satisfy the discontinuity condition for the normal component of the electric field at lateral interfaces, since it deals with laterally continuous functions.
2.4.4 Finite Element Method

All previous methods assumed an analytical dependence on the longitudinal coordinate in every layer composed from forward and backward propagating waves. Finite element method (FEM) utilizes a numerical discretization in this direction as well. This procedure requires careful consideration, since AlGaAs-based VCSELs usually consist of more than fifty pairs of quarter wavelength layers, and numerous cells should be assigned in all of them to resolve the standing wave pattern precisely. Therefore the number of unknowns becomes roughly by a factor of a thousand greater. On the other hand, one gets a sparse matrix, which can be stored more economically in the computer memory than dense matrices encountered in mode expansion techniques. FEM has another clear advantage, as it can be easily adapted to other optoelectronic devices.

The subject of this method is to find a fully numerical solution of the vectorial Helmholtz equation for a given permittivity distribution that is independent of the azimuthal coordinate. To allow reflectionless truncation of the computational domain by means of PEC walls, one should cover the physical region with PML as discussed above. It is realized by introducing an anisotropic diagonal tensor $\Lambda(r)$ into Eq. (2.12), which then takes the form [59, 86]

$$
\nabla \times \left[ \Lambda^{-1}(r) \nabla \times E(r) \right] - \frac{\omega^2}{c_0^2} \Lambda(r) \varepsilon(r) E(r) = 0, \quad (2.31)
$$

with

$$
\Lambda(r) = \begin{bmatrix}
\frac{s_y(r)s_z(r)}{s_x(r)} & 0 & 0 \\
0 & \frac{s_z(r)s_y(r)}{s_x(r)} & 0 \\
0 & 0 & \frac{s_x(r)s_y(r)}{s_z(r)}
\end{bmatrix}. \quad (2.32)
$$

The matrix reduces to unity matrix in the physical region, and can also be given in cylindrical coordinates [76]. It is essential to use the variational principle for the derivation of finite element discretization, which states that the previous equation is equivalent with the stationary point of the following functional:

$$
F(E) = \frac{1}{2} \int_V \left[ (\nabla \times E) \Lambda^{-1}(\nabla \times E) - \frac{\omega^2}{c_0^2} E \varepsilon \Lambda E \right] dV, \quad (2.33)
$$

where the integration must be evaluated for the whole domain including the PML.

One can expand the fields into Fourier-series in the azimuthal coordinate for rotationally symmetric structures:

$$
E(r, z, \varphi) = E_{rz,0}(r, z) + E_{\varphi,0}(r, z)e_\varphi +
+ \sum_{m=1}^{\infty} \left[ E_{rz,m}(r, z) \cos (m\varphi) + E_{\varphi,m}(r, z) \hat{e}_\varphi \sin (m\varphi) \right] +
+ \sum_{m=1}^{\infty} \left[ E_{rz,m}(r, z) \sin (m\varphi) + E_{\varphi,m}(r, z) \hat{e}_\varphi \cos (m\varphi) \right], \quad (2.34)
$$
where $\hat{e}_\phi$ labels the normal unit vector to the $rz$-plane, and the $rz$ subscript the in-plane component. The first sum contains the symmetric fields, the second the asymmetric fields with respect to the $\varphi = 0$ plane. It can be shown that inserting this ansatz into the variational problem, the different terms are decoupled \[86\], and one should solve for the stationary points for each term independently. The boundary conditions along the axis are given by $E_r,0(0,z) = 0$ and $E_{\varphi,0}(0,z) = 0$ for $m = 0$, $E_{z,1}(0,z) = 0$ for $m = 1$, while all components must vanish for $m > 1$.

The 2-D problems are solved by substituting linear combinations of edge and node finite element basis functions into the decoupled functionals. The axial cross section is meshed with triangular or quadrilateral elements, and vectorial basis functions representing $E_{rz,m}$ are assigned to their edges, and scalar ones representing $E_{\varphi,m}$ to their nodes. The number of basis functions depends on the type of the polygons and the desired polynomial order of the solution. One should take care to use axial divisions less than $\lambda/32$ in order to properly resolve the standing wave. This yields

$$F \left( \begin{bmatrix} c_i \\ c_j \end{bmatrix} \right) = \frac{1}{2} \begin{bmatrix} c_i \\ c_j \end{bmatrix}^T \begin{bmatrix} A_{ii} & A_{ij} \\ A_{ji} & A_{jj} \end{bmatrix} \begin{bmatrix} c_i \\ c_j \end{bmatrix} - \frac{1}{2} \frac{\omega^2}{c_0^2} \begin{bmatrix} c_i \\ c_j \end{bmatrix}^T \begin{bmatrix} B_{ii} & B_{ij} \\ B_{ji} & B_{jj} \end{bmatrix} \begin{bmatrix} c_i \\ c_j \end{bmatrix}$$

(2.35)

with $c_i$ and $c_j$ denoting the linear coefficients of edge and node basis functions, while $A$ and $B$ evolve as their cross integrals according to Eq. (2.33). The stationary point is obtained as the solution of the generalized algebraic eigenproblem $A\mathbf{c} = \omega^2/c_0^2 B\mathbf{c}$, that results in the complex angular frequency as eigenvalue and the coefficients as eigenvector. The field can be constructed from the known coefficients in each point. The above analysis has been performed for various cylindrical VCSELs using second order-elements, and led to matrices having a rank of the order of 100000.

2.4.5 Comparison of Optical Models

Eleven optical simulation methods have been reviewed in the preceding sections, and they are classified here from various viewpoints. Despite their different complexity, all methods can find the applications, for which they are appropriate and predict valuable results. The common concept is to build up a hierarchical modeling tree that contains fast methods for prompt information, as well as more sophisticated ones that yield accurate results after longer computational time. The theories are summarized in Table 2.1 and discussed below.

One can recognize that Green method itself does not provide the optical modes of VCSEL resonators, but traces back the active cavity problem to an eigenvalue problem Eq. (A.18), whose solutions can be found by relying on other methods. The second

\[\text{The abbreviations of those discussed in Appendix A are recalled here for the sake of convenience: EFM - effective frequency method, NMM - numerical mode matching method, CAMFR - eigenmode expansion with perfectly matched layers, MoL - method of lines, PWAM - plane wave admittance method, Green - Green’s function model, PREVEU - optimized-waist paraxial eigenmodes method.}\]
<table>
<thead>
<tr>
<th>Property</th>
<th>EIM</th>
<th>EFM</th>
<th>WIM</th>
<th>NMM</th>
<th>CAMFR</th>
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<td>Depends</td>
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<td>PhC-VCSELs (3-D only)</td>
<td>General (3-D)</td>
<td>Preliminary attempt (3-D)</td>
<td>2-D</td>
<td>Separable structure</td>
<td>2-D</td>
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**Table 2.1:** Comparison of optical modes for VCSEL simulation
preliminary statement is that the solutions of PREVEU were based on the minimization of the round-trip gain rather than on the waveguiding behavior of the device. One should also note that the modal wavelengths and threshold gains obtained by PREVEU considerably differed from those of other methods [69]. As an interesting feature one should remember that PREVEU predicted nearly Gauss-Laguerre near fields in contrast to the nearly Bessel-type eigenfunctions of the other methods. It is also unique in the sense that it replaces the VCSEL mirrors by an equivalent homogeneous cavity, and eliminates both axial and radial material interfaces.

The methods can be grouped whether they deal with scalar or vectorial fields. Only EIM, EFM and PREVEU used a scalar variable, related to the dominant transverse electric field component \( E_x \), for instance. Other methods introduce two independent components of the vector potentials (WIM, MoL), expansion coefficients of vectorial basis functions that extend for the whole cross section (NMM, CAMFR, PWAM, CMM), or expansion coefficients of localized vectorial shape functions (FEM). The scalar versions of these approaches could also be easily derived.

One can clearly separate EIM, EFM and WIM from the other approaches, as these three do not reflect the diffraction of the wave on the aperture. Of course, it is possible to estimate this phenomenon quantitatively with further methods [87, 88] that emphasize the importance of the Fresnel-number; nevertheless, these \textit{a posteriori} calculations do not couple self-consistently to the basic resonator mode simulation. The remaining models enable the adaptation of the wave to the actual structure, as they do not fix a single lateral mode profile.

The next object is the mathematical characterization of the models. Although all methods invoke some numerical steps, it is essential to classify them according to the longitudinal and radial treatment and to the numerical complexity of the final mathematical task. The first three methods assumed analytical dependence in all spatial variables, and invoked a root finding of function with two independent scalar variables. Since the Green’s function of an infinite reference structure can also be written in analytical form, one may prefer to call it analytical, as well. Five semianalytical methods solve an analytical axial equation, but use either discretization (MoL) or mode expansion in the radial direction. The expansion basis can be composed either from Bessel-functions (NMM, CAMFR, CMM) or from plane waves (PWAM). PREVEU utilized GL expansion functions, in which analytical variation is prescribed in all coordinates. The final mathematical task is to solve a dense matrix eigenproblem in these six formulations. FEM is the single fully numerical method, which treats the axial and radial dimensions at an equal level, performs a full discretization resulting in a final sparse matrix eigenproblem. It is worth to keep in mind that while the number of unknowns is in the order of 100 for 2-D semianalytical approaches, it may exceed 100000 for the fully numerical FEM.

The advantage of FEM is revealed when discussing the boundary conditions. Most methods cannot satisfy all continuity conditions point-by-point at material interfaces, but
only in averaged or smoothed sense. EIM and EFM takes into account only the core in the axial solution and thus neglects other materials outside, WIM defines weighted material indices instead of exact ones. Mode expansion methods cannot perfectly match different finite expansion basis on two sides of an axial interface. In the lateral dimensions, EIM, EFM and the mode expansion methods assume continuous basis functions, neglecting again material discontinuities. MoL can fulfill the continuity conditions at horizontal interfaces, because it deals with the same discretization points on both sides. In principle, it might also fulfill the radial discontinuity condition in 2-D simulations depending on the difference scheme, but fails for 3-D calculations owing to the finite Fourier-expansion in the azimuthal variable. In contrast, it is possible to satisfy all physical continuity conditions with FEM, as it uses local shape functions. The tangential components are matched point-by-point, while the normal electric field component jumps according to the dielectric constants with an accuracy up to the selected polynomial order of the basis.

One should also comment the truncation of the computational domain. The methods having analytical axial descriptions allow only outgoing waves or enforce the reflection coefficients that are valid for planar surfaces. Only PWAM and FEM covered the laser with PML from the bottom and top sides. Analytical methods, CMM and PREVEU simulate laterally infinite structures, where there is no need to close the structure at some radial distance. NMM simply places a metal wall at some distance, not bothering with the backscattered energy. This effect is corrected in CAMFR by introducing PML, which is also employed in PWAM and FEM. It is also possible to impose periodic boundary condition in PWAM for infinite photonic structures.

Although the correct description of material boundary conditions is theoretically desirable, many groups reported excellent agreement with experimental data even for inexact models. Some researchers argued that abrupt discontinuity did not exist in reality, and the permittivity was always smoothed. We may conclude that simpler continuity conditions could be allowed for most practical purposes, but on the other hand, methods claiming correctness and high accuracy should address the exact physical conditions.

2.5 Rate Equation Approach

Lumped Element Model

The preceding section dealt with the calculation of global properties of laser cavity modes, and with the determination of their normalized intensity profiles. These modes can be interpreted as possible modes of VCSELs, but shall not unconditionally appear on the experimental spectrum, only if they benefit from the actual spatial profile of the population inversion. The absolute intensity thus depends on the current injection profile, or with the spot distribution of the incoming light for optically pumped VCSELs. This interaction can be formulated on the basis of a fundamental rate equation approach
that yields both stationary and dynamical characteristics. Before discussing the spatially dependent description, a simple single-mode lumped element model is reviewed, in which the current, carrier and optical profiles are assumed to be uniform [13, 89]:

$$\frac{dn}{dt} = \eta I(t) eV_{QW} - R_{sp}(n) - R_{nr}(n) - v_g \Gamma g(n, S) S,$$

$$\frac{dS}{dt} = \beta V_{QW} R_{sp}(n) + v_g [\Gamma g(n, S) - L] S.$$

Here $n = p$ is the population inversion density in the QW, $S$ the photon number in the mode inside the cavity, $I$ the total current, and $\eta$ denotes the injection efficiency (defined as the ratio of carriers that recombines in the QWs compared to all incoming). $R_{sp}(n) = Bn^2$ labels the rate of spontaneous emission with the radiative recombination coefficient $B$, $R_{nr}(n) = An + Cn^3$ is the nonradiative recombination rate with the monomolecular recombination coefficient $A$ and the Auger-coefficient $C$, respectively. The last term denotes the density of the stimulated emission rate with $v_g$ group velocity, $\Gamma$ is the axial confinement factor of the mode for the QWs, and $g$ labels the material gain coefficient that generally depends on the free carrier density and also on the photon density, the latter accounting for gain suppression at high laser intensity. One has the volume of the QWs ($V_{QW}$), and the modal loss $L$ (in 1/cm units). Finally, the spontaneous emission factor $\beta$ gives the ratio of spontaneously emitted photons that are coupled into the laser mode. The time scale of these equations is much slower than the one corresponding to the optical frequency.

One can easily deduce some basic parameters from these simple equations. Stationary operation is achieved if the time derivatives vanish, which gives the lasing condition $g(n, S) = L/\Gamma$ having neglected the usually smaller spontaneous emission term. Since the photon number is low at threshold, this provides the threshold gain, the threshold carrier density and the threshold current from the first equation. Beyond threshold, $\Gamma g(n, S)$ can be substituted with $L$ in the first equation, and the closed form of $dS/dI$ can be obtained, which is proportional to the slope of the light power to current curve. The proportionality factor is $\omega''(L_{\text{mirror}}, 1/L_{\text{total}})(\hbar \omega')$, since photon number decays at a rate of $\omega''$ in the absence of pumping, and the first brace labels the ratio of emitted photons in the desired direction through one of the mirrors to all lost (absorbed, for example), and the second brace gives the energy of a single photon. Dynamical characteristics can be simulated by tracing the time evolution numerically or by performing analytical small-signal analysis in the frequency domain.

Local Description

In contrast to the lumped element model, the formulation can be carried out naturally for multimode operation. According to the adiabatic approximation, the time dependent electromagnetic fields can be expanded on the basis of modes, if the maximum frequency at which the laser is modulated, is small compared to the inverse photon round-trip time.
within the laser cavity: \( \mathbf{E}(\mathbf{r}, t) = \sum_i s_i(t) e^{i\omega_i t}/\mathbf{E}_i(\mathbf{r}) + \text{c.c.} \) [71]. The modes depend on the instantaneous value of the dielectric function, which may contain slow explicit time-dependence, and must fulfill Eq. (2.12). It has been shown [59] that the evolution of mode intensities, proportional to their amplitudes \((s_i)^2\), is governed by 
\[
\frac{dS_i}{dt} = -2\omega''_i S_i + R'_{sp,i},
\]
where the spontaneous emission term has been indicated shortly compared to Eq. (2.36).

One can recognize that \(2\omega''\) corresponds to the difference between the modal gain and loss, which is a very important fundamental relationship, and shall be investigated in details at the end of this section. For the moment, Eq. (2.36) is generalized for spatially distributed variables, and the stimulated emission term is weighted with the mode profiles:

\[
\frac{\partial n(\mathbf{r}, t)}{\partial t} = \frac{\eta j(\mathbf{r}, t)}{e d_{QW}} - R_{sp}(n) - R_{nr}(n) + D \Delta n - \sum_i v_g \int_{QW} |\mathbf{E}_i|^2 g_i(n) dV S_i,
\]

\[
\frac{dS_i}{dt} = \beta_i \int_{QW} R_{sp,i}(n) dV + v_g \left[ \int_{QW} |\mathbf{E}_i|^2 g_i(n) dV - L_i \right] S_i.
\]

The explicit spatial and spatial dependence has been indicated for easier understanding, and the \(S\) variable has been omitted from the material gain, although both self- and cross-gain suppression can be taken into account. A new lateral diffusion term has appeared with diffusion coefficient \(D\), and the total width of the QWs is introduced \((d_{QW})\). Several realizations have been published for the solution of the above equations for cylindrically symmetric VCSELs, and most of them employed a scalar description of the optical fields. An elegant analytical approach has been formulated for a simple linear gain function [90], and a similar model with Bessel-function expansion has been proposed [91]. Fully numerical solutions have also been demonstrated [59].

Three extensions of the above model shall be mentioned, which account for carrier transport through the SCH layers, laser linewidth and laser noise, respectively. The first approach replaces the carrier equation with two coupled equations, one for the free carrier density in the SCH and the second for the QW. Current injection appears only in the SCH-layer as a source term, and interacts with the QW through carrier capture and escape, represented by effective times \(\tau_c\) and \(\tau_e\). This theory predicts lower modulation sensitivity by a factor of \(\sqrt{1 + \tau_c/\tau_e}\), which is typically between 1 and 2 at operation temperatures [92]. The second extension introduces a photon phase equation for the determination of laser linewidth with an appropriate phase noise term [89]. The last point is the incorporation of Langevin noise terms for each physical process, and yields the relative intensity noise spectrum after small-signal perturbation analysis [89, 93, 94]. As a final note, it has been mentioned that Eq. (2.21) discussed in EIM was also capable of analyzing laser dynamics.
Cold Cavity and Active Cavity Modes

This paragraph is devoted to the comparison of cold cavity and active cavity modes in the frame of first order nondegenerated perturbation principle. The Helmholtz equation can be viewed as generalized eigenproblem \( A\Psi = \omega^2/c_0^2 B\Psi \), where \( \Psi (r) \) is a vectorial or scalar eigenfunction defined strictly inside the VCSEL cavity and subject to radiation boundary condition, \( A \) denotes the double curl or negative Laplace operator, and \( B \) the multiplication by \( \varepsilon (r) \); both are symmetric operators. As it has already been clarified, it is a non-Hermitian problem even if the permittivity were real everywhere, but mode completeness and orthogonality still hold in a modified sense [68]. Therefore one can also apply perturbation approach for a modified dielectric function \( \varepsilon (r) + \delta \varepsilon (r) \).

Since \( A \) remains unchanged, one obtains for the first-order terms:

\[
\left( A - \frac{\omega^2}{c_0^2} B \right) \delta \Psi = \delta \left( \frac{\omega^2}{c_0^2} B \Psi + \frac{\omega^2}{c_0^2} \delta B \Psi \right),
\]

and the change of the solution can be expressed with the unperturbed eigenfunctions:

\[
\delta \Psi = \sum_j c_j \Psi_j.
\]

By multiplying with \( \Psi_i \) from the left, integration for the VCSEL, and applying mode orthogonality, the left hand side vanishes, and one gets

\[
\frac{2 \delta \omega_i}{\omega_i} = \frac{\delta \left( \frac{\omega^2}{c_0^2} \right)}{\omega^2/c_0^2} = -\frac{\langle \Psi_i \delta B \Psi_i \rangle}{\langle \Psi_i \Psi_i B \Psi_i \rangle} = -\frac{\langle \delta \varepsilon \Psi_i^2 \rangle}{\langle \varepsilon \Psi_i^2 \rangle}.
\]

Now consider an eigenmode of \( \omega = \omega' + i \omega'' \) angular frequency of cold cavity with unlossy materials. The active cavity eigenproblem is obtained by adding \( g\lambda/(4\pi) \) to the imaginary part of the QW refractivity. Since the typical wavelength is 1 \( \mu m \) and the gain is in the order of 1000 1/cm, it only corresponds to an order of 0.01 perturbation in the refractivity. If we substituted the refractivity with its average \( \langle n \rangle \), we would have:

\[
\delta \omega \approx \frac{i \omega \lambda}{4\pi \langle n \rangle} \int_{QW} g \Psi^2 dV \approx \frac{2i c_0}{\langle n \rangle} \int_{QW} g \Psi^2 dV,
\]

where we exploited that \( \omega \) was nearly real. The effects of material losses can be derived similarly. This legitimates the introduction of weighted material gain in Eq. (2.37) and the fundamental \( 2\omega'' = \int_{QW} g \Psi^2 dV - L \) relationship as well.

Cold cavity and active cavity descriptions can be then synthetized as follows. One can once calculate the decay rate in the absence of pumping, which is then simply proportional to the cavity loss. After turning on the injection, the decay rate decreases, and reaches zero at a certain injection level, corresponding to the threshold gain. At this point, cavity loss and round-trip gain become equal, and the frequency becomes purely real. This argumentation is valid until the effect of gain is small enough (as in mainly index-guided VCSELs), otherwise it may influence the mode patterns considerably and first order perturbation fails.
2.6 Description of the Active Region

The aim of this section is to calculate the material gain spectrum of the active region in an appropriate wavelength range as a function of the free carrier density. To this end, one has to know the conduction and valence band structure in the QW, and apply Fermi-Dirac distribution to the carriers. The valence band is perfectly filled and the conduction band is empty at zero degree temperature without electrical or optical pumping, therefore only band-to-band photon absorption occurs. Increasing the pumping first leads to reduced absorption, then equilibrium is formed between absorption and stimulated emission, and finally net gain is achieved.

The compound semiconductors used in optoelectronics possess either zincblende or wurtzite crystal structure, which are characterized by different symmetry properties. Most typical AlInGaAs and GaInAsP alloys used for communication wavelengths or in red lasers belong to zincblende, while AlGaInN families with high N-content aiming blue or green emission crystallize in wurtzite structure. One can study their band diagrams by various methods, such as with the nearly free electron model, pseudopotential and tight-binding methods or density-functional theory; but $k \cdot p$ method is the most common approach [95]. Its main advantage is that bulk, QW and quantum dot active regions can be modeled with the help of the same empirical parameters.

The $k \cdot p$ method for a single-electron wavefunctions of bulk semiconductors is derived by substituting a Bloch-function $\Phi_{nk} = u_{nk} \exp(ikr)$ into the Schrödinger-equation, which yields

$$\left( \frac{k^2}{2m} + \frac{\hbar k \cdot p}{m} + \frac{\hbar^2 k^2}{2m} + V \right) u_{nk} = E_{nk} u_{nk}. \quad (2.41)$$

Here $n$ is a band index, $k$ lies in the first Brioullin-zone, $u_{nk}$ is a lattice-periodic function, $V$ denotes the single-electron potential, $E_{nk}$ denotes the eigenenergy, and $p$ stands for the momentum of the wave. At the band center $k = 0$ the second and third terms vanish, and the eigenfunctions $u_{n0}$ are obtained. Fortunately it is not necessary to calculate these exactly, one should know only their symmetry properties. It turned out that at the band center of zincblende type semiconductors, the lowest conduction band (CB) is nondegenerated, while the highest valence band would be triply degenerated. However, it is detached to doubly degenerated heavy-hole (HH) and light-hole (LH) bands, and to a separated spin-orbit (SO) band owing to spin-orbit interaction. Besides, every band has another double degeneracy due to spin orientation. One can distinguish distinct heavy-hole (HH), light-hole (LH) and crystal-field split-hole (CH) valence bands at $k = 0$ in wurtzite-type materials when considering the spin-orbit interaction.

First order perturbation approach can be applied to calculate the eigenenergies $E_{nk}$ for small wavevectors near the band center. In principle, one would need to take all unperturbed solutions ($u_{n0}$) into account, but since the coupling between bands is inversely proportional to their energy difference, only adjacent bands are explicitly incorporated into the analysis, and distant levels may be involved only as correction parameters. The
2.6. DESCRIPTION OF THE ACTIVE REGION

coupling between HH and LH levels can be described by $4 \times 4$ Hamiltonian, whose elements originate from the bracket of the perturbation operator $\hbar \mathbf{k} \cdot \mathbf{p} / m + \hbar^2 k^2 / (2m)$ with $u_{\text{HH},0}$ and $u_{\text{LH},0}$ functions, and results in the splitting of these bands. Further interactions can be turned on by putting $u_{\text{SO},0}$ and $u_{\text{CB},0}$ into the analysis. Due to the symmetry properties of the unperturbed solutions, only few different matrix elements are obtained, that can be traced back to measurable physical quantities, such as band edges, effective masses and optical transition matrix parameters [96].

The single-electron eigenfunctions of QWs grown in the $z$-direction and infinite in the $(x, y)$-plane are searched as $\Phi_{n_z k_x k_y}(x, y, z) = f_{n_z}(z) u_{k_x k_y}(x, y) \exp\left[i (k_x x + k_y y)\right]$, where $u_{k_x k_y}$ labels a two-dimensional lattice-periodic function, and the longitudinal dependence is described as a slowly varying envelope that hardly changes on the atomic length scale. Since the barriers usually have higher conduction band edge and lower valence band edge than the QW, this structure corresponds to a potential valley of finite height, and only a finite number of $f_{n_z}(z)$ solutions are confined within the well. The $n_z$ subscript indicates this quantization, and the resulting solutions are called subbands. The formal solution is similar to the bulk case, but the $p_z k_z$ term has to be replaced for $-i (\partial f_{n_z} / \partial z)$. The solutions in the QW and barrier regions have to be matched by enforcing continuous wavefunctions and continuous quantum mechanical currents (continuous longitudinal derivatives) [97]. Semiconductors having wurtzite structure can be calculated similarly, keeping in mind their different symmetry conditions [98]. Mechanical strain arising from constrained lattice constants can also be incorporated into this method.

The optical gain can be calculated as follows [99]. The density of states can be easily calculated from the solution of the $\mathbf{k} \cdot \mathbf{p}$ problem. This leads to the reduced density of states, which is defined for the energy difference corresponding to emitted photon energy as independent variable. It is then multiplied by transition strength and the probabilities of free electrons and holes that can contribute to stimulated emission, where probabilities are selected according to Fermi-Dirac distributions. These involve the quasi-Fermi levels, which are calculated for each population inversion level. Finally a convolution is evaluated corresponding to a Lorentzian-broadening. Carrier-carrier interaction (many-body effects) can be taken into account by means of bandgap renormalization. The temperature dependence of the material gain spectrum comes from the Fermi-Dirac distribution and from temperature-dependent band parameters. Gain suppression at high photon densities may be described by the well-known analytical formula.
Chapter 3

Novel Results

3.1 Goals

The ultimate goal of this thesis is to elaborate a real three-dimensional coupled opto-electro-thermal analysis for almost arbitrary index-guided VCSELs, that is capable of predicting realistic single- or multi-mode device behavior. Such a work had not been carried out according to previous publications. This ambitious project can be realized only in a step-by-step procedure, and this chapter follows an appropriate hierarchical structure. This classification reflects also the development history of the methods.

Two semi-analytical optical approaches are discussed first, that are extensions of the weighted index method for noncircular geometries. Due to the assumptions of the original method, these models can provide realistic results only for nearly planar index-guided structures, in which the noncircular contours exist only in a single layer (or few layers). Results are demonstrated for a multi-mode VCSEL comprising a realistic oxide aperture that exhibits a close-to-square contour. It is shown that the simulated mode splitting due to the symmetry breaking agrees well with the measured spectrum, and the near field patterns can be reproduced from calculated ones, as well. Since these models describe only the purely optical resonator problem, the intensity of the laser modes is not calculated at all.

The second phase is the extension of the laser mode calculation for arbitrary index-guided structures, including ones incorporating shallow surface reliefs or deep-etched PhC patterns. In these lasers, the assumption of a single axial standing wave does not hold, since the structure is clearly not separable in the axial and lateral dimensions. Although there were publications that applied variants of the effective index method to study circular VCSELs with a quarter wavelength deep surface reliefs, these can be regarded as drastically simplified models that do not provide the detuning of the standing wave below the relief area. Direct numerical solutions of the scalar and vector Helmholtz equations are employed here to illustrate the features of elliptical and square-like geometries, as well as to compare PhC-VCSELs with and without oxide apertures.
3.2. SEMI-ANALYTICAL OPTICAL MODE CALCULATION

The third section investigates the coupling with thermal and electrical processes, and with the locally formulated rate equation approach that is capable of capturing spatial hole burning. It yields the absolute intensity of the supported laser modes as a function of the strength of the electrical pumping. The temperature dependence of the optical gain responsible for the stimulated emission is also covered by this approach. The cold-cavity description assumes current-independent optical mode profiles, an essential simplification for purely computational convenience. The way of coupling the individual mechanisms also sustains the need for direct optical mode solutions. Calculation results are given for a VCSEL encompassing a square-like oxide aperture and a triangular surface relief, and for another using a circular oxide aperture and an elliptical relief. The fabrication of different surface patterns can be applied to suppress selected laser modes, and to enhance single-mode operation either in the fundamental or in a higher-order mode.

The last section illustrates the utilization of the fully coupled model for a close-to-industry example, if the laser mode properties strongly depend on the current injection level. PhC-VCSELs maintaining stable single-mode operation in the low current regime usually change to multi-mode behavior at higher pumping. This feature is quantitatively studied with respect to the lattice constant of the PhC, and the measured characteristics are interpreted with numerical simulation.

3.2 Semi-Analytical Optical Mode Calculation

3.2.1 Group Theoretical Considerations

As the modes of the electromagnetic field follow the symmetry of the laser diode, they should follow the transformational properties of the respective symmetry group. Accordingly, as a VCSEL of cylindrical symmetry belongs to the $C_{\infty v}$ symmetry group, each optical mode of the diode has the same transformational characteristics as one of the irreducible representations of the group\(^3\). In Table 3.1 a part of the character table of the $C_{\infty v}$ group can be seen together with the shape of the first few LP modes. Only the LP\(_{0n}\) modes belong to the non-degenerated $A_1$ irreducible representation, all the others are doubly degenerated as they belong to any of the E representations.

If the shape of the aperture is distorted, it breaks the cylindrical $C_{\infty v}$ symmetry of the diode and the optical modes follow the transformational properties of the new group. The correlation of the old and the possible new groups can be seen in Table 3.2. For the sake of compatibility, A, B and E symbols are applied for the irreducible representations of the $C_{\infty v}$ point group. If, for example, the aperture has a square-shape, the diode symmetry is $C_{4v}$ and every second, originally degenerated (E-species) pair of modes should split

\(^2\)This section deals with thesis 1 of this dissertation, and follows Refs. [J1, C1].

\(^3\)Here and below we follow the Schönflies notation (see in [100]). This labeling system is generally used in spectroscopy and for the description of molecular symmetry.
**Table 3.1:** The \( C_{\infty v} \) point group and LP-modes

<table>
<thead>
<tr>
<th>( C_{\infty v} )</th>
<th>I</th>
<th>( 2C^\varphi )</th>
<th>Pattern</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_1</td>
<td>1</td>
<td>1</td>
<td></td>
<td>LP_{01}</td>
</tr>
<tr>
<td>A_2</td>
<td>1</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>E_1</td>
<td>2</td>
<td>2 \cos(\varphi)</td>
<td></td>
<td>LP_{11}</td>
</tr>
<tr>
<td>E_2</td>
<td>2</td>
<td>2 \cos(2\varphi)</td>
<td></td>
<td>LP_{21}</td>
</tr>
<tr>
<td>E_3</td>
<td>2</td>
<td>2 \cos(3\varphi)</td>
<td></td>
<td>LP_{31}</td>
</tr>
<tr>
<td>E_4</td>
<td>2</td>
<td>2 \cos(4\varphi)</td>
<td></td>
<td>LP_{41}</td>
</tr>
</tbody>
</table>

**Table 3.2:** Correlation between \( C_{\infty v} \), \( C_{4v} \), \( C_{2v} \) and \( C_{6v} \) symmetry groups

<table>
<thead>
<tr>
<th>( C_{\infty v} )</th>
<th>( C_{4v} )</th>
<th>( C_{2v} )</th>
<th>( C_{6v} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_1</td>
<td>A_1</td>
<td>A_1</td>
<td>A_1</td>
</tr>
<tr>
<td>A_2</td>
<td>A_2</td>
<td>A_2</td>
<td>A_2</td>
</tr>
<tr>
<td>E_1</td>
<td>E_1</td>
<td>B_1 + B_2</td>
<td>E_1</td>
</tr>
<tr>
<td>E_2</td>
<td>B_1 + B_2</td>
<td>A_1 + A_2</td>
<td>E_2</td>
</tr>
<tr>
<td>E_3</td>
<td>E_3</td>
<td>B_1 + B_2</td>
<td>B_1 + B_2</td>
</tr>
<tr>
<td>E_4</td>
<td>A_1 + A_2</td>
<td>A_1 + A_2</td>
<td>E_4</td>
</tr>
</tbody>
</table>

and form individual non-degenerated A_1 and A_2, or B_1 and B_2 modes. If the square-shape breaks further (e.g. rectangular or ellipse shape), the new \( C_{2v} \) symmetry group prohibits any degeneracy. Furthermore, only every third pair of modes should split in case of the hexagonal symmetry (\( C_{6v} \)). On the basis of this simple consideration we can easily estimate the degeneracy or non-degeneracy of a given mode.

### 3.2.2 Effective Radius-Weighted Index Method

The shape of the oxide aperture investigated here is a curvilinear tetragon, as realistic apertures usually have two perpendicular symmetry axes and four edges, and are round elsewhere. A good example illustrating the corners and their possible effects on reliability issues can be found in [101]. From simulation aspects a formula is needed that approximates this shape. Debernardi et al. suggested to describe a general aperture with the
3.2. SEMI-ANALYTICAL OPTICAL MODE CALCULATION

Figure 3.1: Aperture models. a shows the shape defined by Eq. (3.1) with $\Delta_2 = 0$ and $\Delta_4 = 1/16$. Curves b, c and d are given by Eq. (3.2) with $c=0.5, 0.25$ and $0.75$, respectively.

following Fourier-series [84]:

$$r(\varphi) = r_0 \left[ 1 + \sum_k \Delta_{2k} \cos(2k\varphi) \right], \quad (3.1)$$

where $r_0$ is the original (averaged) radius, the $\Delta_{2k}$ values denote the coefficients. $\Delta_4$ controls the square-like shape. A wide spectrum of aperture shapes can be approximated using appropriate values for the $\Delta_{2k}$ parameters (see Fig. 3.1.a). This formula allows, however, only round shapes, and together with effective radius-WIM may lead to unwanted degeneracies as discussed in details at the end of this subsection. The following formula has been found to fit better to the experimental shape (see Fig. 3.1.b):

$$r(\varphi) = cr_0 + (1-c)r_{sq}(\varphi), \quad (3.2)$$

where $r_{sq}(\varphi)$ describes a square in polar coordinate system. With the help of the $c$ ”cylindricity” parameter the circle-to-square transition can be scaled. The realistic experimental oxide shape is closest to the one halfway between the ideal circular and square cases (Fig. 3.1.b). Fig. 3.1.c and d display model apertures for comparison with cylindricity parameter of 0.25 and 0.75, respectively.

The model aperture belongs to the $C_{4v}$ symmetry group, as it still has two symmetry axes and shows a rotational symmetry of 90 degrees. As a consequence of Table 3.2, for odd $\mu$ values the degeneracy of the $LP_{\mu\nu}$ modes remains, while for even ones does not. Since degenerated modes have the same optical properties they can be observed together, and the sum of their intensity distribution forms distorted rings.

Apertures of general shape can be approximated with cylindrical apertures of proper radius from certain point of view. Noble et al. used a circular aperture having the same area instead of the assumed square aperture ($r = a/\sqrt{\pi}$) to compute the optical parameters of the fundamental mode [82]. The simple condition for the areas does not answer the degeneracy splitting. By defining different effective radii for the split transverse modes and executing two WIM-iterations the effect could be reproduced. Therefore the effective
radii are defined as weighted integrals of the \(r(\varphi)\) function describing the shape:

\[
R_{1,2} = \frac{\int_0^{2\pi} r(\varphi) g_{1,2}(\varphi) d\varphi}{\int_0^{2\pi} g_{1,2}(\varphi) d\varphi}.
\]  

(3.3)

Here \(g_{1,2}(\varphi)\) denotes the weighting factors of the two modes, respectively. They must be chosen such a way that the two effective radii should differ in the case of degeneracy splitting (for even \(\mu\) values), and are equal if degeneracy remains (for odd \(\mu\) values). The optical parameters calculated from these radii should also match the experimental data. The right choice for the weighting functions can be the intensity distributions because they intrinsically reflect the existing or nonexisting degeneracies. Assuming that the aperture only slightly deviates from the circle, the \(\varphi\)-dependencies of the known intensity patterns of the circular structure were used:

\[
g_{1,2}(\varphi) = \begin{pmatrix} \sin^2(\mu\varphi) \\ \cos^2(\mu\varphi) \end{pmatrix}.
\]  

(3.4)

This formula gives one effective radius for \(\mu = 0\). It produces the same radii for odd \(\mu\) values with the aperture shape of (3.1) according to the previous expectation. If the last nonzero coefficient in the Fourier-series is \(\Delta_{2K}\), it provides two different radii only if \(\mu \leq K\) even. This means that in order to predict correctly the degeneracy splitting of higher order modes further coefficients must be defined when using (3.1). This problem does not occur when using the shape function (3.2).

### 3.2.3 Hybrid Weighted Index Method

A simple scalar formulation of weighted index method is presented for general non-circular apertures in this subsection. It predicts correctly the splitting of degeneracy due to the distortion of the rotational symmetry, but does not take polarization into account. An improved vectorial version of this method is also feasible, but demands a more difficult handling of the boundary conditions (in which the electric and magnetic field components are coupled) at the core-cladding interface. Let us write one dominant transverse field component in the form of \(E(x, y, z, t) = E(x, y, z)e^{i\omega t}\). The field must satisfy the Helmholtz equation:

\[
\left[\Delta + \epsilon(x, y, z)\frac{\omega^2}{c^2}\right]E(x, y, z) = 0,
\]

(3.5)

where \(\epsilon\) is the piecewise constant dielectric function. In general cases \(E(x, y, z)\) is not separable because of the diffraction at the oxide aperture. By neglecting this effect the following separation is made in the longitudinal and the lateral components, but no harmonical dependence is assumed in the azimuthal angle: \(E(x, y, z) = P(x, y)Q(z)\). Inserting this ansatz into Eq. (3.20):

\[
\frac{\partial^2 Q(z)}{\partial z^2} P(x, y) + \Delta_T P(x, y) Q(z) + \epsilon(x, y, z)\frac{\omega^2}{c^2} P(x, y) Q(z) = 0,
\]

(3.6)
where $\Delta_T = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is the transverse Laplace-operator. By multiplying with $Q^*(z)$ and integrating against $z$ from the lower to the upper boundary planes of the VCSEL, and multiplying with $P^*(x,y)$ and integrating for the $xy$-cross-section of the diode, the original partial differential equation splits into two coupled equations:

$$
\left[ Q \left( \frac{\partial^2 Q}{\partial z^2} \right) + \frac{\omega^2}{c^2} \langle \epsilon | Q \rangle (x,y) \right] P(x,y) + \langle Q | \Delta_T P(x,y) = 0, \tag{3.7}
$$

$$
\left[ P \langle \Delta_T P \rangle + \frac{\omega^2}{c^2} \langle P | \epsilon | P \rangle (z) \right] Q(z) + \langle P | P \rangle \frac{\partial^2 Q(z)}{\partial z^2} = 0. \tag{3.8}
$$

In order to make the following derivations simpler, $P$ and $Q$ are assumed to be normalized. The coordinates in the lower indices in the above expressions indicate that the weighted dielectric constant may depend on the coordinates omitted from the integration. For piecewise constant dielectric functions, $\langle P | \epsilon | P \rangle (z)$ is a step-like function of the $z$-coordinate, and its values can be denoted as $\langle \epsilon \rangle_j^P$, where $j$ refers to the $j$-th layer ($j = 1$ denotes the substrate, $j = N$ is air). The same way $\langle Q | \epsilon | Q \rangle (x,y)$ can be reduced to $\langle \epsilon \rangle_i^Q$, where $i = 1$ for the core region and $i = 2, 3, ..., M$ for the cladding(s). Eq. (3.8) is a second-order ordinary differential equation in the $j$-th layer, and the general analytical solution reads as follows:

$$
Q_j(z) = a_j e^{i\beta_j z} + b_j e^{-i\beta_j z}, \tag{3.9}
$$

and

$$
\beta_j^2 = \langle P | \Delta_T P \rangle + \frac{\omega^2}{c^2} \langle \epsilon \rangle_j^P \quad (j = 1, ..., N) \tag{3.10}
$$

is the squared propagation constant. $Q(z)$ and $\partial Q(z)/\partial z$ must be continuous at each interface between the layers, and only outgoing waves are allowed out of the structure. This problem is solved by the transfer matrix method and a root finding routine on the complex frequency-plane. Knowing the general solution for $Q(z)$, $k_i^2$ is defined as:

$$
k_i^2 = \frac{\omega^2}{c^2} \langle \epsilon \rangle_i^Q + \left[ Q \left( \frac{\partial^2 Q}{\partial z^2} \right) \right] = \frac{\omega^2}{c^2} \langle \epsilon \rangle_i^Q - \langle Q | \beta_j^2 | Q \rangle = \frac{\omega^2}{c^2} \langle \epsilon \rangle_i^Q - \langle \beta_j^2 \rangle^Q \quad (i = 1, ..., M). \tag{3.11}
$$

Eq. (3.7) can be rewritten, and it is clear that $k_i$ plays the role of the lateral propagation constant:

$$
k_i^2 P(x,y) + \Delta_T P(x,y) = 0 \quad (i = 1, ..., M). \tag{3.12}
$$

Before describing in detail how to solve the lateral problem, the iterational procedure is pointed out between the longitudinal and lateral dimensions. Multiplying Eq. (3.12) with $P^*(x,y)$, and integrating over the whole cross-section of the diode:

$$
\sum_{i=1}^{M} \int_{A_i} P^*(x,y) k_i^2 P(x,y) dx dy + \langle P | \Delta_T P \rangle = 0, \tag{3.13}
$$

where $A_i$ refers the $i$-th region. The sum gives the weighted lateral propagation constant $\langle k_i^2 \rangle^P$. Inserting it into Eq. (3.10) the same expression is got for $\beta_j^2$ as Eq. (3.11):

$$
\beta_j^2 = \frac{\omega^2}{c^2} \langle \epsilon \rangle_j^P - \langle k_i^2 \rangle^P. \tag{3.14}
$$
The order of the iteration is the following. At first step the axial part is solved assuming \( \langle k^2 \rangle^P = 0 \). The weighted axial propagation constant \( \langle \beta^2 \rangle^Q \) is calculated next. Substituting it into Eq. (3.11) the lateral problem is computed. With the lateral propagation constant Eq. (3.14) is used to refine the axial solution, etc. The iteration stops if the difference for both the real and imaginary parts of the frequency were lower in a cycle than a previously defined threshold.

Now we move on the solution of Eq. (3.12) in case of non-circular apertures. While for special cylindrical structures analytical solutions are known: the Bessel-functions, here only numerical methods are applicable. Natural options are the finite difference method (FDM) that can be implemented on a non-equidistant rectangular grid, or finite volume method (FVM) that fits to more versatile triangular meshes. Since the problem is an eigenvalue equation for the complex frequencies as eigenvalues and for the field distributions as eigenvectors, a system matrix containing only the inner nodes of the core and cladding(s) is wanted. The nodes at the interfaces must be expressed using the boundary conditions and eliminated from the unknown variables, and simultaneously the fields at the surface were taken equal to zero. In order to give an elegant solution, an algebraic matrix-description of the following differential equation is presented:

\[
\left( \frac{\omega^2}{c^2} \langle \epsilon \rangle^Q - \langle \beta^2 \rangle^Q \right) P(x, y) + \Delta_T P(x, y) = 0.
\]

(3.15)

Let us denote the discretized values of \( P(x, y) \) as \( \overline{P} \). The discretized difference equation has the form of:

\[
\left( \frac{\omega^2}{c^2} \overline{\epsilon} - \langle \beta^2 \rangle \overline{I} \right) \overline{P} + \overline{\Delta P} = \overline{0},
\]

(3.16)

where \( \overline{\epsilon} \) denotes the diagonal matrix of the dielectric constant, \( \overline{I} \) the identity matrix and \( \overline{\Delta} \) the sparse matrix of the transverse Laplace-operator. Rearranging the equation one gets:

\[
\frac{\omega^2}{c^2} \overline{\epsilon} \overline{P} = \left( \langle \beta^2 \rangle \overline{I} - \overline{\Delta} \right) \overline{P},
\]

(3.17)

which is a generalized algebraic eigenvalue problem, and can be solved using standard routines. Finally the propagation constants were expressed using Eq. (3.11). It is important to note that the transverse confinement factor is simply \( \int_{\text{core}} P^*(x, y) P(x, y) dxdy \), the intensity in the core.

### 3.2.4 Optical Modes for Square-Like Aperture

The effective radius-WIM and the hybrid WIM techniques were tested on a GaAs/AlGaAs multi-mode VCSEL designed for 850 nm emission. It consists of a \( \lambda \)-length cavity and 18 pair top- and 25 pair bottom-DBR mirrors. The first low index layer below the cavity was partially oxidized, the aperture shape is parameterized as a square-circle transition with a cylindricity of 0.5 (Fig. 3.1.b). The detailed description can be found in Table 3.3.
3.2. SEMI-ANALYTICAL OPTICAL MODE CALCULATION

Table 3.3: The structure of the simulated VCSEL

<table>
<thead>
<tr>
<th>Periods</th>
<th>Type</th>
<th>Thickness [nm]</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>$\text{Al}<em>{0.2}\text{Ga}</em>{0.8}\text{As}$</td>
<td>60.9</td>
<td>3.492</td>
</tr>
<tr>
<td></td>
<td>$\text{Al}<em>{0.9}\text{Ga}</em>{0.1}\text{As}$</td>
<td>69.4</td>
<td>3.065</td>
</tr>
<tr>
<td>1</td>
<td>Cavity</td>
<td>244.4</td>
<td>3.482</td>
</tr>
<tr>
<td>1</td>
<td>$\text{Al}<em>{0.9}\text{Ga}</em>{0.1}\text{As}$</td>
<td>46.3</td>
<td>3.065</td>
</tr>
<tr>
<td></td>
<td>$\text{AlAs/Al}_2\text{O}_3$</td>
<td>23.6</td>
<td>3.002/1.7</td>
</tr>
<tr>
<td></td>
<td>$\text{Al}<em>{0.2}\text{Ga}</em>{0.8}\text{As}$</td>
<td>60.9</td>
<td>3.492</td>
</tr>
<tr>
<td>24</td>
<td>$\text{Al}<em>{0.9}\text{Ga}</em>{0.1}\text{As}$</td>
<td>69.4</td>
<td>3.065</td>
</tr>
<tr>
<td></td>
<td>$\text{Al}<em>{0.2}\text{Ga}</em>{0.8}\text{As}$</td>
<td>60.9</td>
<td>3.492</td>
</tr>
</tbody>
</table>

Figure 3.2: Calculated wavelength versus aperture diameter. Hybrid WIM results are drawn with continuous, effective radius-WIM results with dashed lines.

The calculated blueshift of the modes versus the aperture diameter can be seen in Fig. 3.2. Both the predicted mode splitting and the absolute wavelength values show reasonable agreement with the experimental data (Fig. 3.3), which was measured according to the configuration shown in Fig. 3.4. A VCSEL wafer of 20 nm × 30 nm was placed on the target holder, and the laser output of a single diode was coupled into a graded-index multi-mode fiber of 50 μm core diameter with the help of two lenses and a mirror. An Ando AQ-6315 spectrum analyzer with 0.05 nm resolution, connected to a PC, was used to record the spectrum. The environmental temperature was fixed on
room temperature, while the VCSEL was driven by a current of 4.5 mA. The redshift of the modal wavelengths due to the slightly increased cavity temperature was calibrated by changing the refractive indices of all layers according to an empirical formula compared to their background values, see Eq. (3.31). The wavelength splitting between the two LP_{21} modes is a direct consequence of the different lateral wavenumbers ($k_i$-s in Eq. 3.12), as the mode with shorter wavelength experiences a shorter effective radius according to its lateral intensity distribution. The mode splitting decreases as the cylindricity parameter increases, finally vanishing in case of the perfect circular aperture.

The dependence of transverse confinement factor on the aperture size is plotted on Fig. 3.5. A small difference between the cutoff aperture diameters of the two LP_{21} modes also appears. The results of the two methods are nearly the same, near cutoff a difference
of 5-10% can be observed between the calculated confinement factors for each mode. In Fig. 3.6 the intensity pattern of the fundamental and some higher order modes can be seen. They were calculated by the lateral part of hybrid WIM with FDM. As previously predicted, the first higher order mode, LP_{11}, has remained degenerated, the degeneracy of LP_{21} has been split (with effective radii of 92% and 87% of r_0, respectively), and LP_{31} is degenerated again. It is important to note that all linear combinations of two degenerated modes are appropriate solutions as well; and since degenerated modes can be seen together, distorted ring-like near fields can be observed. However, if the higher order nondegenerated LP_{21} modes come into play while increasing the current, LP_{21c} will significantly dominate over LP_{21s}, which can be clearly recognized on the experimental near field patterns depicted on Fig. 3.7. The measured fields at different current levels have been reproduced by the superposition of the previous modes. Although the relative intensities have been empirically adjusted here, a predictive calculation is also possible, as it is discussed in Section 3.4.
CHAPTER 3. NOVEL RESULTS

Figure 3.6: Mode patterns calculated with FDM. The aperture shape is indicated with white curve.

3.3 Resonator Modes of Advanced VCSELs

3.3.1 Solution with the Scalar Helmholtz Equation\textsuperscript{4}

The validity of the previous approaches is limited to mainly planar structures, in which the axial standing wave does not depend on the lateral position. This assumption cannot hold in PhC-VCSELs, or in ones employing surface reliefs. The fully numerical solution of the Helmholtz eigenproblem is proposed for these complex structures. This optical mode calculation is the most challenging to solve among the mathematical tasks encountered in this thesis, because very fine discretization is required to resolve the standing-wave pattern in the open resonator. We present a scalar formulation first that neglects the polarization of the light, and may be less accurate for small aperture sizes than a vectorial solution.

\textsuperscript{4}Subsections 3.3.1-3.3.6 discuss theses 2-3, and are based on Refs. [J2, C2, C3].
3.3. RESONATOR MODES OF ADVANCED VCSELS

Figure 3.7: Comparison between calculated and measured near field patterns at different current injection levels. The first six calculated (individual) optical mode profiles were weighted and superposed to approximate the experimental images. All but the first figures show multimode behavior.

The differential form of the scalar Helmholtz equation is recalled:

\[ \nabla^2 \Psi = -k_0^2 \varepsilon \Psi, \]

where \( k_0 \) denotes the free space wavenumber, \( \Psi \) a dominant field component of the linearly polarized mode and \( \varepsilon = (n' + in'')^2 \) the complex dielectric constant. While the real part of the wavenumber provides the mode wavelength, the imaginary part represents the total modal loss including mirror, absorption and scattering losses. To avoid reflection of the electromagnetic waves from the surface of the computational domain, PML media are used to cover the diode from all sides. The discretization scheme and the difficulties of
the eigenvalue solution are discussed later in subsections 3.4.4 and 3.3.3, respectively.

The optical modes can be obtained either simultaneously as eigenvalues of the matrix arising from the discretization for the whole cross-section, or successively if symmetry planes can be taken into account. Then one has to solve four problems with different sets of boundary conditions (Dirichlet- or Neumann-type) for the two symmetry planes, but the rank of the matrices is reduced by a factor of four. As a third option it is also possible to search all modes separately, if good enough initial guess or target eigenfrequency is known for each prior to the eigenvalue iteration.

### 3.3.2 Vectorial Approach for Helmholtz Equation

According to the adiabatic approximation, the time dependent electromagnetic fields can be expanded on the basis of modes, if the maximum frequency at which the laser is modulated, is small compared to the inverse photon round-trip time within the laser cavity. The modes depend on the instantaneous value of the time-dependent dielectric function [71]. The resonator modes are calculated for static dielectric function here, and the total electric field can be written as:

\[
E(r, t) = \sum_{\nu} s_{\nu}(t) e^{i\omega_{\nu} t} E_{\nu}(r) + c.c.,
\]  

with the \(\nu\)-th mode \(E_{\nu}(r)\) satisfying the vectorial Helmholtz equation:

\[
\nabla \times \mu^{-1}(r) \left[ \nabla \times E(r) \right] - \frac{\omega^2}{c^2} \varepsilon(r) E(r) = 0.
\]

In the above equations, \(s_{\nu}(t)\) denotes the time-dependent amplitude of the \(\nu\)-th mode, \(\omega_{\nu} = \omega'_{\nu} + i\omega''_{\nu}\) the angular frequency of the mode, and \(c\) is the speed of light in vacuum. \(\varepsilon(r)\) is the permittivity and \(\mu(r)\) is the permeability of the medium, which may be tensors if material anisotropy is present. Temperature and carrier induced refractive index change, the elasto-optic and electro-optic effects can be incorporated into the permittivity tensor similar to Ref. [83] to calculate their impact on the laser modes.

Eq. (3.20) is solved for a given dielectric profile (which may describe local gain and absorption loss if the refractive index is set to complex), while the permeability is constant 1. Since the time dependence was decoupled, the problem is analyzed in the frequency domain. The unknowns are the electric field profiles as eigenfunctions and the associated complex angular frequencies as eigenvalues. For the sake of easy understandability the mode index is omitted in the following. To obtain a numerical solution one has to select an appropriate computational domain, which must be covered by nonreflecting boundary condition. This task is performed by PML that involves a complex diagonal tensor \(\Lambda(r)\) [78]. Then Eq. (3.20) is rewritten as:

\[
\nabla \times \Lambda^{-1}(r) \left[ \nabla \times E(r) \right] - \frac{\omega^2}{c^2} \varepsilon(r) \Lambda(r) E(r) = 0.
\]

48
The solution of this equation is equivalent to the extremum of the following variational functional:

$$F(E) = \frac{1}{2} \int_V \left[ (\nabla \times E) \Lambda^{-1} (\nabla \times E) - \frac{\omega^2}{c^2} E \epsilon r \Lambda E \right] dV,$$

where the integral is evaluated for the volume of the computational domain including the PML media. If the unknown electric field is approximated as a linear combination of appropriately selected vectorial basis functions, \(E(r) = \sum_i c_i E_i(r)\), an algebraic complex symmetric generalized eigenproblem can be derived:

$$Ac = \frac{\omega^2}{c^2} Bc,$$

where \(c\) denotes the column vector of the unknown coefficients, and \(A\) and \(B\) the following matrices:

$$a_{ij} = \int_V (\nabla \times E_i) \Lambda^{-1} (\nabla \times E_j) dV,$$

$$b_{ij} = \int_V E_i \epsilon r \Lambda E_j dV.$$

It is left to choose the vectorial basis, which must be complete to span any possible solution satisfying the continuity condition for the tangential fields. Therefore curl-conforming basis must be used, which automatically ensures that non-physical spurious solutions are avoided [86]. Owing to a wide range of arguments that are exposed in Subsection 3.4.4, the layer structure of the VCSEL with possibly complicated transverse cross-sections is covered with prism elements. As the basis functions are selected to be nonzero only inside a single prism, the element integrals given by Eqs. (3.24) and (3.25) lead to sparse matrices. The actual sparsity depends on the polynomial order of the basis, and the mesh density may be traded for higher order interpolatory elements [102]. Although the number of unknowns can be lower using coarser mesh together with higher-order elements in order to keep the same accuracy, the numerical solution faces more fill-in and memory cost. Constant tangential-linear normal basis functions are used in the following discussion, and tangential continuity is maintained by fixing the coefficients of the basis functions associated to the same edge to be equal in adjacent prisms. The discontinuity of the normal component across material interfaces will be automatically satisfied, which can be derived by taking the divergence of Eq. (3.20). Three of the total nine unnormalized shape functions are given by formulas below using the normalized coordinates [102]:

$$E_1^1 = \xi_5 (\xi_2 \nabla \xi_3 - \xi_3 \nabla \xi_2),$$

$$E_4^4 = \xi_4 (\xi_2 \nabla \xi_3 - \xi_3 \nabla \xi_2),$$

$$E_7^7 = \xi_1 \nabla \xi_4,$$

and shown on Fig. 3.8. The element integrals can also be found [103]. Note that the material anisotropies do not increase the number of nonzeros and thus complicate the calculation, unless the dielectric tensor contains off-diagonal elements.
CHAPTER 3. NOVEL RESULTS

Figure 3.8: Vectorial basis functions for prism elements. The plots show the normalized electric field distributions associated to three edges of a representative prism, one laying on the bottom (a), one on the top side (b), and one vertical (c), respectively. The vectors plotted with lighter colors correspond to horizontal cross sections of ascending vertical coordinate. The other six shape functions can be obtained by cyclic permutation of the edges.

The optically interesting part of the VCSEL is selected according to the expected confinement, and PML is used to cover this inner region to allow reflectionless absorption of traveling waves. Perfect electric conductor (PEC, $\hat{n} \times \mathbf{E} = 0$, where $\hat{n}$ is the normal unit vector of the surface) boundary condition is associated to the outer surface of the PML. It is always essential to exploit the symmetry of the device to reduce the computational domain. Most practical VCSELs exhibit two perpendicular symmetry axes, along which either PEC or perfect magnetic conductor (PMC, $\hat{n} \cdot \mathbf{E} = 0$) boundary conditions can be applied. More appropriate forms of the symmetry conditions read as follows. PEC condition is given by $E_x = 0, \partial E_y/\partial y = 0, E_z = 0$ on the x-axis, and by $\partial E_x/\partial x = 0, E_y = 0, E_z = 0$ on the y-axis. PMC satisfies $\partial E_x/\partial y = 0, E_y = 0, \partial E_z/\partial y = 0$ on the x-axis, and $E_x = 0, \partial E_y/\partial x = 0, \partial E_z/\partial x = 0$ on the y-axis.

The optical modes can then be classified into four groups with different sets of symmetry boundary conditions, as summarized in Table 3.4. They are labeled as $\text{LP}_{nm}^\alpha$, where the subscripts denote the azimuthal and radial variation of the respective modes of a circularly symmetric device, $\alpha$ can be $c$ for cosinoidal or $s$ for sinusoidal intensity distribution with respect to the x-axis, and $\beta$ is either $x$ or $y$ depending on the dominant transverse field component.

3.3.3 Effective Numerical Treatment of Large Matrix Problems

In order to divide the whole computational domain using only prism elements, one has to create a triangular mesh, which respects all lateral contours present in the VCSEL. To this end the oxide aperture, the surface relief or grating, etched hole patterns, metallic contacts, and also the artificial PML region must be projected into the same transverse plane. Fortunately the triangularization of this domain can usually be easily accomplished resulting in a two-dimensional mesh (see Fig. 3.9), which is then extruded to the 3-D
Table 3.4: Symmetry boundary conditions for transverse modes

<table>
<thead>
<tr>
<th>x-axis</th>
<th>y-axis</th>
<th>x-polarization</th>
<th>y-polarization</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMC</td>
<td>PEC</td>
<td>LP_{mn}^{ex}, m even</td>
<td>LP_{mn}^{sy}, m even</td>
</tr>
<tr>
<td>PEC</td>
<td>PMC</td>
<td>LP_{mn}^{ex}, m even</td>
<td>LP_{mn}^{sy}, m even</td>
</tr>
<tr>
<td>PMC</td>
<td>PMC</td>
<td>LP_{mn}^{ex}, m odd</td>
<td>LP_{mn}^{sy}, m odd</td>
</tr>
<tr>
<td>PEC</td>
<td>PEC</td>
<td>LP_{mn}^{ex}, m odd</td>
<td>LP_{mn}^{sy}, m odd</td>
</tr>
</tbody>
</table>

Figure 3.9: Sample triangular lateral mesh for a hexagonal PhC-VCSEL, in which the central seven unetched positions form the defect zone. Only a quarter cross section is discretized due to symmetry considerations. The optically active region is painted with green, the top metallic contact with deep red, and the etched holes with blue color. The region outside the innermost circle can be oxidized in one layer.
Algorithm 1 Shift-invert iteration

Require: target eigenvalue of $\sigma_0$ and a random starting vector $x$

Ensure: $Ax = \sigma Bx$, where $A$ and $B$ are given complex symmetric matrices, $\sigma$ is the closest eigenvalue to $\sigma_0$, and $x$ is a corresponding eigenvector

repeat
  solve $(A - \sigma_0 B) y = x$ for $y$
  $x := \frac{y}{\|y\|}$
  $\sigma := \frac{(x,Ax)}{(x,Bx)}$ (Rayleigh-quotient associated to $x$)
until the relative error of $\sigma$ becomes negligible

structure.

Matrices $A$ and $B$ are filled according to a global indexing scheme of the edges. It is recommended to order the edges layer-by-layer, taking first the horizontal and then the vertical ones, and matching the local edge directions to the global orientation always pointing to vertices with higher indices. Constrained PEC boundary condition is enforced by erasing the respective columns and rows of the matrices. The large-scale sparse complex symmetric eigenvalue problem given by Eq. (3.23) is solved with a shift-invert iteration with the matrix $A - \sigma_0 B$. The target eigenvalue is denoted by $\sigma_0$, and it may be calculated as a Rayleigh-quotient associated to an eigenfunction obtained on coarse mesh or by an approximate method. The algorithm can be read in Alg. 1, using a modified inner product without complex conjugation: $(v, w) = \sum_i v_i w_i$. Although more sophisticated eigenvalue algorithms like the Jacobi-Davidson method [104] might provide faster convergence towards the eigenvalue, the linear equation solution with an ill-conditioned matrix still remains.

For this purpose a direct solver with complete LU-factorization was proposed for the cylindrically symmetric case [59], but it is definitely not feasible for the general 3-D problem with higher rank and more dense matrices. Therefore an iterative solution with a preconditioner matrix approximating $A - \sigma_0 B$ is inevitable. An incomplete complex Cholesky-factorization is used to accelerate the conjugate orthogonal conjugate gradient (COCG) iteration [105] throughout this work. Without a good preconditioner (or, as an extreme case, if it were selected as the unity matrix) the iteration would converge particularly slowly. On the other hand, the incorporation of a preconditioner complicates the core of the iteration with a linear equation solving (see Alg. 2), takes the longest computational time and demands most memory inside the loop. If one chose $A - \sigma_0 B$ itself as the other extremity, the iteration would reach convergence in a single step, but we would arrive back to the original task to perform a matrix inversion. Therefore the preconditioner should be selected as an easily invertible matrix that approximates the original one in order to reach optimal performance, for example according to Alg. 3. Note that it should be sufficient to store its nonzero elements in single precision format in the computer memory.
Algorithm 2 Conjugate orthogonal conjugate gradient iteration

Require: known initial guess for $x$ and $M$ preconditioner

Ensure: $Mx = b$, where $M$ is complex symmetric

$p := 0; \alpha := 0; r := b - Mx; w := \tilde{M}^{-1}r; \rho_0 := (r, w)$

for $j=0,1,2,\ldots$ do

$p := w + \alpha p; w := Mp; \mu := (w, p)$

if $\mu = 0$ then quit (failure)

$\alpha = \rho_j/\mu; x := x + \alpha p; r := r - \alpha u$

if $x$ is accurate enough then quit (convergence)

$w := \tilde{M}^{-1}r; \rho_{j+1} := (r, w)$

if $\rho_{j+1}$ is small then quit (failure)

$\alpha := \rho_{j+1}/\rho_j$

end for

Algorithm 3 Incomplete complex column-Cholesky factorization

Require: given complex symmetric $M$ matrix of $n \times n$ size

Ensure: $M \approx RR^T$, and $R$ is lower triangular

let $R$ be the lower triangular part of $M$

for $j = 1$ to $n$ do

for $k = 1$ to $j - 1$ do

for $i = j$ to $n$ do

$r_{ij} := r_{ij} - r_{ik}r_{jk}$

end for

end for

$r_{jj} := \sqrt{r_{jj}}$

for $i = j + 1$ to $n$ do

$R_{ij} := \frac{r_{ij}}{r_{jj}}$

end for

drop small elements from the $j$th column except $r_{jj}$

end for

Its main advantage is that the total memory cost is reduced drastically; moreover, the drop tolerance can be continuously varied that allows trade-off between convergence speed and the required memory capacity, see Fig. 3.10. The typical value of the drop tolerance was $10^{-6}$ to achieve acceptable convergence for a discretization counting few million edges. The overall calculation time varied from 10 to 30 hours per mode on 2.4 GHz Opteron processor, depending on the complexity of the structure and on the target eigenvalue, whereas memory cost was between 20 and 50 GByte. The first values refer to a moderate mesh for a VCSEL with elliptical mesas, while the second to a PhC-VCSEL demanding fine discretization. A domain decomposition technique may also be used to
CHAPTER 3. NOVEL RESULTS

![Convergence history of COCG iterations](image)

**Figure 3.10:** Convergence history of COCG iterations. It can be seen that the drop-tolerance level affects drastically the number of iterations required to achieve a selected relative error. On the other hand, this number is fairly constant during the consecutive eigenvalue iterations in the outer loop.

3.3.4 Model Validation

The VCSELs analyzed in this section are based on the thoroughly simulated circular COST268 benchmark example [69], which is given in details in Table 3.5. This AlGaAs VCSEL is designed for operation around 980 nm, and grown on GaAs substrate. The bottom DBR consists of 29.5 pairs of AlGaAs/GaAs mirrors, while the top one has 25 pairs. The lowest layer of the top mirror was selectively oxidized, an accommodates a λ/20-thick oxide aperture. The 5 nm thick single QW is assumed to have a step-index profile with the same dimensions as the oxide aperture. It exhibits loss outside of the aperture, which is implemented by specifying a complex refractivity.

In order to validate the 3-D FEM approach indirectly due to the lack of appropriate experimental data, the same concept is adopted for the circular device as in Ref. [69]. The location of the aperture was varied in five steps from node (1) to antinode position (5) with respect to the optical field. This was performed by adjusting the thickness of the AlGaAs layer \(x\) from 63.71 nm to zero in equal steps, while the diameter of the oxide window was fixed to 8 μm. Since cold-cavity calculations were executed, the threshold gain was not directly calculated. However, it was estimated as the quotient of the modal loss and the total confinement factor. The latter was evaluated as a volume integral of
### Table 3.5: The layer structure of the COST268 benchmark VCSEL

<table>
<thead>
<tr>
<th>Type</th>
<th>Material</th>
<th>Thickness [nm]</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>air</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>24 pair bottom DBR</td>
<td>GaAs</td>
<td>69.49</td>
<td>3.53</td>
</tr>
<tr>
<td>Oxide window</td>
<td>GaAs</td>
<td>69.49</td>
<td>3.53</td>
</tr>
<tr>
<td>window</td>
<td>AlAs/AlOx</td>
<td>15.93</td>
<td>2.95/1.60</td>
</tr>
<tr>
<td>Oxide</td>
<td>AlGaAs</td>
<td>63.71-x</td>
<td>3.08</td>
</tr>
<tr>
<td>Cavity Quantum well</td>
<td>GaAs</td>
<td>136.49</td>
<td>3.53/3.53-j0.01</td>
</tr>
<tr>
<td>29.5 pair top DBR</td>
<td>AlGaAs</td>
<td>79.63</td>
<td>3.08</td>
</tr>
<tr>
<td>Substrate</td>
<td>GaAs</td>
<td>69.49</td>
<td>3.53</td>
</tr>
</tbody>
</table>

**Figure 3.11:** Calculated wavelength and threshold material gain of the fundamental mode for different oxide positions, compared to the reference results obtained with vectorial coupled mode theory (Torino model).

The obtained wavelengths and threshold gains depicted on Fig. 3.11 yield good agreement to the values of the cited article. Only the results of coupled mode method are recalled here, which had been the single vectorial approach implemented in three dimensions to determine VCSEL optical modes. It was found reliable for the polarization-resolved
Figure 3.12: Wavelength and threshold material gain of the fundamental and first order modes versus aperture diameter. The threshold gain is plotted on logarithmic scale.

simulation of various devices that included elliptical mesas [57] or surface gratings [33], and its results were compared to experiments. Note that a systematic shift of about 1.25 nm can be observed for all calculated wavelengths, which originates from the finite discretization in the longitudinal direction (the mean height of the prism elements was $\lambda/32$), and has already been reported [108]. Higher axial resolution provides wavelengths consequently approaching their nominal values without significant changes in other parameters. The oxide was kept at antinode position, and its diameter was decreased from 8 $\mu$m to 1 $\mu$m in the second benchmark simulation, see Fig. 3.12. The blueshift of the fundamental mode, and also the mode spacing match the data of the reference simulations. The higher order mode was not supported for an aperture diameter of only 1 $\mu$m.

3.3.5 Elliptical Devices

Perhaps the simplest example to investigate the effects of non-circular structures is the VCSEL with elliptical oxide aperture. This device has already been studied in terms of polarization splitting of the fundamental and also higher order modes [83]. Nevertheless, the clear demonstration of diffraction around the oxidation edge has not been published by other groups yet. The fundamental mode pattern along the two main axial cross-sections is given here for qualitative comparison with the circular device. The aperture was located halfway between node and anti-node position in the COST268 structure for the next examples. The motivation of this possibly surprising position is the demonstration of scattering effects, which would be week for node oxide, and keeping the number of supported modes relatively low at the same time. The minor axis of the ellipse is chosen
as 3.2 μm, while the major axis as 4.8 μm, corresponding to a circular aperture with 4 μm diameter. The active region followed the geometry of the aperture. Material anisotropies related to the electro-optic effect were omitted from the simulations, as well as thermal effects. The calculated intensity of the fundamental mode on logarithmic color scale is displayed on Fig. 3.13, which shows similar diffracted waves to those obtained numerically for the circular device [108]. Moreover, it can be seen that diffraction is stronger along the minor axis of the ellipse, which agrees to the qualitative expectation.

Fig. 3.14 depicts all field components together for the two orthogonally polarized fundamental modes in the horizontal cross section at the quantum well. It confirms the legitimacy of the introduced LP-notation, since one transverse component always exceeds the other transverse and the vertical ones by few orders of magnitudes. 3.4% loss difference, called also modal dichroism, was obtained favoring the polarization oriented along the major axis of the ellipse, which can lead to strong polarization mode suppression ratio. The modal losses were calculated from the imaginary parts of the calculated eigenfrequencies, and were inversely proportional to the decay times. It is important to note that the FEM optical mode calculation described here can be coupled to the rate equation model to calculate modal intensities, as discussed in Section 3.4.

We computed the fundamental mode of a device with circular aperture of 8 μm diameter and an elliptical surface relief with 3.2 μm and 4.8 μm axes. A quarter wavelength layer has been removed from outside this ellipse to increase the losses of higher order modes and to stabilize the fundamental mode output. A similar laser, although with different dimensions and number of mirror pairs, has already been studied experimentally and theoretically [57]. The dichroism between the two orthogonal polarizations is found
CHAPTER 3. NOVEL RESULTS

Figure 3.14: Calculated electric field components at the quantum well plane for a VCSEL with elliptical aperture with axes of 3.2 µm and 4.8 µm. The elliptical oxide aperture is displayed as white curve.

Figure 3.15: Calculated intensity profiles in horizontal planes at the quantum well and at the output. The contours of the elliptical surface relief and the circular oxide aperture are sketched with white curves.

to be 2.0%, smaller than in the elliptical aperture case, since the non-circular structure breaking the symmetry is formed farther from the maximum of the axial standing wave around the quantum well. The longitudinal attenuation is partly compensated by much smaller radial decay, resulting in comparable loss difference to the elliptically oxidized device. Finally it is demonstrated on Fig. 3.15 that the intensity distribution follows the oxide aperture near the quantum wells, but is distorted at the output plane. The
3.3. RESONATOR MODES OF ADVANCED VCSELS

Figure 3.16: Calculated intensity profiles along the corner of the square-like oxide aperture (left panel) and 45 degrees off (right half) on logarithmic colorscale. The scattering is substantially stronger due to shorter aperture diameter along this section.

intensity has maxima just outside the ellipse along the minor axis due to the local shift of the standing wave caused by the removed mirror.

3.3.6 Square-Like Aperture

The fundamental mode of the same device with a square-like aperture having a diagonal of 4 $\mu$m diameter and a cylindricity value of 0.5 has also been calculated. It can be observed on Fig. 3.16 that stronger scattering appears along the shorter axial section 45 degrees off the corners. The shortest distance between the aperture edge and the center axis is about 1.7 $\mu$m in this section. This behavior agrees with one's qualitative expectation according to diffraction theory.

3.3.7 Photonic Crystal VCSEL\(^5\)

The optical properties of photonic crystal VCSELs were calculated in last years by several methods, but none of them was applied directly to the real 3-D structure. The solution of a laterally 2-D scalar method was published by assuming an effective index step in the regions comprising the etched holes [109]. A simplified structure with hard mirrors instead of DBRs was also analyzed by FDTD approach [110]. The whole structure is exactly taken into account through this thesis, with the possibility to perform a coupled opto-electro-thermal analysis. The combined guiding mechanism in oxide-confined PhC-VCSELs, which is an important practical issue, is also feasible to simulate by using the FEM model. The method is applied first for a basic structure deduced again from the

\(^5\)The purpose of this subsection is to support thesis 4, and it is tightly connected to Refs. [J2, C4].
CHAPTER 3. NOVEL RESULTS

COST268 benchmark.

The lattice constant of the hexagonal PhC pattern is selected as 2.5 \( \mu \)m, the hole diameters as 1.25 \( \mu \)m, and a 7-point defect zone is formed by leaving the center and next ring of nodes intact. Holes are etched in three rings outside the defect, and their depth is assumed to be 21 mirror pairs out of the total 25 top-DBR pairs. Two structures are compared, one of them without oxide confinement, the other with an oxide diameter of 9.4 \( \mu \)m. (A simple oxidized device has also been simulated for the sake of comparison.) A typical lateral mesh for this structure is depicted on Fig. 3.9. The calculated intensity distributions of the fundamental and first order modes are shown on Fig. 3.17. It can be seen that the axial standing wave present in the mirrors is highly distorted in the airholes, where waves having longer geometrical periodicity may be formed if the hole diameter is large enough. The relative intensity inside the holes is related to the transverse confinement of the mode for the defect zone. It has been found with simulations, that at least two or three rings of holes are usually required to confine the fundamental mode effectively, if no other optical confinement is present. On the other hand, the first ring of holes has the largest effect on the increased modal loss, since it interacts relatively strongly with the mode profile.

The local electric field vector was computed as the linear combination of the vectorial basis functions weighted with the obtained eigenvector. The transverse confinement factor was calculated as an area integral of the obtained modal intensity and normalized for the whole cross-section. The area for which the integral was evaluated, was defined as the circular aperture, with the holes themselves subtracted. It was observed that the oxide provided additional transverse confinement of about 5\%, if temperature induced refractive index change was not taken into account. The oxide reduces the scattering on the holes, and smaller portion of the light leaves the cavity through the etched holes, resulting in about 10\% lower modal loss coefficient for the fundamental mode. This phenomenon leads to lower threshold current in oxide-confined PhC-VCSELs, which was also experimentally demonstrated [111]. On the other hand, the oxide aperture decreases the losses of higher modes more significantly, up to 15-20\% for some configurations, and reduces the modal discrimination, deteriorating finally the single-mode operation. This behavior has been studied for different lattice periodicity and relative oxide aperture sizes; and the largest effect was observed for the smallest lattice constant and for the oxide aperture closest to the defect zone, which is usually defined as the circle touching the perimeter of the innermost holes [112]. This tendency is depicted on Fig. 3.18. The thermal effects tend to squeeze all laser modes to the center under higher bias current, therefore the scattering on the holes can be decreased. In order to simulate this phenomenon, one can modify the refractive index element-by-element according to the local temperature distribution. The active cavity model with three guiding mechanisms could also be investigated in this way, as outlined in the subsequent section.
3.3. RESONATOR MODES OF ADVANCED VCSELS

Figure 3.17: Calculated intensity profiles for two PhC-VCSELS and a conventional oxide aperture VCSEL on logarithmic color scale. The upper row displays half axial section of the fundamental (a) and that of the first order mode (b) without oxide aperture, the second row with an additionally incorporated oxide aperture (c, d). The last row depicts the patterns of the fundamental (e) and next modes (f) if only an oxide aperture is employed. White lines indicate the contours of the innermost etched hole and the oxide aperture.
3.4 Coupled Opto-Electro-Thermal Simulations\(^6\)

3.4.1 Electrical Model

One should take into account at least four basic processes to realize comprehensive coupled simulations, namely: current flow, heat flow, optical eigenmode analysis and laser dynamics, all implemented for general 3-D geometry. The scalar and vectorial solutions of the Helmholtz equation discussed above serve as potential candidates for the optical model. The further components are reviewed in the next paragraphs.

Carriers are drifted by the applied field from the metal contacts through the substrate and semiconductor mirrors to the quantum wells, where they may undergo various recombination mechanisms, and also diffuse laterally. Solving the electrical transport problem results in the knowledge of the current density impinging on the active region, which is essential for the calculation of the optoelectronic interaction. It is emphasized that the presented model approximated only the above threshold current-voltage characteristics, and nonlinear semiconductor behavior was omitted from the following analysis.

The electric potential distribution in the VCSEL and thus the current density are governed by the Laplace-equation \([63, 62]\):

\[
\nabla (\sigma \nabla \Phi) = 0. \tag{3.27}
\]

Here \(\Phi\) denotes the electric potential and \(\sigma = ne\mu\) the electric conductivity, where \(n\)

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\(^6\)This part of the dissertation proves thesis 5, and is based on Refs. [J3, C5, C6].
3.4. COUPLED OPTO-ELECTRO-THERMAL SIMULATIONS

is the local free carrier density, $e$ is the unit charge and $\mu$ is the mobility. For doped semiconductor mirrors, the carrier density has been estimated with the dopant concentration. Heterojunctions are modeled with increased anisotropic resistivity in the axial direction [64]. Eq. (3.27) has been associated with homogeneous Neumann boundary condition except the metal contacts, where Dirichlet boundary condition has been applied. An alternative option can be to adopt linear third-order boundary condition to simulate the Schottky-junction. It is given by the expression: $\Phi - r \sigma \hat{n} \cdot \nabla \Phi = \Phi_0$, where $\Phi_0$ denotes the fixed potential of the metal contact and $r$ is the sheet resistivity of the metal-semiconductor interface. To describe the temperature dependence of electric mobility, the following empirical relation has been evaluated [113]:

$$\mu(T) = \begin{cases} 
\mu(T) = \mu(T_0) \left(\frac{T}{T_0}\right)^{2.3} & \text{for n-doped AlGaAs} \\
\mu(T) = \mu(T_0) \left[\left(\frac{T}{T_0}\right)^{-2.3} + 0.016 \left(\frac{T}{T_0}\right)^{-1.5}\right]^{-1} & \text{for p-doped AlGaAs.}
\end{cases}$$

(3.28)

The second term in p-doped AlGaAs has been neglected here for computational convenience, which can cause approximately 1.6% numerical deviation from the original formula under typical operation temperature.

3.4.2 Thermal Model

The evolution of temperature is governed by the thermal conductivity equation, taking into account nonradiative recombination in the active region, distributed Joule-heat and absorption [63, 62]:

$$c \rho \frac{\partial T}{\partial t} = \nabla (\kappa \nabla T) + R_{nr} + R_{Joule} + R_{abs}.$$  

(3.29)

$T$ denotes the local temperature, $c$ the specific heat, $\rho$ the density, $\kappa$ the thermal conductivity, and the last terms the above-mentioned heat power densities. Eq. (3.29) has been associated with homogeneous Neumann boundary condition except the heat sink. The substrate might be alternatively omitted from the computational window by employing linear third-order boundary condition at the lowest mirror, which describes heat transfer to a fixed temperature reservoir. It is given by the mathematical equation: $T - \kappa \alpha^{-1} \hat{n} \cdot \nabla T = T_0$, where $T_0$ is the fixed temperature, and $\alpha$ denotes the heat transfer coefficient characterizing the substrate, which must be calibrated carefully. If one considers fast processes compared to the thermal time constant of the VCSEL (such as current modulation), the temperature distribution is fixed on the stationary solution of Eq. (3.29) with zero left-hand side. For self-consistent simulations, the temperature dependence of thermal conductivity is given as follows [114]:

$$\kappa(T) = \kappa(T_0) \left(\frac{T}{T_0}\right)^{1.25}.$$  

(3.30)

The temperature dependence of the real part of the refractive index is estimated with a linear formula [59]:

$$n'(T) = n'(T_0) \left[1 + n_T(T - T_0)\right],$$  

(3.31)
where $T_0$ is a reference temperature, and $n_T$ denotes the linear coefficient. It is responsible for the redshift of the laser modes and for thermal lensing on high operation temperatures. The imaginary part of the refractive index, being proportional to the local absorption coefficient, is approximated as an exponential [115], with the $T_{\text{abs}}$ material constant:

$$n''(T) = n''(T_0) \exp \left( \frac{T - T_0}{T_{\text{abs}}} \right).$$

(3.32)

The thermal expansion is not investigated in this work. It has negligible effect on the mode wavelengths compared to the temperature-induced increase of the refractivity, as the linear thermal expansion coefficient is of the order of $10^{-6}$ K$^{-1}$ and the index changes roughly $10^{-4}$ for 1 K temperature variation.

### 3.4.3 Laser Model

The multi-mode rate equations for local free carrier density ($n$) in the QWs and modal intensities ($S_i$) read as follows:

$$\frac{\partial n}{\partial t} = \frac{\eta j}{ed} - An - Bn^2 - Cn^3 + D\Delta n - v_g \sum_i g_i(n)|\Psi_i|^2 S_i,$$

(3.33)

$$\frac{\partial S_i}{\partial t} = \beta B \int n^2 dV + v_g \left[ \int g_i(n)|\Psi_i|^2 dV - L_i \right] S_i.$$

(3.34)

$\eta$ is the injection efficiency (which may depend on the current density itself to take current leakage into account [63]), $j$ the current density, $e$ the unit charge, $d$ the width of quantum wells. $A$, $B$ and $C$ denote the coefficients of defect-induced, radiative and Auger recombination processes, respectively. $D$ is the lateral carrier diffusion constant, $v_g$ the group velocity, $g_i$ the local optical gain of the $i$th mode, $\beta$ the spontaneous emission coupling. The material gain is defined either with an empirical linear or logarithmic function of the free carrier density (parameterized with $a_0$ gain coefficient at transparency and $n_0$ transparency carrier density), and is extended with wavelength and temperature dependence. An alternative way may be to use a previously computed gain lookup table. The gain function used here has the following form:

$$g(n, \lambda, T) = a_0 \ln \left( \frac{n}{n_0} \right) \left\{ 1 - \left[ \frac{\lambda_0 + \lambda_T(T - T_0) - \lambda}{\Delta \lambda_0} \right]^2 \right\},$$

(3.35)

where $\lambda_0$ denotes the wavelength where the material gain has a maximum on the reference temperature, $\lambda_T$ the linear coefficient, and $\Delta \lambda_0$ the half width of the gain interval. The free carrier density and the temperature are evaluated as a function of position and time. The modal loss can be calculated from the imaginary part of the free space wavenumber as follows:

$$L = \frac{c \Im(k_0)}{v_g},$$

(3.36)
with $c$ being the speed of light. Modal gains are evaluated as an overlap integral of the local gain and mode profile in the quantum wells. The parameters used in the calculations are summarized in Table 3.6. Although all coefficients could have been associated with specific temperature dependence, the discussion is restricted to those explicitly mentioned above.

As the rate equations are formulated only for the active region, the reduction to the lateral cross-section is obvious. After utilizing a spatial discretization and casting the diffusion term into algebraic form, a standard ordinary differential equation solver provides the time-dependent solution. Steady-state is found also in the dynamical way, as the analytical solution of the rate equations with zero left-hand side seems to be very complex if a suitable gain function such as Eq. (3.35) is incorporated into the model.

To perform small-signal analysis, the rate equations are linearized around pre-calculated steady-state solutions, and the effect of sinusoidal current modulation on modal intensities is obtained analytically. Substituting $j(r,t) = \overline{j}(r) + \delta j(r) \exp(i\omega t)$, $n(r,t) = \overline{n}(r) + \delta n(r) \exp(i\omega t)$ and $S_i(t) = \overline{S}_i + \delta S_i \exp(i\omega t)$ into Eqs. (3.33) and (3.34), and exploiting that the overlined stationary solutions satisfy them, one obtains:

$$ i\omega \delta n = \frac{\eta \delta j}{ed} - (A + 2B\overline{n} + 3C\overline{n}^2) \delta n + D\Delta \delta n - v_g \sum_i |\Psi_i|^2 \left[ \overline{S}_i \left| \frac{\partial g_i}{\partial n} \right| \overline{n} + g_i(\overline{n})\delta S_i \right], $$

(3.37)
\[ i \omega \delta S_i = 2 \beta B \int \nabla \delta \Phi \, dV + v_g \left\{ \int |\Psi_i|^2 \left[ \frac{\delta S_i}{\delta n} \frac{\partial g_i}{\partial \Phi} \delta n + g_i(\Phi) \delta S_i \right] dV - L_i \delta S_i \right\}. \quad (3.38) \]

A linear equation system appears after adopting spatial discretization for the carriers, in which the unknowns are the complex modulation amplitudes of the carrier densities and the modal intensities. The former can be easily eliminated, and one concludes with the dependence of the optical modulation amplitude as a function of the input current modulation. It is reasonable to approximate the lateral profile of the current modulation simply with the stationary current profile for the typical modulation speed, since the transport of carriers is almost quasistationary [62].

### 3.4.4 Discretization

To exploit the underlying symmetries of special VCSELs with square oxide aperture or elliptical surface relief, only one-fourth slice is meshed to calculate multi-mode dynamics (one-eighth section of a fourfold symmetric device is sufficient to obtain the scalar optical modes with even azimuthal number). Other examples such as the triangular holey structure described in Ref. [53] may also have symmetry, which will always decrease the problem size drastically. Since the optical intensity decays exponentially far from the core, it may also be profitable to truncate the optical computational domain in the cladding (using PML) to reduce the problem size. To avoid numerical difficulties arising from different meshes for the physical processes considered, a unified mesh scheme is proposed in the inner region of the diode, where all the equations have to be formulated. The basic mesh contains the same elements in this domain, the natural requirement to resolve optics in better resolution can be fulfilled with subdivision of base cells. This common region may be covered with separate meshes in the PML for the optical eigenmode calculation, and in electro-thermal domain.

An efficient discretization scheme must fulfill several conditions. It should match the physical structure of the VCSEL that exhibits rigorous vertical layer structure and diverse, usually curved lateral contours. The capability to formulate both scalar and vectorial descriptions is of central importance. The discretization should also enable to divide the domain in a non-equidistant manner in order to allow fine resolution in the sensitive regions, where the physical quantities vary rapidly, and to keep a limited problem size by assigning larger elements in relatively featureless zones. If one selected uniform division everywhere, the solution of the resulting 3-D algebraic problem could not be feasible on the available computers.

One of the most obvious and common method is to lay down an orthogonal grid. Although this solution fits to the layers of the laser diode, it either coincides poorly with curved lateral boundaries or requires tremendous cuboids to approximate all contours step-wisely. It is also possible for special geometries to achieve acceptable fitting using less but distorted elements (whose edge lengths differ extremely), but this results in loosing the numerical accuracy. Covering the computational domain employing general hexahedra or
straight columns with general quadrilateral bases is more versatile, but the formulation of finite volume method is not straightforward. The most complex and irregular geometries can be filled with tetrahedra; but this option may lead to the unnecessary increase of the discrete variables, for example when solving the vector Helmholtz equation, as the unknowns are associated to the edges in this case.

Due to the shortcomings of the above schemes, prism elements have been found to be the most suitable and efficient for VCSEL simulation. They are fitted both to the axial layer structure and the lateral contours (such as oxide aperture, surface relief and contacts) of the device. Their bases are generated using relaxed Delaunay triangularization (see Fig. 3.9). Although it can be sufficient for the purpose of electro-thermal computations to assign a single layer of prisms in each physical quarter wavelength layer, and it corresponds also to the theoretical limit of resolving optical waves, the precise laser mode calculation requires more detailed partitioning. In order to achieve acceptable resolution of the axial standing wave, eight layers of prisms have been allocated in average in every quarter wavelength period. The lateral size of the prisms was selected according to the expected profile of the resonator modes and to the available computer resources. If the laser diode supports only few modes, their lateral profiles do not change rapidly within the optical aperture, and few tens of divisions provide good accuracy. On the other hand, as the modes decay nearly exponentially far away from the aperture, a locally rough mesh will not influence the results significantly. Therefore a non-equidistant division of the structure is highly preferred if the computer power is limited.

The representative points are selected as mid-points of axial edges of the prisms, above the vertices of triangles. All equations are integrated over the dual elements of the prisms forming polygon-based straight columns, as shown in Fig. 3.19. The finite volume discretization is derived below for the left-hand side of Eq. (3.27) for a selected dual element. The integral form is first expanded in horizontal and vertical terms as follows:

$$\int_V \nabla (\sigma \nabla \Phi) \, dV = \sum_i (\sigma \nabla T \Phi_i) A_i + \left( \sigma \frac{\partial \Phi}{\partial z} \right)_t A_t + \left( \sigma \frac{\partial \Phi}{\partial z} \right)_b A_b,$$

(3.39)

where $A_i$ refers to the side surfaces, the subscripts $t$ and $b$ to the top and bottom surfaces of the column, respectively. $\nabla T$ is the two-dimensional gradient operator. The evaluation of the first term is performed triangle by triangle using the following linear order approximation for the gradient:

$$\begin{bmatrix} \frac{\partial \Phi}{\partial x} \\ \frac{\partial \Phi}{\partial y} \end{bmatrix} = \begin{bmatrix} x_1 - x_2 & y_1 - y_2 \\ x_1 - x_3 & y_1 - y_3 \end{bmatrix}^{-1} \begin{bmatrix} \Phi_1 - \Phi_2 \\ \Phi_1 - \Phi_3 \end{bmatrix},$$

(3.40)

with subscripts labeling the vertices of the triangle under analysis. The same gradient vector appears in scalar products formed with the normals of two sides of the cell (labeled as $A_1$ and $A_2$, for example). The calculation of the vertical fluxes in Eq. (3.39) needs further consideration since the electric conductivity may be discontinuous between
adjacent nodes. Therefore the total current is written based on Ohm’s law, summing up all contributions in the neighboring third-prisms:

$$I = \sum_i (\Phi_1 - \Phi_2) \left( \frac{\Delta z_{1i}/\sigma_{1i} + \Delta z_{2i}/\sigma_{2i} + r_i}{A_\Delta/3} \right)^{-1},$$

(3.41)

where $\Delta z$ denotes the distance between nodes and the interface, $A_\Delta$ the areas of the lateral triangles, and subscripts label quantities in the two cells. $r$ describes heterojunction sheet resistivity between different materials, $i$ runs for all the adjacent triangles. While Eq. (3.40) and Eq. (3.41) provide the entries of the left-hand side matrices for all problems, the derivation of the mass matrix is straightforward.

The complex coordinate stretching technique [116] adopted in PML in the optical model requires some modifications. When employing the scalar Helmholtz equation, Eq. (3.20) is rewritten in PML as follows:

$$\nabla_s^2 \Psi = -k_0^2 \epsilon \Psi,$$

(3.42)

with

$$\nabla_s = \begin{bmatrix} s_x^{-1} & 0 & 0 \\ 0 & s_y^{-1} & 0 \\ 0 & 0 & s_z^{-1} \end{bmatrix} \nabla,$$

(3.43)

where $s_x$, $s_y$ and $s_z$ are properly chosen complex stretching factors. A quadratic profile is usually utilized for the absorption strength in the PML, which allows the minimalization of numerical backscattering. As a consequence the above derivatives and fluxes will contain the stretching matrix.
3.4.5 Self-Consistent Coupling

Since the effect of the optical fields are relatively weak on the strongly coupled electro-thermal system [59], a two-level iteration is essential. In order to calculate the steady-state solution of the system for a given bias, the electro-thermal part is iterated first until a desired convergence. Nonradiative heat sources are specified homogeneously or with an empirical function in the current-confined section of the quantum wells; Joule-type heat sources are selected according to the local current density and electric potential gradient. While in the first step all material parameters are fixed on the heat-sink temperature, their temperature dependence given by Eq. (3.28) and Eq. (3.30) can be locally specified in the following cycles.

Having obtained the temperature distribution, a given set of optical modes of the active cavity can be computed next using the locally modified complex refractive indices. Finally, rate equations are solved using the current density profile through quantum wells and mode distributions. To make the whole system self-consistent, absorption heat sources can be taken into account as the overlap of the electromagnetic fields and material absorption, and nonradiative heat sources can also be re-distributed according to the second and fourth terms of Eq. (3.33). This leads to a second loop extending the electro-thermal coupling.

The computational efforts of the outer iteration may be very expensive, therefore it is sometimes omitted from practical computations. The effective use of preconditioning can accelerate the iterations and also the calculations on the next bias. As results are expected to change slightly in few steps, significant computational time may be saved by using the same preconditioners.

3.4.6 Non-Circular Oxide Aperture

Calculation has been performed on a GaAs/AlGaAs multi-mode VCSEL growth on GaAs substrate, designed for 850 nanometer emission. It consists of a \( \lambda \)-length cavity and 20 pair top- and 32 pair bottom-DBR mirrors and four quantum wells. The second low index layer below the cavity is partially oxidized, forming an aperture close to node position to reduce the number of transverse modes contributing to the lasing action [85] and enhance modal stability [69]. The real aperture shape is approximated with a curvilinear tetragon halfway between a circle and a square. The purely optical mode properties of such devices have already been calculated, in Ref. [84] for round-, and in Subsection 3.2.4 for cusp-cornered oxide contours; here we follow the second model. The aperture area is approximately 100 \( \mu \text{m}^2 \). The lower metal contact is situated below the substrate, while the inner radius of the ring-fashioned top contact deposited on the semiconductor mirror stack is 15 \( \mu \text{m} \). The detailed description can be found in Table 3.7.

Due to the distortion of the ideal circular aperture, the current profile is expected to be asymmetric. Electrical simulation showed approximately 20-25% difference between
Table 3.7: The layer structure of the simulated VCSEL

<table>
<thead>
<tr>
<th>Periods</th>
<th>Type</th>
<th>Doping [cm⁻³]</th>
<th>Thickness [nm]</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>n− Al₀.2Ga₀.8As</td>
<td>5 × 10¹⁸</td>
<td>60.9</td>
<td>3.492</td>
</tr>
<tr>
<td></td>
<td>n− Al₀.9Ga₀.1As</td>
<td>5 × 10¹⁸</td>
<td>69.4</td>
<td>3.065</td>
</tr>
<tr>
<td>1</td>
<td>Cavity</td>
<td>0 − 2 × 10¹⁷</td>
<td>244.4</td>
<td>3.482</td>
</tr>
<tr>
<td>1</td>
<td>p− Al₀.9Ga₀.1As</td>
<td>2 × 10¹⁸</td>
<td>69.4</td>
<td>3.065</td>
</tr>
<tr>
<td></td>
<td>p− Al₀.2Ga₀.8As</td>
<td>2 × 10¹⁸</td>
<td>60.9</td>
<td>3.492</td>
</tr>
<tr>
<td></td>
<td>p− Al₀.9Ga₀.1As</td>
<td>2 × 10¹⁸</td>
<td>46.3</td>
<td>3.065</td>
</tr>
<tr>
<td>1</td>
<td>p− AlAs/oxide</td>
<td>10¹⁹/−</td>
<td>23.6</td>
<td>3.002/1.7</td>
</tr>
<tr>
<td></td>
<td>p− Al₀.2Ga₀.8As</td>
<td>2 × 10¹⁸</td>
<td>60.9</td>
<td>3.492</td>
</tr>
<tr>
<td>30</td>
<td>p− Al₀.9Ga₀.1As</td>
<td>2 × 10¹⁸</td>
<td>69.4</td>
<td>3.065</td>
</tr>
<tr>
<td></td>
<td>p− Al₀.2Ga₀.8As</td>
<td>2 × 10¹⁸</td>
<td>60.9</td>
<td>3.492</td>
</tr>
</tbody>
</table>

Figure 3.20: Near field CCD image of the VCSEL summarized in Table 3.7 with a non-circular aperture of nearly 100 µm² area. Driving current was 7 mA. Although clear multi-mode emission is observed, the intensity of the LP_{21} mode oriented to the corners of the aperture dominates.

The current density at the corners of the oxide aperture and along its edges, and also significantly lower value at the center axis. Nevertheless the injection profile through the quantum wells is rather homogeneous within 5% limit due to lateral current spreading, although it preserves the shape of the confinement region. As a consequence, different steady-state intensities and also decoupled dynamic behavior are expected for the two LP_{21} transverse modes, one having lobes along the corners of the aperture (labeled as LP_{21c} according to cosine azimuthal distribution), the other along the edges (labeled as LP_{21s} in accordance with sine mode pattern). An experimental evidence of this effect is shown in Fig. 3.20.

A quantitative analysis of the observed symmetry-breaking effect is exposed in the following. Since the first higher order LP_{11} modes are degenerated for the oxide shape of
3.4. COUPLED OPTO-ELECTRO-THERMAL SIMULATIONS

Figure 3.21: Computed light-current characteristics for five optical modes. The inset shows the intensity distribution in the quantum well at 15 mA.

Fourfold symmetry, their combination forms an almost perfect ring. On the other hand, \( \text{LP}_{21} \) modes are known to be split for this aperture shape, and the four separate intensity maxima on the near field image can be explained assuming \( \text{LP}_{21c} \) to be considerably more intense. Therefore one should incorporate at least five modes into the simulation. Although this choice will not provide the full description of the VCSEL, it can adequately describe the consequences of the non-circular oxide and further examples.

The simulated steady-state multi-modes light-current characteristics is displayed for the five lowest order modes on Fig. 3.21. The fundamental mode starts lasing at a moderate threshold current of 3 mA due to increased losses compared to usual designs containing more mirrors. The next higher order, degenerated \( \text{LP}_{11} \) modes are almost suppressed in the whole current range except a small interval between 4-6 mA. At higher bias, the two \( \text{LP}_{21} \) and the fundamental modes deplete the outer and inner injection regions, respectively, preventing \( \text{LP}_{11} \)-s to reach the threshold gain. As afore-mentioned \( \text{LP}_{21c} \) become somewhat stronger than its complementary mode due to advantageous overlap with the carrier reservoir. The intensity ratio is related to the inhomogeneity of the current profile in the vicinity of the quantum wells, which depends mainly on the distance between the active region and the oxide. If the aperture is formed in a layer farther from the cavity, better current spreading and thereby more homogeneous near field are expected. The thermal rollover appears around 16.5 mA as a consequence of the detuning between the gain spectrum and the laser modes given by Eq. (3.35) and caused by the refractive index change according to Eq. (3.31), respectively.
CHAPTER 3. NOVEL RESULTS

Figure 3.22: Large signal analysis for five competitive modes. The insets show near field patterns at 0, 200 and 1000 ps, respectively.

In Fig. 3.22 the evolution of five modes can be seen, when the injection current has been switched to a higher value. The distortion of the circular aperture leads to slightly decoupled dynamic behavior of the two $LP_{21}$ modes, from which the one having lobes at the aperture corners is generally more intense. The other might also be somewhat stronger for a short time, as shown near 200 ps. The steady-state power ratio of these modes depends on the total driving current, and a reduced difference is observed on the graph for the final stage. Rise and fall times can be determined using large-signal simulation.

Small-signal modulation response function is plotted in Fig. 3.23. The effect of thermal detuning between the gain spectrum and lasing modes can be observed as the limitation in the modulation bandwidth. Current leakage [63] can also be a contributing factor, as it decreases the injection efficiency and thus restrains the total light power. Nevertheless, for small currents both the relaxation oscillation frequency and damping increase with the driving current, as expected.

3.4.7 Triangular Surface Relief

The intensity difference between the two split $LP_{21}$ modes can be further influenced by introducing mode selective losses using specially designed surface relieves. To obtain the highest discrimination between the $LP_{21}$ modes of interest, four triangular holes should be etched into the top layer of the VCSEL (see Fig. 3.24), which has otherwise the same structure as in the previous example. In order to invert the existing relationship between
the intensities of the LP_{21} modes, the regular triangles are oriented along the corners of the oxide aperture. This solution is similar to the one reported in [117]. The etch depth dependence of emission wavelength and modal losses has been analyzed in [118] for a circular VCSEL, and the highest discrimination is expected for quarter wavelength deep holes.

The modal losses are analyzed as a function of the position of the holes in the following. Four sets of parameters with increasing distance between the center axis and the inner
corner of triangles have been calculated, while the outer side has been fixed 3 μm far from the oxide aperture. Results of cold cavity computations are depicted for the five lowest order modes in Fig. 3.25. If the holes are located closer to the center of the device, losses become higher since increasing portion of the transverse mode pattern overlaps with high loss etched areas. Due to the shape of the holes, LP_{21c} mode having lobes in the vicinity of the triangles experiences highest loss; while the maxima of LP_{21s} mode are outside, therefore its loss is almost unchanged (with smaller than 5% increase). The fundamental mode has also moderate loss, and both orthogonal LP_{11} modes overlap only with every second holes. The LP_{02} transverse mode shows the most interesting behavior which has the second highest loss for relatively outside positioned holes, as its side lobe significantly overlaps with triangular holes. If holes approach the center axis, however, its loss decreases due to the confinement effect of holes, which squeezes the mode pattern. The guiding contribution of the surface patterns may be usually much lower than that of the oxide aperture, but the structure under consideration has relatively few mirrors to achieve high modal discrimination, and this is the reason of the obtained behavior. The free carrier absorption loss is around 10 cm\(^{-1}\) for all positions and modes, therefore the mirror loss ratio between the two LP_{21} modes can be as high as 4.

The calculated modal losses change at high pumping due to thermal lensing and increased free carrier absorption. The index change confines the transverse modes to the center of the device, thereby reduces their overlaps with the etched holes remarkably.

Figure 3.25: Cold cavity modal losses of the fundamental and few higher order modes versus hole position. Dashed line represents total loss of 188 cm\(^{-1}\) if topmost layer is fully removed, while solid line at 28.4 cm\(^{-1}\) is for unetched VCSEL.
3.4. COUPLED OPTO-ELECTRO-THERMAL SIMULATIONS

Figure 3.26: Calculated light-current characteristics for five lowest order optical modes. The intensity profile in the quantum well at 15 mA is displayed on the inset.

Although the mirror loss may decrease by up to 30% on high temperature, the sequence of the modes remains unaltered.

Fig. 3.26 shows the simulated light power versus current diagram of the VCSEL, where holes are located 3 μm from the axis. In comparison with Fig. 3.21 one can observe that the LP$_{21c}$ mode now possessing the highest loss has been drastically suppressed. Even the fundamental mode has weakened significantly, and exceeds threshold only in the mid current interval. The intensity of the LP$_{21s}$ mode has increased, but cannot retain all the gain the modes had shared together. While the fundamental mode can profit from the carriers injected close to the aperture corners only in a limited amount, LP$_{21s}$ is almost totally disjunct from this most effectively pumped region. As approximately 17% of the area of the total current aperture lays below the triangular holes in this particular example, at least 10-15% of the carriers are not exploited by stimulated emission. Together with the slight increase of the optical losses, it leads to a diminished maximum light power. By approaching the holes to center, single higher-order mode emission could be possible, similar to the situation obtained in [117].

The opposite orientation of the holes, 45 degrees off compared to the aperture corners, can also be simulated. The LP$_{21c}$ transverse mode profits from this arrangement, and LP$_{21s}$ becomes suppressed. The maximal output power is about 7.6 mW, somewhat higher than in Fig. 3.26, due to the more advantageous overlap with the injected carriers.
3.4.8 Elliptical Surface Relief

A third VCSEL depicted schematically on Fig. 3.27 shares a similar structure with the previous examples except a circular oxide aperture and a quarter wavelength deep elliptical surface relief. The axis ratio is fixed 1:2 in all samples, and the length of the shorter axis is changed from 2 to 4 \( \mu \text{m} \).

A similar laser diode has been thoroughly studied with respect to single-mode, single polarization emission [57]. It was found that the elliptical relief resulted in a threshold gain difference of about 1% between the two fundamental modes of orthogonal polarization, but the impact on modal intensities was not calculated. Since a scalar optical model is here, the polarization control is not addressed in the following discussion. This approach is, however, capable of a sophisticated single-mode device design including electric, thermal and optical aspects. A numerical example is given for a multi-mode VCSEL, and the inherent calculation of the light power versus current diagrams exceeds the frames of the already published algorithm.

One should note in advance that if the guiding contribution of the elliptical relief were negligible, mode patterns would be expected to be unchanged, only the losses of the originally degenerated linearly polarized mode could split. However, as this example contains relatively few mirror pairs, mode patterns may be distorted due to the symmetry breaking caused by the elliptical relief. Moreover, for large eccentricity the original mode labeling for rotationally symmetric structures might not be kept due to overlapping of the lobes.

The cold cavity modal losses of five modes have been calculated and plotted in Fig. 3.28. For small ellipse sizes, the fundamental mode experiences the lowest loss, because it is well squeezed below the unetched part of the top layer. The low loss of the LP\(_{11c}\) mode oriented along the long axis of the ellipse is also reasonable (and may drop below the
3.4. COUPLED OPTO-ELECTRO-THERMAL SIMULATIONS

Figure 3.28: Cold cavity modal losses of the fundamental and four higher order modes versus elliptical relief size. Dashed line represents total loss of 188 cm$^{-1}$ if topmost layer is fully removed, while solid line at 28.4 cm$^{-1}$ is for VCSEL without surface pattern.

loss of the fundamental mode if the long axis of the ellipse exceeds the aperture radius), while the orthogonal orientation experiences always higher loss, since it is located rather below the etched areas. The LP$_{21c}$ mode should have medium loss if its mode pattern were similar to that of circular VCSEL. The elliptical relief, however, modified the distribution, and resulted in a pattern with overlapping lobes along the short axis, also squeezed inside. Therefore its loss is lower than expected. Finally, the loss of the LP$_{21s}$ mode having zero intensity along axes exceeds even the loss of the LP$_{11s}$ mode, as all its lobes are partially below the etched region.

Fig. 3.29 shows the calculated light power versus current diagram for elliptical relief with 3.3 and 6.6 $\mu$m long axes. Compared to Fig. 3.21 one can point out that all modes having lobes outside the ellipse are practically below threshold. Only the fundamental and the long axis oriented LP$_{11c}$ and LP$_{21c}$ modes operate in the whole current range. They start lasing in the sequence of their threshold gains, and reach roll-over at different currents, when their modal wavelengths become equal with the gain maximum. One may observe that the threshold current has increased and the total power has decreased remarkably. This is the direct consequence of the increased losses for all modes (even the fundamental mode exhibits 33% increase) and the assumed logarithmic gain function. In order to keep the losses of a few modes low and obtain high discrimination at the same time, the growth of one additional mirror pair is proposed, which can compensate the loss increase of the preferred modes caused by the relief.
3.5 Design of a Single-Mode PhC-VCSEL\(^7\)

One of the most important and attractive characteristics of PhC-VCSELs is that they potentially offer high optical power in the single fundamental mode. This feature is borrowed from large area single-mode PhC fibers, which can be employed for high power fiber lasers as well. The geometry of PhC lasers is obviously more complex, and their modal behavior has been investigated only recently.

Several papers were published, in which PhC-VCSELs were studied by means of quasi 2-D analysis [109]. The basic assumption in these approaches was that the axial structure can be compressed into an etching depth dependence factor, and the single mode condition can be traced back to a two-dimensional waveguide problem defined with appropriate effective indices. For example, the effective frequency parameter was defined as:

\[
\nu_{\text{eff}} = \frac{2\pi \Lambda}{\lambda} \sqrt{n^2 - (n - \gamma \Delta n)^2},
\]

with \(\Lambda\) being the lattice constant, \(\lambda\) the emission wavelength, \(n\) the average refractivity of the DBR, \(\Delta n\) the reduction of the index extracted from photonic band diagram calculations. The \(\gamma\) etching depth factor was selected according to the axial overlap between the standing wave and the depth of the etched holes [119]. If the effective frequency was

\(^7\)This section relies on Refs. [P1, C7, C8, C9, C10], and contains the results for thesis 6.
3.5. DESIGN OF A SINGLE-MODE PHC-VCSEL

Figure 3.30: Calculated transverse confinement factors of the two lowest order modes as a function of the total dissipated heat power on logarithmic scale. Three PhC-VCSELs with different lattice constants have been studied. Notice that only the fundamental mode is supported for small lattice constant and low current injection, corresponding to single-mode PhC or conventional fibers having narrow core diameter and low normalized frequency.

smaller than 2.405, single-mode operation was expected in a single-point defect structure [120]. These methods, however, neglected the scattering effect of the etched holes on the modal losses, as well as any thermal effects. A 3-D simulation model has recently been presented to determine the optical modes more accurately on the basis of PWAM (see Subsection A.5), but has still neglected thermal effects. It has been experimentally confirmed meanwhile, that the simple condition for the effective frequency does not explain stable mode operation, and the modal loss difference can play more important role in this question [121].

The 3-D coupled opto-electro-thermal model outlined in the preceding section is capable of handling all these mechanisms in a natural way. The resonator modes can be calculated under cold-cavity conditions, as well as for continuously varying temperature distributions that evolve under bias. The temperature profile has been calculated for a discrete number of total heat powers that were distributed homogeneously in the pumped region of the QWs, and have been used to correct the background refractive indices. The important properties of the modes at interior heat dissipation values have been adjusted by numerical interpolation in order to keep a reasonable running time.

The two lowest order optical modes of three PhC-VCSELs have been calculated under 0, 2.5, 5, 10, 15, 20, 25, 30, 40, 50 and 60 mW heat power dissipation. All devices
incorporated a thick proton-implanted zone that formed an electrical aperture having 7.9 \( \mu \text{m} \) diameter, but did not influence the resonator system. The optical confinement was guaranteed by etching three rings of holes into the top DBR in a hexagonal pattern, leaving the center position intact. The depth of all holes was assumed as 24 mirror pairs from a total of 30 pairs, while the lattice periods were 3, 4 and 5 \( \mu \text{m} \), respectively. The diameter of the holes was half of the lattice constant in all cases.

Fig. 3.30 displays the transverse confinement factor for the defect area, which has been defined as the difference of the circle passing through the centers of the innermost etched regions and the holes. One can see that the higher order mode is unsupported (crowded out from the defect zone) for the smallest lattice constant below 10 mW heat power, and therefore the laser must be unconditionally single-mode in this regime. The thermal lensing tends to squeeze the modes towards the center axis, and increases their confinement for the active defect area.

Fig. 3.31 shows the calculated modal losses for the same modes and structures. They decrease in the low current regime, because the dominant component, scattering on the holes, diminishes due to the extra mode guidance caused by thermal lensing. After passing beyond the minimum, the free carrier absorption loss strengthens with temperature; but the loss ratio between the LP\(_{11}\) and LP\(_{01}\) reduces monotonically. One can also determine that smaller lattice constant brings better modal discrimination (equivalent with higher loss ratio) and higher overall modal loss, which forecasts the possibility of extended single mode regime at the cost of higher threshold current.
3.5. DESIGN OF A SINGLE-MODE PHC-VCSEL

![Graph showing simulated light power versus injection current characteristics of three PhC-VCSELs of various lattice constants.](image)

Figure 3.32: The simulated light power versus injection current characteristics of three PhC-VCSELs of various lattice constants. The fundamental modes are displayed with dashed, the first higher modes with dash-dotted lines, while the total powers are indicated with solid curves. The highest single mode power can be achieved using the device of 4 µm lattice constant, due to the competing effects of larger active area and diminishing modal discrimination.

Knowing the laser modes and the current density profile through the QWs from the electrical analysis, the rate equation approach has been employed to find the steady-state solutions and thus simulate the light power versus current characteristics. The dissipated heat power has been estimated with the help of the measured current-voltage curves, assuming negligible emitted power. Although only the two lowest modes have been incorporated into this simulation, the single mode regime should be rendered correctly, as all other modes exhibit less confinement and higher scattering loss, and come into play only at larger current injection. The results are given on Fig. 3.32. They clearly prove that single mode operation can be maintained even if LP_{11} is supported by the structure, but cannot reach its laser threshold. More importantly, it can be observed that highest single mode power can be achieved using the device possessing 4 µm lattice constant, due to the competing effects of larger mode area and diminishing discrimination at increasing lattice period. Lower threshold current and higher slope efficiency have also been found as the mode area became wider. This evidence shows convincing agreement with the measured behavior plotted on Fig. 3.33. Note that since only the two lowest modes were taken into account, the multi-mode regime can alter after introducing other modes. Therefore this particular simulation cannot predict the experimental characteristics correctly in the high current range.
Figure 3.33: Experimental light power versus current diagrams (solid lines) and side-mode suppression ratio plots (dashed lines) of PhC-VCSELs possessing different lattice constants. Single-mode condition is defined as higher than 30 dB mode suppression.
Chapter 4

Summary and Outlook

The realization of a coupled, real three-dimensional opto-electro-thermal simulation model has been demonstrated in this dissertation, and applied for various realistic VCSELs that do not possess cylindrical symmetry. It has been developed in a step-by-step procedure, first semianalytical methods providing relatively fast data have been proposed, keeping in mind that their applicability is limited to planar geometries. The fully numerical solution of the scalar or vector Helmholtz equation has yielded accurate laser mode profiles, wavelengths and optical losses for a pre-defined arbitrary refractive index distribution. These calculations can be thus employed for novel diodes like photonic crystal lasers, as well. The vectorial approach also carries the information on polarization mode splitting, and the individual components of the electric and magnetic fields can be reconstructed.

While approximate laser mode calculation tools had already been described for three-dimensional VCSELs before this work, it has brought forth the first comprehensive method of analyzing the complex behavior for noncylindrical cases that covers thermal and electrical aspects. Its unique feature is in this context that the three subproblems were solved in a similar fashion, employing a unified lateral triangular mesh. Therefore the mathematical efforts have been greatly simplified. Although the computer demands have become clearly higher than before, realistic device characteristics can be yet modeled even for relatively weak index-guiding, when the laser mode properties depend considerably on the injection strength.

The major results of this dissertation are summarized in the following points.\(^8\)

1. I have developed two new semianalytical extensions of the weighted index method, and applied for the simulation of a multi-mode VCSEL incorporating an oxide aperture that exhibits a realistic contour between an ideal circle and the encased square. The calculated wavelength spacing among the fundamental and the next three modes has agreed convincingly with the recorded spectrum, and the measured near field patterns have also been reproduced by weighting the first few predicted transverse mode profiles \([J_1, C_1]\).

\(^8\)Thesis 1 is discussed in Section 3.2, subsections 3.3.1-3.3.6 comprise theses 2-3, Subsection 3.3.7 is related to thesis 4. Theses 5 and 6 correspond to Section 3.4 and to Section 3.5, respectively.
2. I have realized the direct numerical solution of the Helmholtz equation for noncylindrical VCSELs, and demonstrated the diffraction of the light near their oxide windows. Two model apertures have been simulated, one possessing a curved tetragonal shape, the other an ellipse with moderate eccentricity. Both cases have shown agreement with one’s qualitative expectation that stronger scattered waves should appear along the shorter sections of the aperture [J2, C2].

3. I have revealed significant cold-cavity modal loss difference with the fully numerical solution of the vector Helmholtz equation between the two orthogonally polarized fundamental modes of a VCSEL that possesses an elliptical oxide aperture. The structure, in which only the topmost quarter-wavelength thick layer was partially etched to form an elliptical surface relief, has yielded smaller loss difference; and an exciting intensity distribution at the top surface due to the detuning of the axial standing wave below the etched region. [J2, C3].

4. I have confirmed and explained the previous experimental finding that an oxide aperture could lead to reduced threshold current in PhC-VCSELs, by invoking the Helmholtz equation solver. It has been proved that the extra guiding introduced by the oxide squeezed the laser modes further towards the center axis, and decreased the scattering loss on the deep etched holes. As stronger effect has been found for the higher modes, the dielectric aperture can deteriorate single-mode operation in PhC lasers [J2, C4].

5. I have predicted the static light power versus injection current characteristics of various noncircular VCSELs using the coupled three-dimensional opto-electro-thermal approach, and assuming cold-cavity laser modes. In a laser diode possessing a square-like aperture shape, the degeneracy splitting between the second-order modes and the asymmetric current distribution have together resulted in noticeable peaks on the calculated near field pattern, which has matched to the experimental image. I have pointed out with numerical modeling that this behavior could be reversed, if quarter-wavelength deep triangular holes are etched into the top mirror above the corners of the aperture. A similar light power versus current diagram has also been estimated for a VCSEL with an elliptical surface relief but cylindrical structure elsewhere, and it has indicated the suppression of transverse modes that overlap substantially with the etched region [J3, C5, C6].

6. I have optimized with simulation the lattice constant of a proton-implanted PhC-VCSEL to achieve the highest single-mode output power. To this end, the coupled opto-electro-thermal analysis has been utilized, and the laser modes have been consequently recalculated at different injection levels. It has been obtained that higher order modes
became more easily unsupported by the PhC, and the modal discrimination strengthened as the lattice constant decreased. On the other hand, the threshold current has decreased and the maximal laser power has scaled naturally for larger optical mode area. These competing effects have made clear the existence of an optimal lattice constant that corresponds to the highest single-mode power, which has been verified experimentally, as well [P1, C7, C8, C9, C10].

The following future directions are worth considering. Although the presented approximate electrical calculation has been sufficient for studying the device characteristics above threshold and explaining noncylindrical effects, it has not captured the nonlinear diode behavior and has been inappropriate to predict more realistic current-voltage behavior. Therefore the realization of a drift-diffusion type semiconductor model is essential. Another challenging topic would be the quantum-mechanical description of the QWs, and its interaction with the electronic system. To mention new promising applications, the investigation of VCSELs incorporating surface gratings and asymmetric PhC patterns attracts high interest. Although the list of possible extensions seems almost infinite, the discussed approaches have been proved useful not only for academic purposes but also in industrial environment, and the utilization of the accompanying software has been gradually strengthening.
Appendix A

Further Optical Approaches

A.1 Effective Frequency Method

The effective frequency method (EFM, [122]) is very similar to EIM. The only remarkable difference is that it takes into account the temporal dispersion of the dielectric function in the frequency domain. If the permittivity depends on the frequency, the second term of Eq. (2.14) is expanded around its reference value:

\[
\frac{\omega^2}{c_0^2} \varepsilon(\omega, \mathbf{r}) \approx \frac{\omega_0^2}{c_0^2} \varepsilon(\omega_0, \mathbf{r}) + \left[ \frac{2\omega_0}{c_0^2} \varepsilon(\omega_0, \mathbf{r}) + \frac{\omega_0^2}{c_0^2} \frac{\partial \varepsilon(\omega, \mathbf{r})}{\partial \omega} \right]_0 (\omega - \omega_0) =
\]

\[
\frac{\omega_0^2}{c_0^2} n_p^2(\mathbf{r}) + \frac{2\omega_0}{\omega_0^2} n_p(\mathbf{r}) n_g(\mathbf{r})(\omega - \omega_0)
\]

The phase index \( n_p(\mathbf{r}) = \varepsilon^{1/2}(\omega_0, \mathbf{r}) \) and the group index \( n_g(\mathbf{r}) = \partial[\omega \varepsilon^{1/2}(\omega, \mathbf{r})]/\partial \omega|_{\omega_0} \) have been introduced. Then one gets a modified scalar Helmholtz equation with the nominal free space wavenumber \( k_0 = \omega_0/c_0 \) and the dimensionless frequency parameter \( \nu = 2(\omega - \omega_0)/\omega_0 \):

\[
\Delta \Psi + k_0^2 n_p^2(\mathbf{r}) \Psi = \nu \kappa^2 n_p(\mathbf{r}) n_g(\mathbf{r}) \Psi.
\]

(A.2)

The eigenfunctions are searched in a separable form \( \Psi(z, r, \phi) = \psi(z; r) \phi(r) \exp(i m \varphi) \), but with a possibly continuous radial dependence instead of discrete region index \( j \). Nevertheless, \( r \) is only a parameter in \( \psi(z; r) \), not a truly independent variable. Equation (A.2) can than be regrouped as follows:

\[
\frac{\partial^2}{\partial z^2} + k_0^2 n_p^2(\mathbf{r}) \psi(z; r) = \nu \kappa^2 n_p(\mathbf{r}) n_g(\mathbf{r}) \psi(z; r)
\]

(A.3)

and

\[
\left[ \frac{\partial^2}{\partial \varphi^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} + \nu \kappa^2 \right] \phi(r) \exp(i m \varphi) = \nu \phi(r) \exp(i m \varphi),
\]

(A.4)

where \( \langle n_p n_g \rangle_{(r)} \) denotes averaged indices with \( \psi(z; r) \) similar to Eq. (2.18), and the role of \( \nu_{\kappa^2} \) is similar to the correction parameters \( \xi_j \) in EIM. The original equation can be obtained apart from the averaging, after multiplying the first one with \( \phi(r) \exp(i m \varphi) \);
A.2. NUMERICAL MODE MATCHING METHOD

rearranging the second to have only the transverse derivatives on the left, then multiplying it with $\psi(z; r)$, finally adding the two equations. One can also recognize that the second equation is Bessel-type, and is solved practically using the same method as in EIM, provided that discrete regions can be distinguished.

There are two differences between EIM and EFM. The first one is only conceptual, since EIM focuses on the effective indices $\langle \varepsilon \rangle$, while EFM emphasizes the effective frequency parameter $\nu_{\text{eff}}$. The main argument of EFM arises from a comparison with Schrödinger’s equation: while the frequency parameter corresponds to the confining potential, the effective index plays the role of the effective mass with weak spatial variation. The second is about the temporal dispersion of the dielectric constant. If the group indices were replaced with phase indices, the original scalar Helmholtz equation and EIM would be obtained. However, the group indices of the relevant semiconductors are by more than 10% larger than phase indices, and all wavelength shifts should be reduced consequently by comparable amount.

A.2 Numerical Mode Matching Method

The disadvantage of the previous model is the inability to take the diffraction of the wave into account. It follows from its separable analytical solution in radial and axial directions, but the real mode profile should expand by some amount far from the aperture. A popular approach detaches a single laser mode into numerous layer modes, among which energy transfer is possible at the material interfaces according to the local continuity condition for the tangential fields. This enables the change of the relative amplitudes of layer modes, possibly resulting in the expansion of the average spatial mode width, or in other kind of adaptation to the actual laser geometry. A global resonator mode is found by a self-consistency condition, such as the mode must be mapped into itself after back-and-forth propagation in the diode.

The selection of the initial modes, on which basis the actual mode expression takes place, is not an obvious task. One faces first a theoretical problem, since guided modes do not form a complete basis without radiation ones. Numerical mode matching method (NMM) circumvent this fact by placing the semiconductor laser into a metal cylinder, which reflects back any outgoing radiation, and enforces the completeness of the basis for the truncated domain [58]. Although it seems an arbitrary manipulation of the physical device, it may provide acceptable results provided the metal cylinder is located far away from waveguiding structure. One should also pay attention on the analytical behavior of the basic modes, since the final solution retains it automatically. The global mode would therefore inherit the radial continuity and smoothness of the basis, even if it were nonphysical at radial material discontinuities. The third issue is of practical type: it must be verified how finite expansion basis (their number is denoted by $N$) affects the accuracy of the results.
APPENDIX A. FURTHER OPTICAL APPROACHES

NMM starts from the known Bessel eigenfunctions of a finite radial region truncated by a metal wall, referred as basic modes. The VCSEL is placed in the same enclosure, and the basic modes are combined in each layer with \( \exp(i\beta z) \) longitudinal dependence. This representation is substituted to Maxwell’s equations, which leads to an \( N \times N \) eigenproblem resulting in the knowledge of layer modes, that can propagate in the layers. This step can be omitted in homogeneous layers, since the solutions are well known. The resonator mode can be then expressed as the superposition of vectorial layer modes as follows:

\[
\mathbf{E}_k(r, z, \varphi) = \sum_{p=1}^{N} \left[ a_{k,p}^+ \mathbf{E}_{k,p}(r, \varphi) \exp(i\beta_{k,p} z) + a_{k,p}^- \mathbf{E}_{k,p}(r, \varphi) \exp(-i\beta_{k,p} z) \right], \quad (A.5)
\]

\[
\mathbf{H}_k(r, z, \varphi) = \sum_{p=1}^{N} \left[ a_{k,p}^+ \mathbf{H}_{k,p}(r, \varphi) \exp(i\beta_{k,p} z) - a_{k,p}^- \mathbf{H}_{k,p}(r, \varphi) \exp(-i\beta_{k,p} z) \right], \quad (A.6)
\]

where the \( k \) index refers the \( k \)th layer, and the \( p \)th layer mode exhibits an electric field distribution \( \mathbf{E}_{k,p}(r, z, \varphi) \) and a magnetic field \( \mathbf{H}_{k,p}(r, z, \varphi) \).

Reflection and transmission matrices from layer \( k - 1 \) to layer \( k \) are defined for the fields consisting a single incident layer mode with index \( q \) and local amplitude \( a_{k-1,q}^+ \exp(i\beta_{k-1,q} z_k) = 1 \). Then \( \mathbf{R}_{pq}^k = a_{k-1,p}^+ \exp(-i\beta_{k-1,p} z_k) \) and \( \mathbf{T}_{pq}^k = a_{k,p}^+ \exp(i\beta_{k,p} z_k) \) follow by definition. The matrices are obtained by enforcing the best possible matching of the tangential fields. To this end, one evaluates the vector products of the tangential components of the previous equations with the tangential components \( \mathbf{E}_{k-1,s}^t \) and \( \mathbf{H}_{k-1,s}^t \) for every \( s = 1, 2, ..., N \), integration for the cross section, and invoking orthogonality relations:

\[
\delta_{qs} \left\langle \mathbf{E}_{k-1,q}; \mathbf{H}_{k-1,s} \right\rangle + \sum_{p=1}^{N} \mathbf{R}_{ps}^{k+} \left\langle \mathbf{E}_{k-1,p}; \mathbf{H}_{k-1,s} \right\rangle = \sum_{p=1}^{N} \mathbf{T}_{ps}^{k+} \left\langle \mathbf{E}_{k,p}; \mathbf{H}_{k-1,s} \right\rangle, \quad (A.7)
\]

\[
\delta_{qs} \left\langle \mathbf{E}_{k-1,q}; \mathbf{H}_{k-1,s} \right\rangle - \sum_{p=1}^{N} \mathbf{R}_{ps}^{k-} \left\langle \mathbf{E}_{k-1,s}; \mathbf{H}_{k-1,p} \right\rangle = \sum_{p=1}^{N} \mathbf{T}_{ps}^{k-} \left\langle \mathbf{E}_{k,s}; \mathbf{H}_{k,p} \right\rangle, \quad (A.8)
\]

with the \( \delta_{qs} \) Kronecker-symbol and the definition \( \langle \mathbf{v}; \mathbf{w} \rangle = \int (\mathbf{v} \times \mathbf{w}) \hat{S} \) comprising only the tangential components. The \( 2N^2 \) unknown matrix entries can be easily derived from the equations. It is worth noting that the previous condition does not guarantee the continuity everywhere on the interface, but only the best possible matching of the layer modes, which can even be disjunct on the two sides. The transmission and reflection matrices are then determined for incident waves traveling from layer \( k \) to \( k - 1 \).

The transmission and reflection matrices of stacks can be obtained by chain multiplication of single interface matrices, taking into account the additional complex exponential terms describing the propagation inside the layers, as well. If one divides the resonator with an arbitrary plane, it is possible to calculate the reflection matrix \( \mathbf{R}^+ \) of the top part as seen from the bottom, and \( \mathbf{R}^- \) vice versa. A laser mode is given by its expansion
coefficients $a^+$ at the selected plane if it satisfies $R^{-}R^+a^+ = a^+$. This complex condition selects the resonator frequency as well as the threshold gain, which is required to compensate the optical loss and maintain stable laser operation. It has been shown that a reformulation into a singular value decomposition problem for the matrix $I - R^{-}R^+$ was advantageous for numerical stability (the first term denotes the unity matrix). One may also apply the scattering matrix formalism that relates the incident fields from both sides to the outgoing fields. It has been proved numerically stable, because it eliminated the exponentially increasing factors. More than 200 basic modes should be be chosen in order to provide accurate results for 2-D simulations.

A.3 Eigenmode Expansion with Perfectly Matched Layers

It has been mentioned in the previous section that the VCSEL under study must have been enclosed in a metallic volume, therefore the radiated fields were completely reflected back to the structure. In order to alleviate this, an absorbing boundary condition should be applied. This paragraph reports about the extension of the previous method with the incorporation of a PML, and the outcome is referred shortly as CAMFR after its computer implementation called Cavity Modeling Framework [123]. The complex coordinate stretching approach can be readily incorporated into the NMM, since only the radial variable should be modified in the expressions. The modal expansion and the evaluation of transfer matrices proceeds otherwise unchanged.

A.4 Method of Lines

The method of lines (MoL) utilizes a numerical discretization scheme in the transverse directions instead of mode expansion [124, 125]. This feature would enable to prescribe exact boundary conditions instead of continuous layer modes along the radial direction in layers with material discontinuities. Despite of the discretization procedure, the method consist of a step that involves the transformation to layer modes that can be resolved on the selected mesh. An impedance/admittance matching condition yields the transformation between adjacent layers. MoL was applied for the optical mode calculation of a noncircular benchmark VCSEL, but not for practically interesting ones.

The vector potential $\Pi(r, z, \varphi)$ serves as the primary unknown in this method, with which the electric and magnetic fields can be expressed as $E = 1/(\varepsilon_0 \varepsilon) \nabla \times \nabla \times \Pi$ and $H = i/(\mu_0 \omega) \nabla \times \Pi$, respectively. It satisfies the vectorial Helmholtz equation

$$\Delta \Pi - \frac{\nabla \varepsilon}{\varepsilon} \cdot \Pi + \frac{\omega^2}{c_0^2 \varepsilon} \Pi = 0 \quad (A.9)$$

in each axially uniform layer. $\Pi_z$ is decoupled and can be chosen as zero, and only two components remain: $\Pi_r$ and $\Pi_{\varphi}$. Substituting them into the Helmholtz equation leads to two lengthy scalar equations. In order to keep the number of unknowns low,
APPENDIX A. FURTHER OPTICAL APPROACHES

Spatial discretization is performed only in the radial variable, and an absorbing boundary condition is also employed. The azimuthal variations are expanded in Fourier series:

\[ \varepsilon(r, \varphi) = \sum_{m=0}^{M} \varepsilon_m(r) \left\{ \cos (m \varphi) \right\}, \quad \Pi_{r/\varphi}(r, \varphi) = \sum_{m=0}^{M} \Pi_{r/\varphi,m}(r) \left\{ \cos (m \varphi) \right\}, \tag{A.10} \]

and the axial derivation is preserved in analytical form. Having approximated the radial partial derivatives by their appropriate difference forms, one gets algebraic equations:

\[ \sum_{m=0}^{M} \left[ \left( \frac{\partial^2 \Pi_{rm}}{\partial z^2} - D_{rm} \left\{ \frac{\Pi_{rm}}{\Pi_{\varphi m}} \right\} \right) \right] \cdot \left\{ \cos (m \varphi) \right\} = 0, \]
\[ \sum_{m=0}^{M} \left[ \left( \frac{\partial^2 \Pi_{\varphi m}}{\partial z^2} - D_{\varphi m} \left\{ \frac{\Pi_{rm}}{\Pi_{\varphi m}} \right\} \right) \right] \cdot \left\{ \cos (m \varphi) \right\} = 0. \tag{A.11} \]

The values of the functions at different positions have been arranged into column vectors \( \Pi_{r/\varphi,m} \), and the coupling terms arising from the derivations into matrices \( D_{\varphi m} \). These equations can be further simplified formally by collecting the unknowns into a hypervector \( \Phi = [\Pi_{r0}; \Pi_{\varphi0}; \Pi_{r1}; \Pi_{\varphi1}; \Pi_{rM}; \Pi_{\varphiM}; ...; \Pi_{rM}; \Pi_{\varphiM}] \) (the superscripts labeling the type of the azimuthal dependence) and the matrices into a dense hypermatrix \( D \), accordingly.

The resulting second-order differential equation has a formal general solution \( \Phi = a^+ \exp (i\sqrt{D}z) + a^- \exp (-i\sqrt{D}z) \), but the matrix exponential cannot be calculated efficiently. It is therefore essential to diagonalize it using a transformed potential \( \Phi = T^{-1} \Phi \), resulting in \( \Gamma^2 = T^{-1} D T \). This mathematical step is equivalent to the calculation of layer modes (their values can be extracted from the columns of \( T \) on the given mesh) with propagation constants appearing in the diagonal of \( \Gamma \). The matrix exponentials can then be evaluated economically in the transformed domain.

The values of the electric and magnetic fields can also be approximated by matrix multiplications on \( \Phi \). The tangential continuity is written for the Fourier components in \( \varphi \) at all radial positions, and realized with an impedance/admittance transfer condition. Selecting a matching plane arbitrarily leads to an implicit eigenvalue problem, yielding the complex frequencies and field distributions characterizing the optical modes.

The essence of the Fourier-transformation in the azimuthal variable was to keep the number of unknowns at a reasonable level. As a consequence, the material discontinuities are smoothed for any finite number of harmonic basis. It were theoretically possible to use difference formulas in both \( (r, \varphi) \)-variables, or in \( (x, y) \)-coordinates for (nearly) rectangular cross sections; which would allow the matching of the interfaces and setting exact conditions for the tangential fields. Nevertheless, this has not been accomplished for the simulation of realistic noncircular VCSELs yet.
A.5 Plane Wave Admittance Method

This method is particularly suitable for the 3-D simulation of periodic structures such as PhC-VCSELs. It was first proposed to describe the electromagnetic modes of infinite photonic crystal slabs [126], but can be extended to other geometries that exhibit only truncated periodicity or a complicated layer structure [127]. Plane wave admittance method (PWAM) can be traced back for the combination of MoL with plane wave expansion.

MoL equations are rewritten for the tangential electric and magnetic fields in Descartes-coordinates. The longitudinal components are expressed with the transverse ones from two scalar components of Maxwell’s curl equations, and substituted into the remaining four:

\[
\begin{align*}
\frac{\partial}{\partial z} \begin{pmatrix} -E_y \\ E_x \end{pmatrix} &= -\frac{i}{\omega \varepsilon_0} \begin{pmatrix}
\frac{\partial}{\partial y} \varepsilon_{z-1} \frac{\partial}{\partial y} + k_0^2 \\
-\frac{\partial}{\partial x} \varepsilon_{y-1} \frac{\partial}{\partial x} + k_0^2
\end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix}, \\
\frac{\partial}{\partial z} \begin{pmatrix} H_x \\ H_y \end{pmatrix} &= -\frac{i}{\omega \mu_0} \begin{pmatrix}
\frac{\partial^2}{\partial x^2} + \varepsilon_y k_0^2 \\
\frac{\partial^2}{\partial y^2} + \varepsilon_x k_0^2
\end{pmatrix} \begin{pmatrix} -E_y \\ E_x \end{pmatrix}.
\end{align*}
\]

(A.12)

Instead of using the discretization approach, one can expand any of the four fields (Ψ) in some truncated basis as \( \Psi = \sum_\mathbf{G} \Psi^\mathbf{G} | \phi_\mathbf{G} \rangle \). The plane wave basis \( | \phi_\mathbf{G} \rangle = \exp(i \mathbf{G} r_t) \) is a natural choice for two-dimensional periodic structures, where \( r_t \) denotes the position on the transverse \( (x, y) \)-plane, and \( \mathbf{G} \) is a reciprocal lattice vector. Thanks to the orthogonality of this basis, Eq. (A.12) can be cast into differential equations for the linear coefficients:

\[
\begin{align*}
\frac{\partial}{\partial z} \begin{pmatrix} E_y^\mathbf{G} \\ E_x^\mathbf{G} \end{pmatrix} &= -\sum_\mathbf{G'} \frac{i}{\omega \varepsilon_0} \begin{pmatrix} \phi_\mathbf{G} \frac{\partial}{\partial y} \varepsilon_{z-1} \frac{\partial}{\partial y} + k_0^2 \\
-\frac{\partial}{\partial x} \varepsilon_{y-1} \frac{\partial}{\partial x} + k_0^2
\end{pmatrix} \begin{pmatrix} \phi_\mathbf{G'} \langle H_x^{\mathbf{G'}} \\ H_y^{\mathbf{G'}} \rangle \\
\phi_\mathbf{G'} \langle H_x^{\mathbf{G'}} \\ H_y^{\mathbf{G'}} \rangle \end{pmatrix}, \\
\frac{\partial}{\partial z} \begin{pmatrix} H_x^\mathbf{G} \\ H_y^\mathbf{G} \end{pmatrix} &= -\sum_\mathbf{G'} \frac{i}{\omega \mu_0} \begin{pmatrix} \phi_\mathbf{G} \frac{\partial^2}{\partial x^2} + \varepsilon_y k_0^2 \\
-\frac{\partial}{\partial y} \varepsilon_x k_0^2 + \varepsilon_x k_0^2 \end{pmatrix} \begin{pmatrix} \phi_\mathbf{G'} \langle E_y^{\mathbf{G'}} \\ E_x^{\mathbf{G'}} \rangle \\
\phi_\mathbf{G'} \langle E_y^{\mathbf{G'}} \\ E_x^{\mathbf{G'}} \rangle \end{pmatrix}.
\end{align*}
\]

(A.13)

One can expand the transverse permittivity components and the reciprocal longitudinal component also into Fourier-series: \( \varepsilon_{x/y}(\mathbf{r}_t) = \sum_{\mathbf{G''}} \varepsilon_{x/y}^{\mathbf{G''}} | \phi_{\mathbf{G''}} \rangle \) and \( \varepsilon_{x/y}^{-1}(\mathbf{r}_t) = \sum_{\mathbf{G''}} \gamma^{\mathbf{G''}} | \phi_{\mathbf{G''}} \rangle \), and the bracket finally simplifies to an analytical matrix expression. However, the finite basis expansion and the usual convolution of the dielectric function with a two-dimensional Gaussian \( \exp(-r/t^2) \) that improves the convergence, blur the real transverse contours of the device.

The further algorithm is similar to that encountered in the discussion of MoL. The matrix of the differential equations is transformed to principal axes in each layer, and the general solution takes the form of forward and backward propagating waves along the axial direction. The coefficients are matched at the interfaces according to tangential field continuity, which is assured by the admittance transfer condition. PML should cover the system from the bottom and top to prevent reflections from the surfaces of the finite
computational domain. The transverse periodic boundary condition cannot be applied for PhC-VCSELs with few rings of holes, and must be replaced by PML, as well. While the numerical procedure is straightforward for rectangular PhC pattern, special attention must be paid for hexagonal lattice. Since not all coordinates of a \( (1, 0) \) and \( (1/2, \sqrt{3}/2) \) basis vectors can be represented by rational numbers, the computer implementation may split the natural sixfold degeneracy of the system, and yield unphysical mode distributions as in Ref. [128].

A.6 Green’s Function Model

The basic idea behind this approach is to separate the dielectric function into passive and active contributions: \( \varepsilon(r, \omega) = \varepsilon_{\text{cavity}}(r, \omega) + \chi_{\text{gain}}(r, \omega) \) [129, 130]. The active term may rapidly change owing to current injection, and is defined as susceptibility.

The vectorial Helmholtz equation can then be rewritten as follows:

\[
\nabla \times [\nabla \times E(r, \omega)] - \frac{\omega^2}{c_0^2} \varepsilon_{\text{cavity}}(r, \omega)E(r, \omega) = \frac{\omega^2}{c_0^2} \chi_{\text{gain}}(r, \omega)E(r, \omega),
\]

whose formal solution can be expressed using the tensorial Green’s function of the same equation with vector-valued Dirac-delta right-hand-side. Therefore we have

\[
E(r, \omega) = \int G(r, r', \omega)\frac{\omega^2}{c_0^2} \chi_{\text{gain}}(r', \omega)E(r', \omega)dr',
\]

with

\[
\nabla \times [\nabla \times G(r, r', \omega)] - \frac{\omega^2}{c_0^2} \varepsilon_{\text{cavity}}(r, \omega)G(r, r', \omega) = \delta(r - r').
\]

One can define an integral operator \( G_{\text{gain}}(\omega) \) that acts on a vector-valued function as indicated in Eq. (A.15), except that a normalized \( \chi_{\text{gain}}^0(r', \omega) \) is included in the integral. This is motivated by the fact that in many circumstances the gain profile looks similar under different bias, and only its magnitude changes. After introducing the prefactor

\[
\Xi(\omega) = \chi_{\text{gain}}(r', \omega)/\chi_{\text{gain}}^0(r', \omega),
\]

one arrives to an operator eigenproblem

\[
\frac{1}{\Xi(\omega)}E(r, \omega) = G_{\text{gain}}(\omega)E(r, \omega),
\]

whose solution yields the mode patterns and the gain amplitudes that define the stationary lasing condition. The complex gain amplitude is a continuous function of the angular frequency. In order to obtain the frequencies at which the VCSEL can actually operate, the complex gain susceptibility must be matched to that available from the electronic system in both magnitude and phase. This condition only occurs at discrete frequencies characterizing the resonator modes.

It is possible to repartition the susceptibility to take part of the cavity out of the Green’s function, and put it into the eigenvalue problem instead. For example, the contribution of thermal lensing is separated in the second term of \( \varepsilon(r, \omega) = \varepsilon_{\text{cavity}}(r, \omega) + \)
\( \chi_{\text{cavity}}(r, \omega) + \chi_{\text{gain}}(r, \omega) \). A similar operator \( G_{\text{cavity}}(\omega) \) can be defined with the incorporation of \( \chi_{\text{cavity}}(r, \omega) \) instead of \( \chi_{\text{gain}}(r, \omega) \) into the integral in Eq. (A.15). That takes us to the generalized eigenproblem

\[
\frac{1}{\Xi(\omega)} \left[ 1 - G_{\text{cavity}}(\omega) \right] E(r, \omega) = G_{\text{gain}}(\omega) E(r, \omega).
\] (A.18)

This formulation allows greater computational speed by avoiding the slow numerical techniques needed to find the tensor Green’s function of complex VCSELs. For example, an analytical Green’s function is available for planar cavities [131]. The solution of Eq. (A.18) still requires either discretization or mode expansion, and leads to an algebraic eigenproblem. This method has been used for the simulation of a gain-guided VCSEL having a rectangular active region, as well as for a cylindrical oxide-confined one, in which the gain profile was chosen as an ideal step-function.

### A.7 Optimized-Waist Paraxial Eigenmodes Method

The previous theories relied mainly on index guiding caused by either by the oxide aperture, etched mesa or thermal lensing. This approach, abbreviated as PREVEU after Paraxial Radiation Eigenmodes for VCSEL Emulation, is better suited for the simulation of purely gain-guided lasers and also embodies diffraction effects naturally by introducing a Gauss-Laguerre (GL) mode representation of the cavity modes [132]. GL beams given in cylindrical coordinates are well-known eigenmodes of spherical resonators in the paraxial approximation. In order to resemble VCSELs with simple resonators, the DBRs are substituted with hard, thin mirrors placed at equivalent effective distances that combine multiple-reflection and finite-diffraction effects. The alternating quarter wavelength mirror structure is omitted, and the beam envelope of an equivalent homogeneous medium is analyzed. Wide angle scattering out of the cone of the paraxial propagation, which occurs at an oxide aperture, is calculated applying the Born approximation to the electromagnetic diffraction integral.

The scalar optical field inside the equivalent resonator is decomposed into a superposition of orthonormal GL beams:

\[
\Psi(r, z, \phi) = \sum_{nm} c_{nm} \psi_{nm}(r, z, \phi),
\]

where \( \psi_{nm}(r, z, \phi) \) denotes a single beam possessing \( n \) node rings and \( m \) azimuthal node planes. It can be written with the help of the associated Laguerre-Gauss functions \( U_n^m \) [132] as follows:

\[
\psi_{nm}(r, z, \phi) = U_n^m \left[ \frac{2r^2}{W^2(z)} \right] \exp(i m \phi) \exp \left[ ik \frac{r^2}{R(z)} \right] \exp \left[ -i(2n + m + 1)\zeta(z) \right],
\] (A.19)

after decoupling the fast axial variation. The longitudinal dependences of the beam waist \( W(z) \), curvature \( R(z) \) and phase shift \( \zeta(z) \) are similar to those of the simple Gaussian-beam [87].

The evolution of any wave front \( \Psi(r, 0, \phi) \), which originates from the middle of the cavity, along a round trip involves an amplification through the active region \( G \), propagation between the mirrors \( T \), and reflection from the mirrors \( R \). Tracing the light
APPENDIX A. FURTHER OPTICAL APPROACHES

path from bottom to top through the center, and both reflections, the cavity eigenmodes should be mapped into themselves apart from a complex multiplier \( \Theta \):

\[
\Psi(r, 2L, \varphi) = S \Psi(r, 0, \varphi) = T_c R_c G T_{ch} R_{ch} G \Psi(r, 0, \varphi) = \Theta \Psi(r, 0, \varphi). \tag{A.20}
\]

Here \( S \) labeled the total round trip operator, which is represented as an \( S \) matrix in the basis holding GL beams. The advantage of this expansion is that the paraxial propagators \( T \) act as similarity transformations rescaling the waist and the curvature of each GL mode, and their respective matrices are diagonal. After reflection from an infinite mirror, the outgoing radiation can be obtained simply as the mirror image of the incoming waist, and the intensity is multiplied by the same reflection coefficient for all GL modes. For a finite mirror, however, the reflected profile is truncated at the mirror rim, and thus the reflected profile of a single incoming GL mode couples into others. Fortunately, modes with different azimuthal parameter do not interact in cylindrical geometry, and the resulting matrix remains block-diagonal. The gain period can also be described as a block-diagonal matrix for a nonuniform carrier profile along the radius. Finally, diffraction losses occur even for perfectly reflecting mirrors of infinite extent and infinite gain region, since the beam waist of the GL modes expand and their wave fronts keep curving. The spread, curved wave-front mode must be projected into modes of the original waist size and flat wavefront after one cavity pass. This transformation can be described by a projection matrix, whose entries can be calculated analytically.

The losses due to wide angle scattering around the edges of an oxide aperture can be calculated from the following integral for the vector potential \( A \) [133]:

\[
A_{\text{total}}(r) = A_{\text{in}}(r) + \frac{1}{c_1} \int j(r') \exp\left(\frac{ik_1|r-r'|}{|r-r'|}\right) dr', \tag{A.21}
\]

where \( j = \partial P/\partial t = i \omega \chi E_{\text{total}} \) is the current response of the medium to the electric field (\( \chi \) denotes its susceptibility), \( c_1 = c_0/\sqrt{\varepsilon} \) is the speed of light and \( k_1 = \omega/c_1 \) is the wavenumber in the material. The scattered power can be approximated analytically for each GL incoming field, provided it is negligible compared to the incoming power, and thus replacing \( E_{\text{total}} \) by \( E_{\text{in}} \) in the expression for the current. Scattering losses are finally included by multiplying the round-trip gain expression by an additional matrix \( \Sigma \).

The resonator modes are determined from the eigenproblem \( Sc = \Theta c \), where the expansion coefficients have been arranged in the column vector \( c \). They are ordered according to decreasing round-trip gain \(|\Theta|\), with the highest eigenvalue for the fundamental mode. Until now, the minimum beam waist \( w \) has been left a free parameter, since an arbitrary choice would constitute a full set of modes. However, there exist an optimal value for which the laser modes become nearly pure GL beams with only small corrections from other terms. A very small \( w \) would lead to the increase of diffraction losses and beam spreading, while a large value would result in increasing losses due to finite active region and mirror size. The number of the basic modes and the computational demands can be reduced considerably by selecting the optimal beam waist parameter.
List of Publications

Publications Related to the Dissertation


95
LIST OF PUBLICATIONS


Further Publications


Bibliography


BIBLIOGRAPHY


